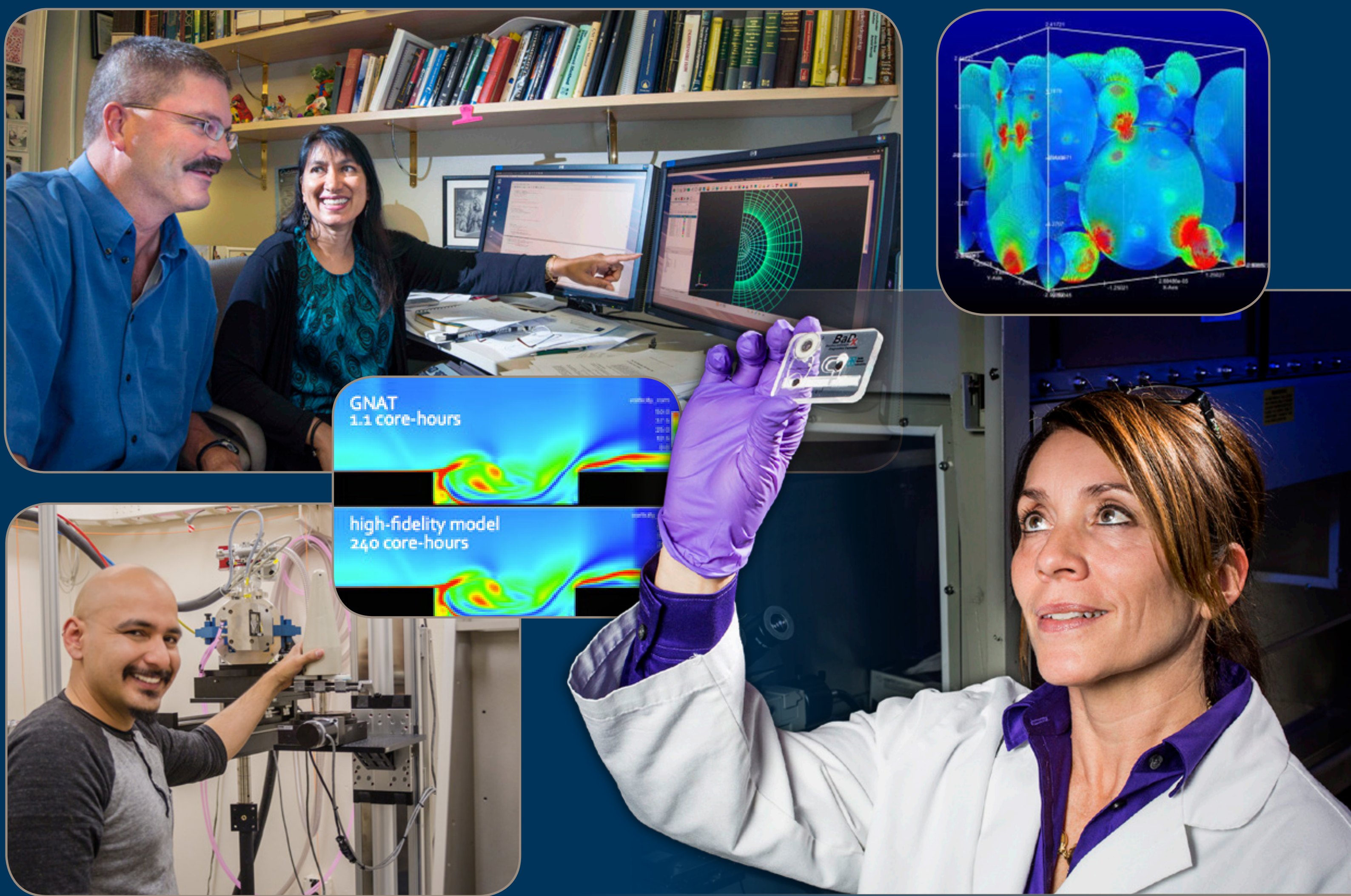
LDRD

Laboratory Directed Research and Development

2014 ANNUAL REPORT



Exceptional service in the national interest

Sandia National Laboratories

NNSA
National Nuclear Security Administration

Cover photos (clockwise):

Randall Schunk and Rekha Rao discuss an image generated by Goma 6.0, an R&D 100 Award winner that has origins in several LDRD projects.

A modeled simulation of heat flux in a grandular material, showing what appear to be several preferential "channels" for heat flow developed in Project 171054.

Melissa Finley examines a portable diagnostic device, for *Bacillus anthracis* detection in ultra-low resource environments, developed in Project 158813, which won an R&D 100 award.

The Gauss–Newton with Approximated Tensors (GNAT) Reduced Order Models technique applied to a large-scale computational fluid dynamics problem was developed in Project 158789.

Edward Jimenez, Principal Investigator for a "High Performance Graphics Processor-Based Computed Tomography Reconstruction Algorithms for Nuclear and Other Large Scale Applications" for Project 158182.

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Abstract

This report summarizes progress from the Laboratory Directed Research and Development (LDRD) program during fiscal year 2014. In addition to the programmatic and financial overview, the report includes progress reports from 419 individual R&D projects in 16 categories. Information for 176 projects in their final year is presented in a more comprehensive format, while for those 243 in their pre-final years, only an abstract is presented herein.

Sandia is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000.

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March 2015

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Message from Julia Phillips, Vice President and Chief Technology Officer

Sandia is the nation's most diverse national security laboratory in both the breadth of its mission and the capabilities it can bring to bear on important challenges. What that means for our Laboratory Directed Research and Development (LDRD) program is that we perform research informed by our understanding of national needs in a unique multidisciplinary environment.

Our researchers work together across a broad spectrum of disciplines, collaborating to advance the frontiers of science and engineering in ways that are critical to Sandia's eight national security mission areas, which range from carrying out our unique responsibilities for the nation's nuclear arsenal to securing a sustainable energy future.

LDRD is an essential component of Sandia's strategy for sustaining and developing the world-class science, technology, and engineering capabilities (ST&E) it needs to execute its mission. LDRD research has contributed to scientific and technical advancement at a level that far exceeds what would be expected from a program of its size, currently capped at 6% of the Laboratories' budget.

Over the past five years, over 70% of Sandia's R&D 100 Awards, including the three R&D 100 Awards received by Sandia researchers in 2014, resulted from LDRD-supported research. In addition, 52% of the Laboratories' invention disclosures, 49% of its patents, and 23% of its software copyrights resulted from LDRD investments. These achievements, along with hundreds of peer-reviewed publications and many awards, invited talks, journal covers, research grants, and professional society fellowships demonstrate the innovative and leading edge nature of our LDRD investments.

The LDRD program, especially in the opportunity it provides for Sandia staff to propose and pursue self-defined research and through its funding of early career projects, is crucial in helping to attract and retain researchers by creating an invigorating and productive research environment. The program has been particularly valuable in recent years as Sandia recruits and trains a new generation of talented scientists and engineers. LDRD is a particularly potent weapon in the fierce competition with industry and academia for top talent.

In 2014, Sandia continued to sharpen the alignment of its LDRD investments with the Sandia Strategic Plan, giving particular attention to a small set of mission-critical research challenges and both near- and long-term capability needs that support the national security mission.

In this report, you will find more information about the results of Sandia's FY 2014 LDRD program and descriptions of each of the funded projects. From this current snapshot, you will get a glimpse of Sandia's investments in its ability to meet emerging national needs. You will also read about some of the significant impacts of previous LDRD investments, which demonstrate how the program has enabled current mission success by anticipating future mission requirements.

Program Overview

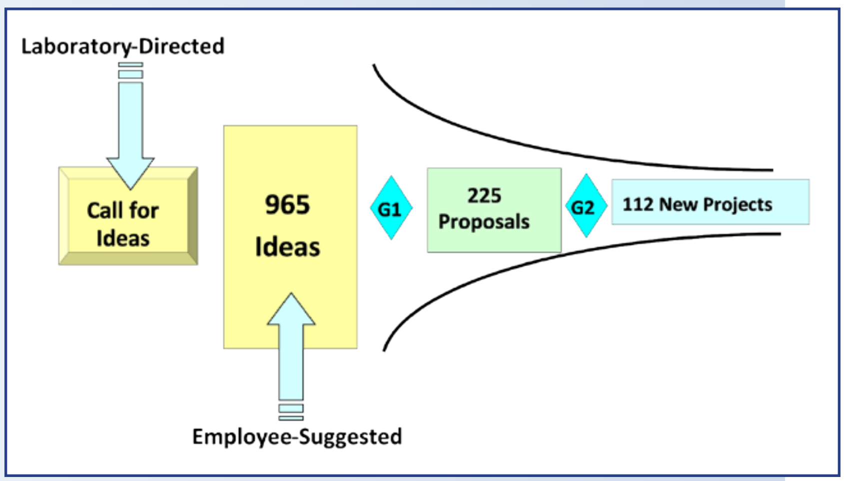
Sandia and other Department of Energy (DOE)/National Nuclear Security Administration (NNSA) laboratories use the congressionally authorized LDRD program to:

- Maintain the scientific and technical vitality of the Laboratories
- Enhance the Laboratories' ability to address current and future DOE/NNSA missions
- Foster creativity and stimulate exploration of forefront science and technology
- Serve as a proving ground for new concepts in research and development
- Support high-risk, potentially high-value research and development

LDRD is foundational, leading-edge research and development (R&D) that nurtures and enhances core science and engineering capabilities, supports national security missions, and leads to the creation of new capabilities. This long-range, forward-looking R&D anticipates technical solutions to future mission challenges. LDRD is Sandia's sole discretionary R&D program and has the following goals:

- Enable our national security missions
- Advance the frontiers of science and technology
- Attract and retain a world-class research community

LDRD projects are chosen for their technical quality, differentiating and programmatic value to Sandia, and relevance, not only to DOE/NNSA's missions but also to the national security missions of the Department of Homeland Security, Department of Defense, and other federal agencies. As a result, the scientific advances and technology innovations from LDRD provide multiple benefits to all Sandia stakeholders, consistent with congressional intent and Sandia's strategic goals.



FY 2014 annual call for ideas and project selection statistics

Sandia's research strategy arises from its laboratory strategy and is organized through program elements known as Investment Areas, each of which is focused on discipline- or mission-based research priorities set by upper management. Each year the LDRD program issues a Labs-wide Call for Ideas organized through the Investment Area leadership teams. In response, staff members generate ideas and proposals that are directed to the appropriate Investment Area selection committee for evaluation.

The Sandia LDRD program is highly competitive. In FY 2014, 965 short idea proposals were submitted; the Investment Area selection committees invited 225 of those to submit full proposals. Ultimately, 112 new projects were funded, with 74 additional projects funded throughout the fiscal year. When added to ongoing projects, 419 projects were active in FY 2014. Each project, new or existing, undergoes a rigorous review process, including peer review by subject-matter experts.

Average annual funding for each LDRD project in FY 2014 was $363,000. Projects ranged in size from slightly less than $20,000 to slightly more than $5,000,000 per year. The goal is to achieve a balanced array of leading-edge R&D projects that align with Sandia's research strategy and have potential impact on Sandia's future national security mission needs.

Supporting a vibrant world-class research community

The LDRD program has been particularly valuable in recent years as Sandia recruits and develops a new generation of talented scientists and engineers. Fierce competition for research talent comes from industry and academia, but LDRD is a powerful tool that helps attract the best and brightest — and retain them. Talented people are what make Sandia a vital and world-class R&D institution, one that can deliver on national security missions while advancing the frontiers of science and engineering.

LDRD funding for postdoctoral researchers and new staff at Sandia is an important contributor to talent development for mission support. Over the period FY 2010 to FY 2014, 52% of Sandia's postdoctoral population was supported by LDRD, which clearly bolsters the pool of new-hire candidates. Moreover, LDRD is used deliberately as a workforce development tool through the Early Career LDRD program element, which funds new strategic hires. Since FY 2010, over 200 new PhD researchers hired at Sandia have led Early Career LDRD projects and by FY 2013, over 50% of these new staff were supporting Sandia's core nuclear weapons mission programs.

Postdocs (FY 2010–2014)	**945**
LDRD-supported Postdocs	489
% due to LDRD	52%

Postdoc Conversions (FY 2010–2014)	**126**
LDRD-supported Postdoc Conversions	90
% due to LDRD	71%

Surveys have shown that many participants in Sandia's Early Career R&D program credit LDRD funding as a significant contributing factor for continuing their career at Sandia. Many principal investigators have also cited LDRD as an important factor in their decision to join the Labs.

Sandia's specialized missions require highly motivated, qualified staff with deep expertise, committed to advancing the frontiers of science and engineering through continual growth and development. LDRD projects give staff the opportunity to keep moving forward, with numerous compelling examples, like those of Stephanie Hansen and Edward Jimenez in 2014.

Stephanie Hansen received a $2.5 million, five-year Early Career Research Program award from the Department of Energy's (DOE) Office of Science for her fundamental science proposal to improve existing atomic-scale models for high-energy-density matter. Hansen's winning submission, "Non-Equilibrium Atomic Physics in High Energy Density Material," describes an approach to improve simulation tools used to design high-energy experiments in dense hot plasmas, as well as the diagnostic tools used to interpret data from them.

"I think that being able to show that more than half my funding was coming from LDRD sources probably increased my competitiveness for this kind of intensive/cutting edge research award," Hansen stated.

Edward Jimenez was named a 2014 HENAAC (Hispanic Engineer National Achievement Awards Conference) award winner as Most Promising Engineer/Advanced Degree by Great Minds in STEM (Science, Technology, Engineering, and Math).

As the principal investigator of an Early Career LDRD that ended in FY 2013, Jimenez developed ways to reconstruct big data using computer tomography and multiple processors, cutting a process that can take years down to less than a day, while conserving energy. As a member of an LDRD project in radiography, Jimenez currently leads an effort to develop a way to identify the composition of a material from an x-ray image. Since becoming a Sandia staff member, Jimenez has published nine peer-reviewed publications, four pending patents, and one provisional patent. He also reaches out to high school students in Albuquerque through Sandia's outreach programs and encourages young people to pursue science in a "Science Central" promotional spot produced by a New Mexico PBS TV station.

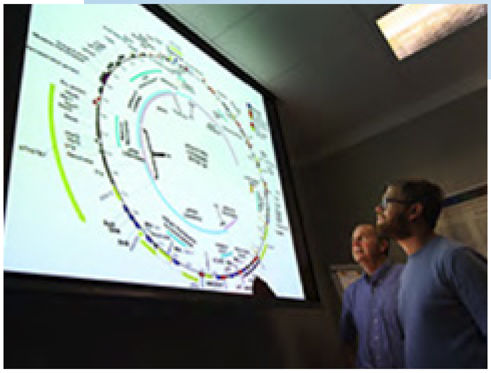
Advancing the frontiers of science and engineering and maintaining scientific vitality

Sandia is a 21st century, broad-spectrum national security laboratory, and LDRD research plays an essential role in maintaining the Labs' scientific vitality. As the nation's most diverse national security laboratory, Sandia is uniquely equipped to tackle groundbreaking interdisciplinary research challenges. Tackling these challenges allows Sandia to fulfill its responsibilities and core national security mission work, while simultaneously advancing related mission areas of value to our nation. To fulfill its national security mission, Sandia must remain at the forefront of multiple scientific areas.

LDRD research has contributed extensively to scientific and technical advancement, disproportionately relative to its cost: LDRD research represents less than 8% (6% starting in FY 2014) of Sandia's overall costs. Over the last five years, 52% of the Laboratories' invention disclosures, 49% of its patents, and 23% of its software copyrights resulted from LDRD investments. These achievements — along with hundreds of peer-reviewed publications and many awards, invited talks, journal covers, research grants, and professional society fellowships — demonstrate the innovative and leading-edge nature of our LDRD investments.

Refereed Publications (CY 2009–2013)	**4052**
LDRD-supported publications	1112
% due to LDRD	27%
Technical Advance/Records of Invention (FY 2010–2014)	**1614**
LDRD-supported Technical Advances	833
% due to LDRD	52%
Patents Issued (FY 2010–2014)	**488**
LDRD-supported Patents	240
% due to LDRD	49%
Software Copyrights (FY 2010–2014)	**363**
LDRD-supported software copyrights	84
% due to LDRD	23%

Sandia's LDRD-funded research projects advance the frontiers of science and engineering. This research is crucial to maintaining the Labs' scientific and technical vitality and enhances our ability to address current and future national security missions. In FY 2014, the following two projects exemplify the role of LDRD in this regard.



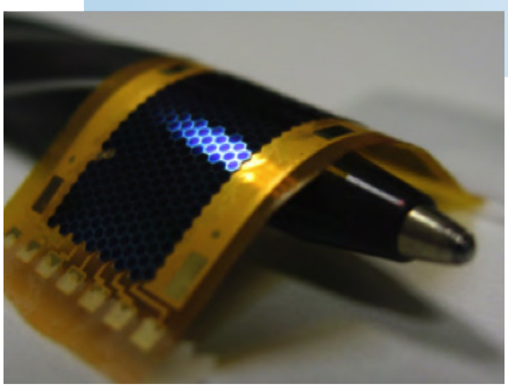
Sandia National Laboratories' researchers Kelly Williams (left) and Corey Hudson look at the mosaic pattern of one of the *Klebsiella pneumoniae* plasmids and discuss mechanisms that mobilize resistance genes. *(Photo by Dino Vournas)*

Detection of engineered biothreats

Kelly Williams and his LDRD team are developing new methods to detect bioengineered threats, in particular, unnatural changes to pathogenicity and/or drug resistance in bacteria.

This team was the first to sequence the entire genome of a *Klebsiella pneumoniae* strain, while developing several new bioinformatics tools that might have multiple uses beyond detecting mechanisms of genetic movement and bioengineering. *Klebsiella pneumoniae* is the most common kind of carbapenem-resistant enterobacteriaceae (CRE) in the United States. As carbapenems are considered the antibiotic of last resort, CREs are a triple threat for their resistance to nearly all antibiotics, high mortality rates, and ability to spread their resistance to other bacteria. Researchers are beginning to understand the bacteria's multifaceted mechanisms for resistance. These findings are also being applied to a related LDRD project developing new approaches for treating drug-resistant organisms.

"Once we had the entire genome sequenced, it was a real eye-opener to see the concentration of so many antibiotic-resistant genes and so many different mechanisms for accumulating them," explained Williams, a bioinformaticist. "Just sequencing this genome unlocked a vault of information about how genes move between bacteria and how DNA moves within the chromosome."



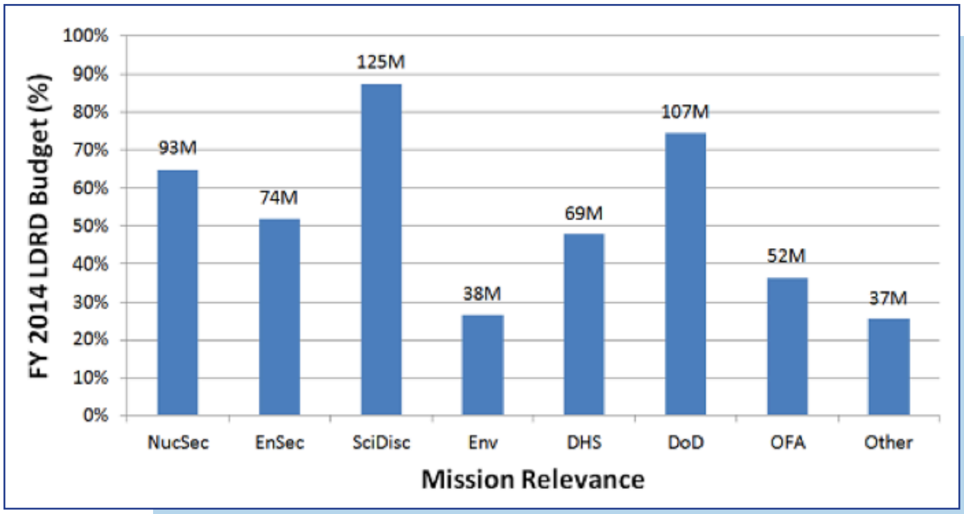
Revolutionary solar glitter

With seven patents awarded and 42 more in process, microsystems-enabled photovoltaics (MEPV) technology is changing solar photovoltaics. Already on the International Space Station, these tiny solar cells can be embedded into devices, used to create small charging pads, and even colorized and integrated into clothing. A just-completed, three-year LDRD project explored the use of MEPV in a concentrating solar application for grid-tied power, moving the tiny devices closer to utility-scale use.

With dimensions as small as 100-µm wide and 1-µm thick, these PV building blocks can be installed in flexible, moldable, or flat-plate formats in sizes that conform to the shapes and contours of natural terrain, large structures, vehicles, and mobile electronics. The MEPV LDRD team used microdesign and microfabrication techniques common to the semiconductor, liquid-crystal display, and microsystem industries to produce miniaturized solar cells that are then placed or "printed" onto a low-cost substrate with embedded contacts and microlenses for focusing sunlight onto the cells. The R&D 100 award-winning MEPV technology's use of microsystems techniques for solar cells results in improved performance, reduced cost, and new capabilities at the cell, module, and system level.

Contributing to mission success

The LDRD program invests in research to enable mission success. As a multidisciplinary laboratory, Sandia brings together researchers from all areas of science and engineering, working together in LDRD projects to develop leading-edge solutions to both current and future challenges. Ranging from building foundational science capabilities to applied research and development of technology, each LDRD project supports one or more national security mission areas. Time and again, mission relevant LDRD investments have opened the door to novel mission solutions.



The FY 2014 LDRD portfolio supports multiple missions. DOE/NNSA missions: nuclear security (NucSec), energy security (EnSec), scientific discovery (SciDisc), environmental responsibility (Env); and Department of Homeland Security (DHS), Department of Defense (DoD), Other Federal Agencies (OFA), and other organizations, e.g., industry (Other).

Copperhead MiniSAR

Detecting improvised explosive devices (IEDs) requires constant, intensive monitoring and rugged equipment. Sandia's Copperhead, a miniature synthetic aperture radar system (MiniSAR) has been locating IEDs since 2009 in Afghanistan and Iraq, where it has been credited with saving hundreds of lives. Copperhead detects disturbances in the earth, such as those made when IEDs are buried. It can find them day or night and in many weather conditions, including fog and dust storms. The proven technology is now being transferred to the US Army to support combat military personnel.

Had it not been for Sandia's R&D process, including LDRD investments in accelerated data acquisition and image processing, as well as miniaturized radar circuitry that led to MiniSAR, Copperhead might never have been ready in time to help the Army with their mission. Department of Energy Secretary Ernest Moniz honored the team that developed Copperhead with an Achievement Award in 2014.

Above: MiniSAR on the Sky Spirit Mini Unmanned Aerial Vehicle (UAV) (funding provided by Lockheed Martin Corporation)

Radiation-hardened trusted application specific integrated circuits (ASICs)

Radiation-hardened (rad-hard) application specific integrated circuits (ASICs) are critical to the performance of nuclear weapons and for systems that operate in space, at high altitude, and in defense systems. Sandia is scheduled to provide more than 25,000 rad-hard ASICs for the nation's weapons modernization programs (FY 2016–FY 2025). These programs include the B61 Bomb and W76 Warhead.

Between FY 1996 and FY 2007, multiple LDRD projects analyzed an assortment of materials that restrict the flow of electrons freed by gamma radiation and neutrons to understand how to limit damaged caused by ionizing radiation. Two complementary approaches were developed: one that designed rad-hard characteristics into the chip and another that applied special techniques to mitigate radiation effects during processing. These investments helped create the sole ASICs technology for the W76-1 life extension program (LEP) and reduced development costs by more than 30 million dollars.

Research excellence in service of the nation

Sandia National Laboratories, like all DOE/NNSA laboratories, is charged with working on tough technical problems on behalf of the nation. These challenges require innovative solutions, which can only be created in an invigorating research environment.

LDRD supports Sandia's mission by investing in leading-edge research that advances the frontiers of science and engineering critical to national security. The program is also instrumental in attracting and developing a world-class workforce of scientists and engineers, the people who make it possible for Sandia to achieve its mission and goals.

To learn more, visit www.sandia.gov/ldrd.

External collaboration and R&D 100 awards

Roughly 40% of current and recent LDRD projects involve external collaborations with academia or industry. These strategic partnerships enhance the Labs' future capabilities through an influx of knowledge and skills. Sandia's partners also benefit from collaborative research results and interaction with peers from outside their organization. In addition to furthering science, partnerships with academia often provide a unique opportunity for Sandia to recruit the world-class scientists and engineers needed for development of mission-critical lab capabilities. Partnerships with industry enable technological breakthroughs developed through the LDRD program to be commercialized under licensing agreements and brought to market for the US public good.

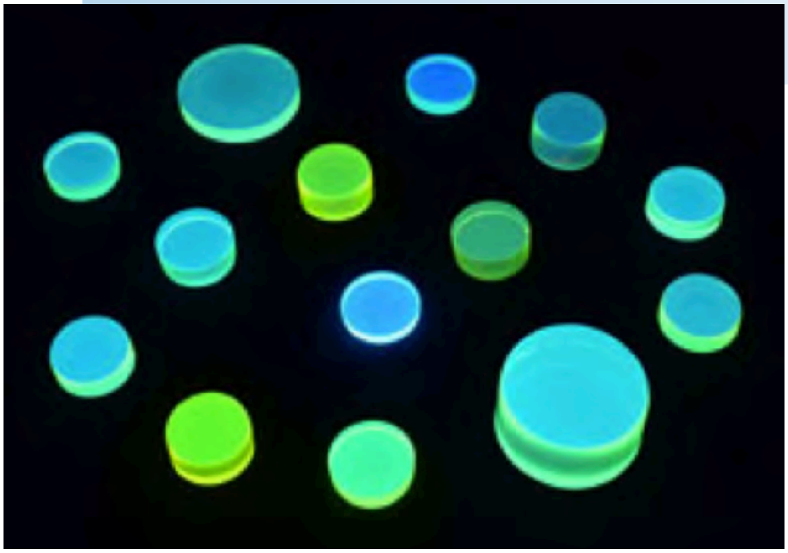
R&D 100 awards recognize the quality and innovation of LDRD investments. Widely recognized as the "Oscars of Invention," these awards from R&D Magazine identify and celebrate the top technology products of the year from industry, academia, and government-sponsored research. Over the past five years, over 70% of Sandia's R&D 100 Awards, including the three awards received by Sandia researchers in 2014, resulted from LDRD-supported research.

R&D 100 Awards (CY 2010–2014)	19
LDRD Supported R&D 100 Awards	14
% due to LDRD	74%

2014 Sandia LDRD-Supported R&D 100 Winners

BaDx

A lab-in-a-pocket device that can detect bacteria that cause anthrax, *Bacillus anthracis* Diagnostics (BaDx) operates with no power, refrigerated storage, or laboratory equipment. The credit-card-sized device requires little training to operate and after use, it "self-destructs" by sterilizing its contents. It is a rapidly deployable platform that can be adapted for other emerging biothreats. The device was developed in an LDRD project that concluded in FY 2014.



Triplet-harvesting plastic scintillators

Automated sensors screen cargo at ports of entry for controlled radiological materials that could be used to make a nuclear weapon. These new detectors scintillate (glow) when they pick up telltale emissions. They also give off more light at less cost, and respond faster than current scintillators. LDRD investments established the foundational concepts that led to Department of Energy funding to develop the award-winning technology.

Goma 6.0

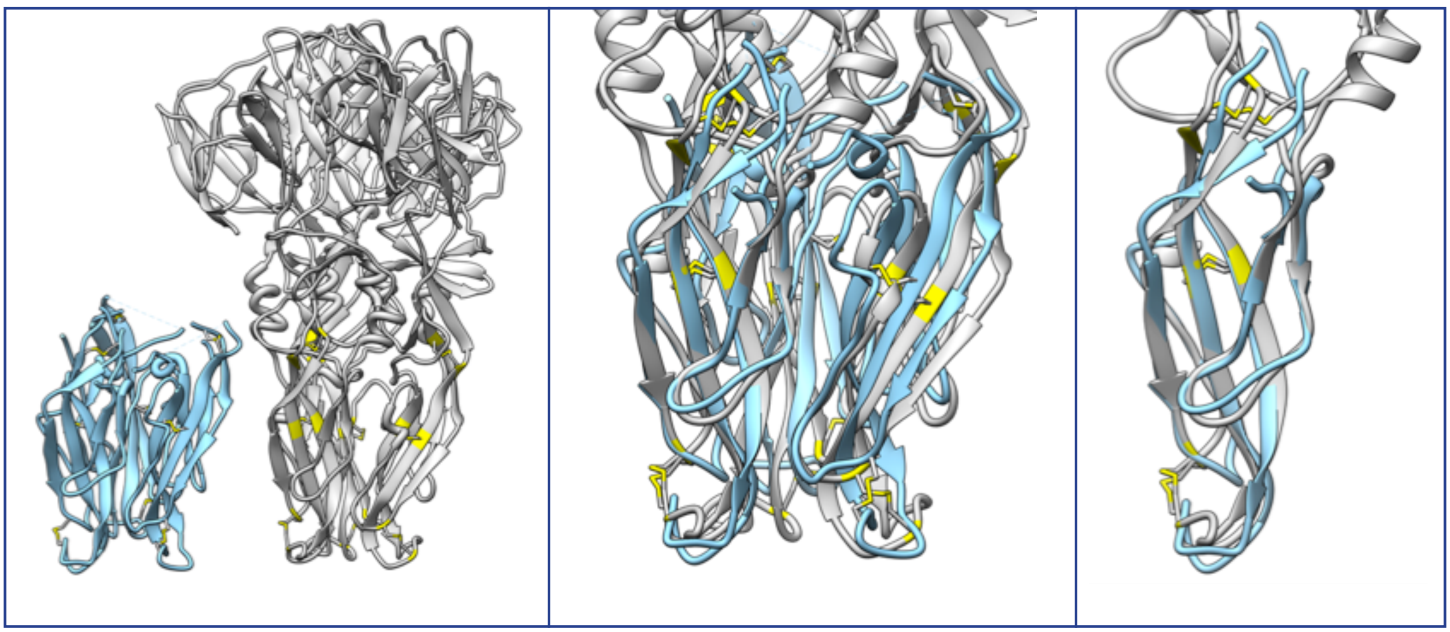
An open-source software, Goma 6.0 helps solve material-processing problems. Goma is designed as a general mechanics code, with no features that tie it to any particular application. Problems to be solved are specified completely in input files, which include code and material properties specifications. Several of Goma's unique capabilities were developed with LDRD funding, most notably, the novel way in which free and moving boundaries between material phases are treated. Goma has been instrumental in the understanding and design of the nuclear weapon component manufacturing process. Other applications include drying polymers, making flat-panel glass, producing reinforced materials for power lines, and creating plastic wrap

BIOSCIENCE

The overarching goal of the Bioscience Investment Area is to develop new competencies in biological science to address two application areas in Sandia's broad national security mission — biodefense and emerging infectious disease, and biofuels.

The research in biodefense includes developing better ways to detect, characterize, and contain harmful pathogens. The strategy integrates advanced technologies with an understanding of human health and immune response. The goal is to improve the response to disease outbreaks and to limit their spread.

The research regarding the nation's reliance on fossil fuels focuses on developing efficient, economical biofuels that can replace or reduce current gasoline, diesel, and aviation fuel consumption. The research includes two sources of energy: lignocellulose, or dry plant matter, and algae. The aim is to find efficient and economical methods to convert lignocellulose into fuels and to understand the factors that govern algal pond stability and identify molecular mechanisms that can be used for lipid/fuel production.



A depiction of a molecular dynamics simulation run on Red Sky, used to understand how viral proteins catalyze the fusion of viral membranes within host cell endosomes, leading to infection. (Left panel) Side by side comparison of the truncated sE trimer (blue) and the full protein. (Middle) Overlap of the two protein structures after simulating each system for 100 ns. (Right) Structural alignment between the simulated truncated and full monomers. Disulfide bonds shown in yellow. (Project 158832)

BIOSCIENCE

Mechanism of Fusion of Pathogenic-Enveloped Viruses with the Endosomal Membrane

158832
Year 3 of 3
Principal Investigator: M. S. Kent

Project Purpose:

Pathogenic membrane-enveloped viruses including flaviviruses, arenaviruses, and paramyxoviruses cause devastating infectious diseases (e.g., hemorrhagic fever, encephalitis) and pose major biodefense threats. For these viruses, fusion of the viral membrane with the cellular endosomal membrane is essential for viral replication and infectivity. Fusion of the two membranes is driven by pH-dependent conformational changes of a dedicated protein, called E in flaviviruses. Crystal structures have been determined for the pre-fusion and post-fusion states of E, but only for truncated mutants lacking important flexible and membrane-spanning portions. Thus, a huge gap in knowledge exists regarding conformational changes of E upon binding to the endosomal membrane and during the intermediate stages of fusion, and also regarding the mechanism by which E anchors into the endosomal membrane. The goal of the project is to address: 1) E protein membrane-bound structure and 2) E protein anchoring to endosomal membranes.

In this study, the following hypotheses were examined: 1) E inserts to the same depth for membranes containing anionic lipids (AL) or cholesterol, 2) five trimers per virus-like particles (VLP) or virus interact with the endosomal membrane, 3) strong affinity requires AL (cholesterol alone is not sufficient), 4) strong anchoring requires AL (cholesterol alone is not sufficient), 5) fusion (lipid mixing) occurs only with AL (cholesterol alone is not sufficient), 6) trimerization of E either does not occur or occurs very slowly in membranes lacking AL (cholesterol alone is not sufficient), and 7) the fusion peptide (FP) plays a critical role in the fusion process beyond simply anchoring E into the host membrane. To test these hypotheses, we have developed entirely novel methods to: 1) measure the structure of E in association with lipid membranes, 2) model the interaction of E with lipid membranes, 3) measure the strength and kinetics of the binding of E and VLPs with lipid membranes, and 4) measure the anchoring (pullout) energy of E imbedded in lipid membranes.

Summary of Accomplishments:

We developed unique experimental and modeling capabilities for studying virus-membrane interactions. The experimental data and molecular dynamics (MD) simulations both showed that E inserts into lipid membranes with compositions similar to those of plasma membrane/early endosomes (plasma membrane [PM], no AL, 30% cholesterol) and late endosomes (LE, 30% AL). For both membrane compositions, E inserts to a depth such that the fusion loop (FL) is slightly inserted into the lipid tail groups. Combining the data for the quartz crystal microbalance (QCM) binding measurements of the free protein and VLPs for the two membrane compositions indicates that 3-4 trimers interact with the endosomal membrane per VLP. The QCM binding measurements show a factor of 6-8 greater binding affinities for the LE composition compared with PM. Affinity is clearly important at such low concentrations. The new biophysical technique for measuring anchoring energy revealed a value of 60kT per trimer for PC:PG 80:20 membranes, or at least 180 kT per VLP. That value greatly exceeds the value of 50 kT estimated to be needed for membrane bending during fusion; we conclude that anchoring of

E in the membrane is not limiting for the LE composition (30% PG). Trimerization of E occurs upon membrane binding for both PC:PG 70:30 and PC:PE:CH 49:21:30 bilayers. The fusion data for liposomes containing cholesterol but no AL show that fusion occurs but requires higher concentrations of virus. The MD simulations indicate that mutations in the FL (W101F, F108W, K110E) that have been reported to block fusion have very little impact on binding and certainly do not block binding and insertion of the FL. Experiments suggest FL mutations impact maturation (residual prM levels).

Significance:

The present work suggests a new therapeutic approach to blocking DV replication that may have clinical significance for human health. Since fusion of DV occurs in endosomes, developing a drug strategy to block fusion is substantially more challenging. In particular, the fact that E rearranges from dimer to trimer while in the endosome, thereby exposing many possible drug targets only when in the endosome, presents a serious obstacle. Our work suggests that blocking the residues that are responsible for binding and/or anchoring of E to the endosomal membrane could be a promising alternative strategy. This research may facilitate the development of medical countermeasures against pathogenic membrane-enveloped viruses including flaviviruses, arenaviruses, and paramyxoviruses that are potential biothreat terrorist agents and the causative agents of important emerging infectious diseases.

Utilizing Biocomplexity to Propagate Stable Algal Blooms in Open System — Keeping the Bloom Going

158835
Year 3 of 3
Principal Investigator: T. Lane

Project Purpose:

One of the most significant barriers facing commercialization of algal biofuels is maintaining long-term culture stability. Cultivation of algae in open ponds, while the most economically viable option for biomass production, suffers from instability and inability to sustain high production rates. Although higher algae productivities are regularly touted, established algae facilities can only produce ~ 2 $g/m^2/day$. Achieving biological stability (limiting invasion of undesirable species, grazers, and pathogens) is, therefore, critical in mass algae production. In nature, microorganisms exist as a consortium of functionally specialized and interacting individuals that collectively adapt to dynamic environmental cues, resulting in stability. Algae naturally grow in complex ecosystems and it has been demonstrated that these mixed microbial populations coexist through niche partitioning and are robust to environmental fluctuations, able to weather periods of nutrient limitation, and more capable of resisting various insults (invading species, predators, pathogens). Utilizing mixed communities necessitates an understanding of how interactions among individual system components contribute to global population dynamics. We will investigate the microbial community dynamics and response of algal ecosystems in order to understand the essential niche roles (or symbiotic relationships) necessary to achieve and maintain a stable algal consortium. Specifically, we will: 1) investigate algal-microbial consortia from various sources, identify the community structure (metagenomics) as function of system perturbations (i.e., addition of predator, pathogen or temperature excursions), 2) identify critical functions that stabilize the community by constructing and interrogate representative mixed cultures in vitro for functional validation, and 3) develop models to understand the relationship between biocomplexity (biodiversity) and stability. We will initially focus on predation as stressor and move on to other frequently encountered system stressors. We will then apply this knowledge to develop stable, high biomass producing artificial consortia that is better suited for outdoor algal biofuels production.

Summary of Accomplishments:

Maintaining pond stability is one of the most significant barriers facing commercialization of algal biofuels, and understanding the factors that promote biological stability and the means by which stable communities naturally limit invasion of undesirable species is a critical first step to mass algae production. We investigated the microbial community dynamics in natural and manipulated algal ecosystems to understand the niche roles (symbiotic relationships) necessary to achieve and maintain a stable algal consortium. We investigated the community structure (metagenomics) of natural algal consortia as function of system perturbations and identified critical microbes that are important to the community by constructing and interrogating the network of microbial community. In doing so, we discovered novel strains of bacteria that demonstrated a probiotic or growth enhancing affect on the algae when grown in co-culture. We characterized the effects of the presence of these probiotic strains in laboratory and outdoor culture systems. We carried out an initial transcriptomic analysis of the response of the algae to presence of the probiotic strains. This analysis revealed that several genes in carbon acquisition and oxidative phosphorylation pathways were differentially expressed in the algae when grown in the presence of the probiotic bacterial strains. This leads us to postulate that the probiotic strains could be enhancing algal growth by relieving carbon limitation and/or oxidative stress in the algal mass culture. We characterized the ability of isolated bacterial strains to protect our eukaryotic algae test species, *Nannochloropsis salina*, from biomass loss from predation by rotifier (*Brachionus plicatillis*). We demonstrated that low concentrations of a specific bacterial strain were sufficient to prevent predation.

Significance:

The knowledge gained from research carried out under the auspices of this project will be applied to develop stable, high-biomass-producing, artificial, consortia that are better suited for outdoor algal biofuels production. By increasing annualized real production of open algal mass culture systems, the results of this research will contribute to the eventual economic production of algae based biofuels. Algal-based biofuels are sustainable and can be produced domestically. This will reduce the reliance on foreign petroleum and, thus, increase the energy of the US. This work has also advanced the fundamental understanding of algal/microbial community structures and the interactions between bacteria and eukaryotic microalgae. This work extends to an analysis of the gene expression response of the algae to the presence specific probiotic bacterial strain that enhance algal growth.

Genomic Functionalization: The Next Revolution in Biology

162034
Year 3 of 3
Principal Investigator: P. Imbro

Project Purpose:

Next-generation sequencing, multiple ‘omics’ technologies and computational methodologies have provided an exponential growth in biological data relevant to national priorities in biodefense and bioenergy. The backbone of the data edifice is our greatly expanded knowledge of organisms’ genomes. Genomic data has enabled revolutionary advances in areas such as detection and diagnosis of biological agents, forensics, and bioenergy. The potential of the sequence data has yet to be fully realized, however, in that we often simply do not understand the function or significance of most genome subsequences. This knowledge gap greatly complicates diverse tasks such as assessing the potential pathogenicity of an agent, or the health implications of human genomic sequence variations. Improved interpretation of the biological and operational implications of genomic regions and of their associations with measurable functions would enhance and accelerate the discovery of new solutions to our national needs, with crosscutting impacts in defense, energy, and health care. Approaches to the identification and characterization of gene and genomic potentials, herein referred to as genomic functionalization, vary widely, can follow multiple paths to resolution, and entail different degrees of risk, cost, and efficiency. This project will develop a prototype genomic functionalization capability, a critical stepping-stone to the next revolution in biological sciences, and test this capability for clinical metagenomics applications to national defense and health care. This project will define an architecture for gathering and intersecting genomic and other ‘omic’ data with operational and functional metadata and use advanced data integration tools and knowledge extraction tools to establish useful correlates of genome sequence patterns.

Summary of Accomplishments:

We have implemented a ligand-alignment algorithm into our developed computational pipeline for identifying specificity-determining features (SDFs) in protein-ligand complexes. Given a set of protein-ligand complex structures, the algorithm aligns the complexes by ligand rather than by the C-alpha root mean square deviation (RMSD) or standard approach, providing a single reference frame for extracting SDFs. We anticipate that this ligand-alignment capability will be highly useful for protein function prediction. We already have a database containing >20,000 ligand-protein complex crystal structures taken from the Protein Data Bank. By aligning these proteins to single reference frames using ligand alignment, we can submit the complexes to our pipeline for SDF extraction. The SDFs derived from this training procedure can be used as thumbprints that are hallmarks of individual enzyme classes. These SDF thumbprints may then serve as guides to the prediction of function of new unknown proteins.

Significance:

Our results are significant because this is the first demonstration that enzyme functions can be accurately assigned based on their binding profiles to standard metabolites as predicted by virtual screening. In addition, the binding profiles themselves can be clustered in order to yield insight into SDFs. These findings have dual utility: 1) we have proof of principle of the feasibility of accurate enzyme function prediction in a sequence-independent, high-throughput fashion and 2) the body of data that we generate can feed into the creation of a SDF database for proteins of diverse functional classes.

Developing a bioinformatic capability to associate “-omic” data and clinical metadata to desired predictive outcomes, such as the early detection of an unknown pathogenic biological agent, will potentially accelerate Sandia’s discovery of new solutions to national priorities in energy, remediation, human and animal health, homeland security and national defense.

Self-Deconstructing Algal Biomass as Feedstock for Transportation Fuels

164662
Year 3 of 3
Principal Investigator: R. W. Davis

Project Purpose:

The potential for producing biofuels from algae has generated much excitement, based on projections of large oil yields with relatively little land use. However, numerous technical challenges remain for achieving market parity with conventional non-renewable liquid fuel sources. Among these challenges, the energy-intensive requirements of traditional cell rupture, lipid extraction, and residuals fractioning of microalgae pose great opportunities for translational research in the nascent field of algal biotechnology. To date, solutions to the aforementioned problems have been sought using technology developed primarily for petrochemical applications. A targeted biological approach to these issues could dramatically reduce both the capital and operating costs of producing fuels from algae. Our novel solution to address these problems is to employ methods of biological engineering to eliminate the need for hardware- and energy-intensive methods for cell rupture, lipid extraction, and residuals fractioning by introducing a triggered cell lysis and enzymatic conversion functionality in a halophilic microalgae suited for mass culture. The output of the planned enzymatic deconstruction process will consist of a slurry of phase segregated lipid and aqueous algal metabolites for subsequent transformation to transportation fuels by transesterification, fermentation, and anaerobic digestion.

Until recently, very little progress has been made employing biological engineering for microalgal biofuels applications. However, achievements in genetic analysis and minimally perturbative methods of algal transformation have opened the gates for new research in this area. A prime target for employing biological engineering is the development of biochemically triggered expression of deconstruction genes for decomposing the algal extracellular matrix (ECM). Not only will this process lead to a low-cost lipid extraction process, but the polysaccharides that compose the ECM will be converted to sugars for fermentation. Our strategy will focus on coupling expression of exogenous mesophilic sulphatase and protease enzymes to genes involved in responding to nutrient limitation. This approach will facilitate maximal biomass accumulation prior to deconstruction.

Summary of Accomplishments:

Based on our previous work to identify the best performing enzymes for deconstruction of *Nannochloropsis*, we performed heterologous expression of three different enzymes, including arylsulfatase B (EC 3.1.6.1), alcalase (EC 3.4.21.62), and lysozyme (EC 3.2.1.17). The three enzymes were also combined on a single plasmid for co-expression. Because expression of the stated heterologous gene products was known to be toxic to *Nannochloropsis*, we adopted the protocols developed for expression using a lipid droplet surface protein (LDSP) promoter targeted to nutrient-limitation based lipid accumulation and a 35S terminator sequence (Vieler, et al., 2012). This approach targets algae production in batch culture, where nitrogen limitation is concomitant with onset of lipid production and peak biomass accumulation, thus preventing unwanted detriment to overall biomass productivity during active growth. The DNA sequences and primers were employed for polymerase chain reaction (PCR) addition into plasmids. The sequences were assembled into an interrupt descriptor table (IDT) vector with a xeocin selection marker. This was achieved using PCR assembly using 20-30 PCR cycles per addition and a commercial stabilized T5 exonuclease. The largest plasmid, containing all three heterologous genes, selection marker, and promoter/terminator sequences was confirmed to be

~9.6kB by gel chromatography. The resulting plasmids were introduced into axenic *N. salina* cells using the electroporation protocol established by Kilian, et al. Zeocin-resistant colonies obtained by transformation were resuspended in F/2 medium lacking any nitrogen source, and were subsequently spotted on agar plates containing KNO_3. After ~2 days, the cells were observed to bleach, indicating depletion of the nitrogen source and expression of the heterologous enzymes. Immunoblot analysis was used to confirm presence of the enzymes. Quantification was performed densitometrically using ImageJ software on immunoblots with immunoreactive proteins visualized using alkaline phosphatase.

Significance:

This work addresses a fundamental challenge for low-cost production of renewable bio-based fuels to support the nation's energy efficiency and renewable energy goals. The results of the work provide tangible guidance for efficient processing of high productivity algae biomass and the efforts for genetic modification of *Nannochloropsis* should be applicable for production of intermediate value bio-based products from algae culture. The algae biotechnology techniques that were developed in support of this work could potentially contribute to DOE's technology roadmap and multi-year program plan for algae biofuels development.

Refereed Communications:

R.W. Davis, B.J. Carvalho, H.D.T. Jones, and S. Singh, "The Role of Photo-Osmotic Adaption in Semi-Continuous Culture and Lipid Particle Release from *Dunaliella Viridis*," *Journal of Applied Phycology*, DOI: 10.1007/s10811-014-0331-5, May 2014.

R.W. Davis, H. Wu, and S. Singh, "Multispectral Sorter for Rapid, Nondestructive Optical Bioprospecting for Algae Biofuels," in *Proc. SPIE* 8947, *Imaging, Manipulation, and Analysis of Biomolecules, Cells, and Tissues XII*, San Francisco, CA, 2014.

R.W. Davis, H.D.T. Jones, A.M. Collins, J.B. Ricken, M.B. Sinclair, J.A. Timlin, and S. Singh, "Label-Free Measurement of Algal Triacylglyceride Production using Fluorescence Hyperspectral Imaging," *Algal Research Journal*, DOI: 10.1016/j.algal.2013.11.010, 2013.

Unknown Pathogen Detection in Clinical Samples: A Novel Hyperspectral Imaging and Single Cell Sequencing Approach

165607
Year 2 of 3
Principal Investigator: B. Carson

Project Purpose:

Detection of pathogens in pre-symptomatic stages of infection is challenging. Most diagnostic techniques are insufficiently sensitive to detect infection and identify viruses, particularly at these early stages. Recently, second-generation sequencing has been applied to this problem. However, despite substantial progress, the signal-to-noise ratio inherent in this technique makes pathogen identification in clinical samples prohibitive, thus, leaving treatment decisions dubious. We will address this critical problem by identifying spatial and spectral signatures of host response that differentiate uninfected human blood cells from those infected with a pathogenic virus without requiring a priori knowledge of its identity. We will integrate hyperspectral imaging with microfluidic cell sorting to: 1) separate individual infected and uninfected cells and 2) use high-throughput sequencing to analyze individual cells. We envision this will greatly improve the ability to identify pathogens in clinical samples since pathogen-negative cells from the same sample will serve as control. Moreover, this new capability would transform not only our ability to diagnose infection with unknown pathogens early in disease, but also identification, characterization, and countermeasure development for emerging and engineered viruses.

No current technology can isolate infected cells without knowing pathogen identity, thus, there is presently no way to identify unknown viral pathogens in individual infected blood cells. State-of-the art cell sorters lack the ability to sort on spatial characteristics, so cannot utilize the majority of information contained in a stained cell. This project presents a novel solution to these problems, integrating key Sandia capabilities in hyperspectral imaging and single cell microfluidics. This is high risk because it requires developing new integrated technology to identify cell state-specific but pathogen-independent markers, and data processing with extreme speed and efficiency of optics, analysis algorithms, and system control.

The Engineering and Understanding of Nanoparticle/Cellular Interactions

165609
Year 2 of 3
Principal Investigator: C. J. Brinker

Project Purpose:

Engineered nanoparticle/cellular interactions encompass a broad spectrum of emerging topics in national security and the health and well being of the nation. Engineered nanoparticles could detect the onset of cancer or infectious disease as well as selectively deliver customized therapeutic 'cocktails' and imaging agents to treat the disease and provide in vivo diagnostics of the progress of therapy. Understanding and engineering nanoparticles (NP)/cellular interactions on scales ranging from the sub-cellular to the organism level are crucial to targeted drug delivery, as well as assessing potential ES&H hazards of NPs and engineering new safer-by-design nanoparticles. Although hundreds of engineered nanocarriers are under development, they all fall short of addressing the multiple challenges of targeted delivery and they cannot be systematically varied or engineered to establish structure-activity relationships or address personalized medicine.

We recently invented a new composite nanocarrier termed a "protocell." Targeted protocells, reported in a 2011 *Nature Materials* cover article are formed by fusion of a lipid bilayer — essentially a cell membrane — on a nanoporous, cargo-loaded nanoparticle core followed by modification with targeting and trafficking ligands. They combine the advantages of FDA-approved liposomes (low inherent toxicity, immunogenicity, long circulation times) and porous particle nanocarriers (stability and an enormous capacity for multiple cargos). However, the protocell's supported lipid bilayer (SLB) uniquely represents a reconfigurable surface that can engage in complex biomolecular interactions with a cell surface, directing internalization and intracellular trafficking. As recognized in a *Nature Materials* News and Views commentary accompanying our initial publication, "The properties engineered into this [protocell] system elegantly synergize to approach the goal of an ideal targeted-delivery agent," that is exploiting the modular nature and synergistic characteristics of the protocell. The goal of this project is to design and fabricate next-generation protocells that overcome multiple grand challenges of current nanocarrier platforms with respect to cargo capacity and diversity, circulation time, controlled release, targeting and cell-specific toxicity, and safety.

Consolidated Bioprocessing and Biofuels Production Platform

165822
Year 2 of 3
Principal Investigator: R. W. Davis

Project Purpose:

Depleting fossil fuel reserves and environmental concerns are the major catalysts for research into alternatives for transportation energy that are renewable and carbon neutral. To achieve current US renewable fuels goals, approximately 1 billion tons of residual biomass would need to be converted to biofuels. This research aims to reduce biofuel production costs by building a consolidated bioprocessing (CBP) platform, reducing processing steps. We plan to utilize the thermophilic, cellulolytic bacterium *Clostridium thermocellum* as a chassis to engineer a microbial bioreactor that both degrades biomass feedstocks and produces advanced infrastructure compatible biofuels. We will consolidate biomass pre-treatment and advanced biofuel production to a single bioreactor platform. CBP will reduce unit operations and increase process efficiency by reducing mass transport phenomena and processing steps and costs.

Our proposed CBP chassis, *C. thermocellum*, is a rapid cellulose degrader. Although there are published reports of recombinant DNA transfer into *C. thermocellum*, genetic techniques are not well established to manipulate the organism routinely and no heterologous gene expression has been reported in the literature. The goal of the planned research with UCLA is to: 1) establish a tunable expression system in *C. thermocellum* and 2) use this platform for CBP of protein rich cellulosic biomass to produce advanced biofuels, namely fusel alcohols. We intend to first develop a heterologous expression system driven by a single subunit RNA polymerase (ssRNAP) such as phage T7RNAP instead of attempting to understand native transcriptional regulation of *C. thermocellum*. Our strategy leverages decades of knowledge of ssRNAPs that exhibit specificity for their consensus promoter sequence with minimal expression using host machinery. Furthermore, these features may allow this platform to be transferred to other thermophilic organisms. Secondly, we will introduce optimized pathways for biofuel production under the transcriptional control of these promoters. Anticipated challenges during this research are thermostability of polymerase and optimization of biofuel production pathways and expression systems.

A Modular Nanoparticle Platform for Treatment of Emerging Viral Pathogens

166539
Year 2 of 2
Principal Investigator: E. C. Carnes

Project Purpose:

Anti-viral drugs must typically be administered in large, frequent doses to effectively treat viral infections, including those caused by emerging and engineered viruses. High doses can cause toxic side effects to the host and, if taken improperly, can accelerate the evolution of drug resistant pathogens. There is, therefore, a need to develop biocompatible nanoparticle delivery vehicles in order to reduce the number, frequency, duration, and dosage of treatment, delay treatment beyond the current limit, and prevent recurrent disease. Most state-of-the-art nanocarriers, including liposomes and polymeric nanoparticles, suffer from low capacity, poor stability, and minimal uptake by target cells. This project seeks to address these limitations by designing a modular, highly adaptable nanocarrier, termed a "protocell," which synergistically combines advantages of liposomes and mesoporous silica nanoparticles.

Protocells are comprised of a mesoporous silica nanoparticle (MSNP) core, encased within a supported lipid bilayer, and simultaneously exhibit extremely high loading capacities (>1000-fold higher than comparable liposomes) for chemically disparate therapeutic and diagnostic agents, long-term stability in complex biological fluids, and sub-nanomolar affinities for target cells at low ligand densities. Our ability to precisely control loading, release, stability, and targeting specificity, as well as our ability to engineer the particle size, shape, charge, and surface modification(s) allow us to dramatically reduce dosage and off-target effects, mitigate immunogenicity, maximize biocompatibility and biodegradability, and control biodistribution and persistence. As we reported in the May 2011 cover article of *Nature Materials*, protocells, due to their unique biophysical properties, are one million times more effective at treating human liver cancer than state-of-the-art liposomes. In this project, we seek to extend the utility of protocells to emerging viruses that have relevance as potential biothreats, and will assess the prophylactic and therapeutic potential of protocells loaded with traditional and novel anti-viral agents (such as siRNAs) and targeted to both potential host cells and already infected cells.

Summary of Accomplishments:

Nipah virus (NiV), a biosafety level 4 agent due to its numerous routes of transmission and the high mortality rates associated with infection, is of serious concern globally due to the lack of any efficacious therapeutic treatment. Despite recent advances in understanding the cellular tropism of NiV, however, treatment remains primarily intensive supportive care. To this end, we have developed mesoporous silica nanoparticle-supported lipid bilayers ("protocells") that specifically deliver high concentrations of therapeutic nucleic acids and/or traditional small molecule anti-viral drugs to host cells that were either stably transfected with NiV genes or pre-infected with a NiV pseudovirus. Liposome fusion to nucleic acid-loaded cores results in a supported lipid bilayer (SLB) that promotes long-term (>1 month) cargo retention and provides a fluid interface for ligand display. To generate targeted protocells, we employed phage display to identify peptides that bind to human ephrin B2 (EB2), the primary cellular receptor for NiV. We have found that protocells targeted using the resulting peptides have a nanomolar affinity for EB2-positive cells. When co-modified with a peptide known to trigger macropinocytosis, these protocell nanoparticles are rapidly internalized by target cells but not by EB2-negative cells. Selective design of the supported lipid bilayer results in rapid release of therapeutic cargo upon internalization of protocells by target cells. Using this system, we have demonstrated highly efficacious silencing of NiV genes in target cells. By varying the nucleic acid construct, long-term (> 4 weeks) silencing of viral genes can be achieved. Due to their enormous cargo capacity, as well as their stability and specificity, protocells show promise as delivery vehicles for therapeutic agents capable of preventing viral replication and transmission.

Significance:

The new materials and processes created during this project enable us to better respond to potential biological acts of terrorism at home and abroad. Beyond developing new biodefense countermeasures, these new materials could also be adapted to address persistent and emerging public health issues, such as HIV and Ebola. These new materials may even enable a new generation of prophylaxis beyond traditional vaccines.

Recombinant Vesicular Stomatitis Virus for Therapeutic Antibody Epitope Mapping and Vaccine Development

170801
Year 2 of 3
Principal Investigator: O. Negrete

Project Purpose:

Identification and characterization of antibody binding sites (epitopes) are important for the development of novel vaccines, therapeutics, diagnostics, and affinity reagents. Several methods have been established to map epitopes on target antigens, including x-ray co-crystallography of antibody-antigen complexes, array-based peptide scanning, and 'shotgun' mutagenesis mapping. Combinatorial techniques, such as phage display, are less labor and cost intensive but are unable to reliably map complex 3D conformational epitopes. Rapid and cost effective methods to map neutralizing antibodies binding sites at high resolution are currently lacking. This project seeks to develop a novel technology based on recombinant vesicular stomatitis viruses (rVSV) that provides rapid information about the amino acid sequences of therapeutic neutralizing antibody epitopes to aid in vaccine development for priority pathogens of national security concern.

Many priority pathogens classified as potential agents of bioterrorism by the National Institute of Infectious Diseases (NIAID) require handling in high-level biocontainment facilities and a complex biosafety infrastructure (e.g., high containment labs, select agent registration/permits). This project seeks to create a rapid capability for the high resolution mapping of antibody epitopes for biosafety level (BSL)-3 and BSL-4 biothreat pathogens under BSL-2 containment. We will accomplish this goal by creating libraries of pseudotyped rVSV variants displaying high-complexity randomly mutagenized biothreat antigens. Once the rVSV libraries are developed, we aim to recover detailed information about the amino acid sequences of conformational epitopes recognized by multiple monoclonal antibodies or polyclonal antisera in less than one week using minimal amounts of each antibody.

Systems-Level Synthetic Biology for Advanced Biofuel Production

170804
Year 2 of 3
Principal Investigator: A. Ruffing

Project Purpose:

The US is currently reliant upon foreign fossil fuel resources, representing a significant threat to national security. The limited supply of fossil fuels presents a significant challenge for future energy provision, and the accumulation of carbon dioxide from fossil fuel combustion may lead to significant changes in the global climate. The development of a renewable energy source, such as biofuels derived from microalgae, will help lead to energy independence for the US while also addressing concerns of fossil fuels supply and climate change. However, microalgal fuel production is currently limited by the low natural productivities of microalgae. Synthetic biology techniques may be applied to improve the fuel-producing capacity of these microorganisms, yet the impact of this strategy is limited by the one part (or circuit) at a time approach of traditional synthetic biology. To reach the fuel production rates necessary to make this process economically viable, microalgae must be genetically modified at a systems level to optimize the entire genome for fuel production. Hence, new methods and synthetic biology tools must be developed for these microalgal hosts.

This project will develop a systems-level synthetic biology approach for targeted genetic manipulation of microalgae. With this technique, multiple genetic targets will be modified in a single transformation step, leading to a significant reduction in the time required for strain development. As an example, consider a strain requiring 10 genetic modifications for improved fuel production: the traditional approach would typically require 10 months for strain development, assuming a conservative four weeks per genetic modification. The projected systems-level approach would construct the same strain in only one month. Additionally, the systems-level synthetic biology technique would generate variants with different combinations of the 10 targeted modifications. Given the inherent non-linearity of biological systems, these combination variants may have unknown synergistic effects, resulting in increased fuel production and informing our basic understanding of fundamental microalgal biology.

Understanding and Engineering Lignolysis for Renewable Chemical Production

173019
Year 1 of 3
Principal Investigator: S. Singh

Project Purpose:

Lignin is the only source of renewable aromatics, and utilization of lignin for high value coproducts will enable biofuel industries to become cost competitive with petrochemicals. The potential US market for a lignin-derived octane enhancer alone is estimated to be 2.2 billion gallons per year. The major bottleneck in lignin valorization is the lack of efficient technologies for converting mono-, bi- and tri-aryls into renewable aromatics. In order to address this gap, a mechanistic understanding of the molecular basis of microbial lignolysis, and the discovery of efficient pathways that can be integrated into a commercially viable microbial chassis, must be realized.

The beta-aryl ether (beta-O-4) linkage constitutes a major portion (50% - 80%) of the linkages present in lignin. The lignolytic proteins (ligDEFG) gene cluster that is responsible for the breakdown of the beta-O-4 linkage has been well characterized in *Sphingomonas paucimobilis* SYK-6. For heterologous expression of these four genes in *Bacillus subtilis*, we have designed the synthetic operon to include a signal peptide at the N-terminus of the synthesized proteins, for translocation of the lignolytic proteins LigDEFG across the cell envelope. A preliminary toxicity study was performed on *Bacillus subtilis* with the monomeric compounds of lignin such as vanillin and guaiacol. Our results revealed that even in the presence of 1g/L of these toxic compounds, the growth rate was not hindered significantly. In an effort to expand the molecular tools available for *B. subtilis*, a promoter engineering work is being carried out simultaneously. Different IPTG inducible promoters (Ptac, Ptrc, Ptic, and Pgrac100) and constitutive promoters (PgroE100, Pveg and P43) are being tested in *B. subtilis* by using mCherry as a reporter protein. To obtain high-strength constitutive promoters, a library of promoters is being generated by creating mutations in the spacer region of the -10 and -35 motifs. In addition, experiments are under way on testing lignin transporters from various organisms.

EKSG: A Universal Sample Prep Technology for Multidimensional Bioscience

173020
Year 1 of 2
Principal Investigator: A. Hatch

Project Purpose:

Systems-level understanding of biological states and disease mechanisms typically requires multidimensional analysis of key samples. Unfortunately, multidimensional analysis is often difficult or impossible using current sample preparation methods, due to inherent challenges purifying multiple analytes from small samples (e.g., human clinical, animal model). Each method generally recovers only certain sub-classes of analyte, yet splitting samples for multidirectional processing is problematic or, for small samples, not feasible. Moreover, treatments of sample and sample-derived analytes can lead to analyte degradation and other undesirable effects (e.g., mixing of intra- and extra-cellular analytes), making interpretation difficult. We aim to address current deficiencies by developing a powerful new sample preparation competency. We will develop a novel electrokinetic step gradient (EKSG) device for continuous processing of blood sample input, enabling precise segregation of different analyte classes (nucleic acids, proteins, nanoparticles, and cells) into separate collection reservoirs for downstream analysis. EKSG will be applied to small volumes (<0.1 mL) of healthy whole blood, tuned for simultaneous isolation of informative analytes: 1) mRNA, microRNA, and proteins from white blood cells; 2) microRNA from extracellular vesicles; 3) mRNA, microRNA, and proteins from extracellular RNA/protein nanoparticles; and 4) “free” extracellular DNA, microRNA, and proteins. We will similarly apply EKSG to infected blood for additional isolation of such analytes from viral or bacterial pathogens. Nucleic acid fractions will be analyzed using qPCR and high-throughput sequencing and proteins using mass spectrometry. This R&D work explores a novel and significant “disruptive” sample prep technology that could dramatically improve bioanalytical methodologies.

In Vivo High Throughput Transcriptomics to Elucidate the Spatial and Temporal Dynamics of Host-Pathogen Interactions

173021
Year 1 of 3
Principal Investigator: R. Meagher

Project Purpose:

Massively parallel transcriptome sequencing (RNA-Seq) has the potential to revolutionize studies of microbial pathogenesis by providing information on the spatial and temporal dynamics of gene expression in both the host and pathogen. However, conventional RNA-Seq methodologies focus almost exclusively on the host because host transcripts vastly outnumber those of the pathogen. A novel Sandia-developed approach called Pathogen Capture can enrich microbial transcripts 100-fold, allowing complete recovery and sequencing of the microbial transcriptome without altering host transcripts. This allows coupled, quantitative analysis of both the host and pathogen transcriptome in a single sequencing run. However, Pathogen Capture is a labor-intensive, low-throughput technique that is a bottleneck in performing large studies.

We intend to develop a high-throughput, fully automated Pathogen Capture system to enable a host-pathogen interactions study using primary cell infection with multi-drug resistant *Klebsiella pneumoniae*. Multi-drug resistant gram-negative pathogens such as *K. pneumoniae* are an important class of emerging, difficult-to-treat pathogens with associated high mortality and morbidity, and represent a biodefense threat due to the ease of transmission of drug resistance genes. We will discover the transcriptional sequence of events by which these "opportunistic" pathogens infect the host, overwhelm the immune system, and resist treatment with antimicrobial drugs.

Our planned pathogenesis investigation is uniquely enabled by the envisioned high-throughput platform for Pathogen Capture, which demands a new approach to engineering devices for highly parallel sample prep. The Pathogen Capture technique is unique to Sandia and is distinct from the "subtractive" approaches developed in the RapTOR Grand Challenge for detection of unknown pathogens. The device and methods are broadly applicable to understanding the dynamics of any microbial or viral pathogen in any host system, and the coupled host/pathogen transcriptomic data is a fundamentally new, innovative technique to studying host/pathogen interactions and microbial communities in general. Fundamental studies of biodefense-relevant pathogens support missions in countering bioterrorism and biodefense.

Bio-Inspired MOF-Based Catalysts for Lignin Valorization

173022
Year 1 of 1
Principal Investigator: M. D. Allendorf

Project Purpose:

Lignin is potentially a plentiful source of renewable organics, with ~50 million tons/year produced by the pulp/paper industry and 200-300 million tons/year projected production by a US biofuels industry, which must process ~1 billion tons of biomass to meet the US renewable fuel goals. However, there are currently no efficient processes for converting lignin to value-added chemicals and drop-in fuels. Lignin, therefore, represents an opportunity for production of renewable valuable chemicals, but presents staggering technical and economic challenges due to the quantities of material involved and the strong chemical bond characteristic of lignin. The latter typically requires multiple aggressive chemistries and high temperatures to degrade. Lignin chemical non-uniformity also leads to complex product mixtures that tend to repolymerize. Conventional petrochemical approaches (pyrolysis, catalytic cracking, gasification) are energy intensive (400-800 °C), require complicated separations, and remove valuable chemical functionality. Low-temperature (25-200 °C) alternatives are clearly desirable, but enzymes are thermally fragile and incompatible with organic solvents, making them impractical for large-scale biorefining. Alternatively, homogeneous catalysts, such as recently developed vanadium complexes, must be separated from product mixtures, while many heterogeneous catalysts involve costly noble metals.

The objective of this project is to develop an entirely new class of biomimetic, efficient, and industrially robust synthetic catalysts based on nanoporous metal-organic frameworks (MOFs). Catalysts designed to perform both oxidative cleavage of beta-O-4 and C-C linkages will be developed, as well as a novel approach employing hydrogen radicals. We will apply first-principles computational biology and in situ optical diagnostics to establish a connection between enzyme active site structure and the structural features of MOFs. The resulting fundamental knowledge will be translated into catalytic activity using the exceptional synthetic versatility of MOFs. Although catalytic MOFs are known, catalysis of bond cleavage reactions needed for lignin degradation is new. Thus, fundamental research is required that industry and most sponsoring agencies are currently unwilling to undertake.

Summary of Accomplishments:

We synthesized MOFs and infiltrated them with titanium and nickel species to create catalysts for the hydrogenolysis of aryl-ether (C-O) bonds in model compounds that mimic the beta-O-4, alpha-O-4, and 4-O-5 linkages of natural lignin. The versatile IrMOF-74(n) series was selected as a platform for creating efficient hydrogenolysis catalysts, as it provides tunable pore sizes from 1-10 nm and has the required thermal and chemical stability. We found that using these MOFs, the catalytic C-O bond cleavage occurs at 10 bar hydrogen pressure and mild temperatures in the 90 to 120 °C range. The conversion efficiency of the aromatic ether model compounds into the corresponding hydrocarbons and phenols varies as $PhCH_2CH_2OPh$ > $PhCH_2OPh$ > PhOPh (Ph = phenyl), while the catalytic activity follows the trend: Ni@IRMOF-74 > Ti@IRMOF-74 > IrMOF-74. Conversions as high as 80%, coupled with good selectivity for hydrogenolysis vs. hydrogenation, highlight the potential of MOF-based catalysts for the selective cleavage of recalcitrant aryl-ether bonds found in lignin and other biopolymers.

Significance:

The transformation of lignin into value-added chemicals is a critical, unsolved problem in the development of carbon-neutral biorefineries. New chemistries and catalytic approaches are required to achieve this in a cost-effective manner. In this context, the results of this project, which demonstrate hydrogenolysis of lignin linkages using a novel class of heterogeneous catalysts, are particularly promising, since hydrogen is a widely available, inexpensive consumable reactant. MOF catalysts for lignin degradation have never been reported; consequently, this work represents an important advance for both catalysis and MOF science.

Refereed Communications:

M.D. Allendorf, R.W. Davis, P. Ramakrishnan, K.L. Sale, and V. Stavila, "MOF-Based Catalysts for Lignin Degradation," presented (invited) at the *248th American Chemical Society National Meeting*, San Francisco, CA, 2014.

Metal Organic Frameworks for Targeted, Triggered, Sustained, and Systemic Delivery of Antibiotics

173493
Year 1 of 2
Principal Investigator: C. E. Ashley

Project Purpose:

Engineered nanoparticles promise to revolutionize the prevention, detection, and treatment of biological and chemical threats by enabling development of next-generation adjuvants, affinity reagents, and therapeutics. Nanotechnology is especially critical in improving the bioavailability of antibiotics and antivirals through targeted accumulation of nanoparticles at sites of infection and subsequent release of therapeutic payloads in response to an appropriate stimulus. However, many existing nanoparticle delivery vehicles, including liposomes and polymerosomes, suffer from limited capacities, uncontrollable release profiles, and complex, specialized synthesis procedures that must be re-adapted for each new cargo molecule, leading to drug- and disease-specific approaches. To address these limitations, we intend to develop metal-organic frameworks (MOFs) for targeted, triggered, sustained, and systemic delivery of antibiotics to cells, tissues, and organs infected with the Category A biothreat, *Francisella tularensis*. Our effort will result in a new, differentiating Sandia capability that enables pre-administration of therapeutics to laboratory, first-responder, or military personnel who are at risk of being exposed to a biological threat. Our effort will also facilitate event recovery by enabling effective decontamination of surfaces or buildings after accidental or intentional release of a biothreat. Furthermore, MOF technology should be easily extendable to delivery of nerve agent countermeasures, treatment of traumatic brain injury, and creation of broad-spectrum vaccine adjuvants. Consequently, this work could help establish Sandia as a leader in the development of nanotherapeutics and nanoadjuvants.

When compared to other porous nanoparticles (e.g., mesoporous silica), MOFs have higher surface areas and more tunable chemistries, which should translate into higher loading capacities and optimal drug-MOF interactions. However, MOFs have historically been used for catalysis and gas storage and have only recently been adapted for therapeutic and diagnostic applications. Therefore, the planned effort could have an immediate high impact, with potential to further establish Sandia as a leader in engineering porous nanomaterials for biological and chemical defense and other national security applications.

A Novel Application of Synthetic Biology and Directed Evolution to Engineer Phage-Based Antibiotics

178849
Year 1 of 1
Principal Investigator: M. Wu

Project Purpose:

The emergence of multiple drug resistant bacteria poses threats to human health, agriculture, and food safety. Annually over 100,000 deaths and up to $20 billion in losses to the US economy are attributed to multiple drug resistant bacteria. With only four new chemical antibiotics in the drug development pipeline, dire need exists for new solutions to address the emerging threat of multiple drug resistance.

We envision a paradigm-changing approach to address the multi-drug resistant bacteria problem by utilizing Synthetic Biology (SynBio) methodologies including microfluidic engineering and ultra-high throughput screening to create and evolve "designer" bacteriophages or phages — viruses that specifically infect bacteria to infect and kill newly emerging pathogenic bacterial strains without the need for chemical antibiotics. A major advantage of using phage to combat pathogenic bacteria is that phages can co-evolve with their bacterial host. Sandia can be the first in the world to establish an industrial scale SynBio pipeline for phage directed evolution for safe, targeted, customizable solution to bacterial drug resistance. The synthetic biology and screening approaches will lead to fundamental knowledge of phage/bacteria co-evolution.

Summary of Accomplishments:

The purpose of this project was to perform proof-of-principle studies using SynBio and directed evolution to evolve bacteriophages to expand host range and increase lethality in order to create a new class of evolvable antibiotics to combat the emergence of multiple drug resistant bacteria.

Key accomplishments are:

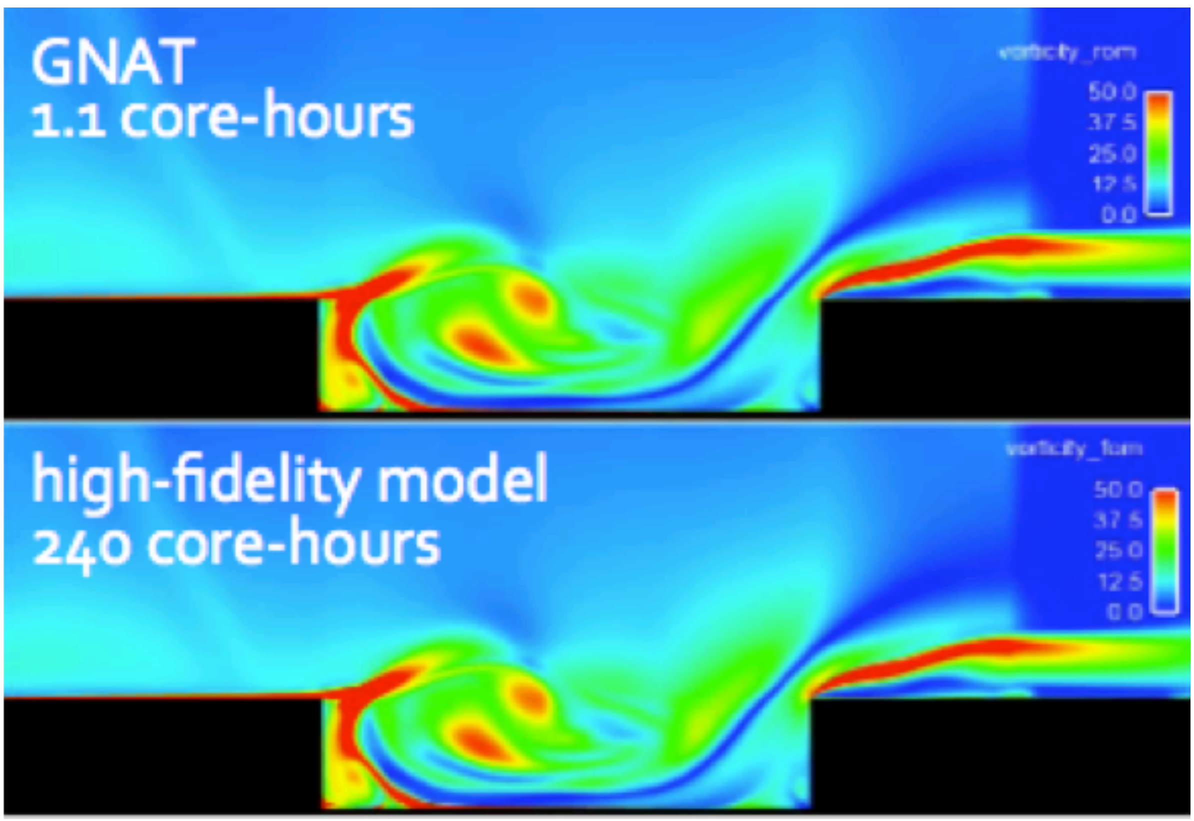
1) The results from this project indicate that bacteriophages can be easily manipulated and subjected to SynBio efforts and be the subject of automated directed evolution processes which become the custom-tailored "live" antibiotics that could potentially be safe for human and animal patients.
    - Random mutagenesis libraries were successfully developed using the newest commercial Directed Evolution reagents. Random mutagenesis was carried out and a total of four mutant phagemid libraries were generated, with different mutagenesis parameters
    - A mutagenesis library was successfully introduced into a suitable recombinant host and phages were successfully produced
    - Screening in a phage plaque assay was demonstrated using *E.coli* as the model "pathogen"
2) A SynBio pipeline for the directed evolution of bacteriophages with increased host range and infectivity for applications as novel evolvable antibiotics was established.
3) Rules of thumb for designing phage mutagenesis experiments for directed evolution were developed.
4) It was determined that the sheer volume of phage screening required for even a small, evolutionary change in phage infection phenotype is overwhelming when conducted by traditional plaque assay methods and manual manipulations. An ultra-high-throughput technology for the library screens will be essential in future related studies.

Significance:

"Live" antibiotics address the challenge of both natural emergence and evolution of antibiotic resistance and also pathogenic organisms that have been engineered to resist standard therapeutics. This approach of custom-evolvable antibiotics should enable specific responses to resistant pathogens as they emerge. The synthetic biology and screening approaches could lead to fundamental knowledge of phage/bacteria co-evolution. The results of this project could potentially impact missions to protect civilians and military personnel from the threat of infectious disease, including re-emerging drug-resistant bacteria.

COMPUTING AND INFORMATION SCIENCES

The Computing and Information Sciences Investment Area (IA) sponsors innovative research and development that advances the state of the art in mathematics and computing relevant to Sandia's national security missions. As the applications of computing continue to deepen and broaden across the Labs, there is a continual need to refresh and advance the underlying technical base in computing and information sciences. The scope of the IA includes computer and computational science and engineering, information science (including mathematics and cognitive sciences), and some aspects of cyber science and engineering. The IA is pursuing several strategic objectives. First, we want to develop the technologies that will underpin the success of future generations of Sandia computers. These technologies include architectures, system software and computational methods and tools for both scientific and data-centric computing. They also include approaches to building future machines out of non-CMOS (complementary metal-oxide semiconductor) technologies. Second, we want to develop and exploit synergy between computing and cyber capabilities. Third, we want to advance the science and engineering of trust in information systems.



The Gauss–Newton with Approximated Tensors (GNAT) Reduced Order Models technique applied to a large-scale Computational Fluid Dynamics problem. The results demonstrated a sub-1% error rate and reduced the computational cost (in core-hours) by a factor of 229. (Project 158789)

COMPUTING AND INFORMATION SCIENCES

Scheduling Irregular Algorithms

158787
Year 3 of 3
Principal Investigator: E. G. Boman

Project Purpose:

Scheduling is the assignment of tasks to processors for execution, and it is an important concern in parallel programming. Most prior work on scheduling has focused either on static scheduling of applications where the dependence graph is known at compile time or on dynamic scheduling of independent loop iterations. However, many algorithms are irregular, which generally means that loop iterations are not independent and the dependence graph is not known at compile time. In addition, scheduling traditionally focuses on improving locality or maintaining good load balance, but for irregular algorithms, even the amount of work may vary with the scheduling policy. The purpose of this project is to investigate novel strategies for partitioning the computations of a simulation into tasks that can be assigned dynamically to processors or processes or threads, so that irregular applications can run efficiently and scalably on thousands to millions of processors.

Irregular applications include traditional scientific applications (partial differential equations ([PDEs], grids, and particles), which are dynamic, either in their geometry or their time dependence. It also includes data-centric applications such as those in informatics or graph analysis where huge volumes of data are processed and the computation is often more memory-bound than compute-bound. Achieving high parallel performance for these kinds of applications is difficult for programmers to achieve due to load imbalances and the dynamic nature of the problems. As supercomputer architectures move to more processors and accelerated hardware such as manycore central processing units (CPUs) and graphic processing units (GPUs), the challenge is exacerbated. One possible solution is to automate more of the parallelization process by appealing to the compiler or a run-time system to partition the simulation's workload effectively and schedule the large number of small tasks on available resources. This project aims to extend the state of the art for that model and apply it to large-scale scientific applications. This year we will study optimal scheduling strategies. This work is in collaboration with University of Texas at Austin.

Summary of Accomplishments:

We developed a new parallel computing framework, Galois, which automatically finds parallelism (concurrency) in irregular applications. The potential impact was demonstrated by multithreaded parallel sparse matrix reordering (reverse Cuthill-Mckee [RCM] and Sloan), which reduced run time for parallel sparse matrix-vector products, a kernel in many iterative solvers. The novel accomplishment was that the ordering itself is parallel so the setup (reordering) cost is low enough that this optimization pays off.

Significance:

This work shows that there is great potential for improving the concurrency in irregular applications via automatic tools. This technology can lead to faster computation and simulation times for a wide range of applications in science and engineering (e.g., renewable energies, climate modeling, and computational fluid dynamics), and also emerging fields such as cybersecurity.

Refereed Communications:

D. Nguyen, A. Lenharth, and K. Pingali, “Deterministic Galois: On-Demand, Portable and Parameterless,” in *Proceedings of International Conference on Architectural Support for Programming Languages and Operating Systems*, *ASPLOS ’14*, 2014.

K.I. Karantasis, A. Lenharth, D. Nguyen, M. Garzaran, and K. Pingali, “Parallelization of Reordering Algorithms for Bandwidth and Wavefront Reduction,” in *Proceedings of SuperComputing 2014*, 2014.

Breaking Computational Barriers: Real-Time Analysis and Optimization with Large-Scale Nonlinear Models via Model Reduction

158789
Year 3 of 3
Principal Investigator: K. T. Carlberg

Project Purpose:

Despite the development of parallel solution algorithms and high performance supercomputers, the computational cost of analyzing large-scale, high-fidelity mathematical models remains a significant barrier in many engineering applications. For example, uncertainty quantification requires simulations to be completed in mere seconds or minutes; embedded control applications require high-fidelity models to be optimized in real time. For nonlinear systems, typical surrogate modeling methods (e.g., response surfaces, proper orthogonal decomposition [POD] Galerkin model reduction) often fail to meet these time constraints without introducing unacceptable errors.

This project is discretized into three parts that will enable real-time analysis and optimization of high-fidelity nonlinear models. The resulting framework will be generalizable, so that it can be applied to a wide range of problems including real-time control and uncertainty quantification (UQ) of power grids, design optimization of nanoporous gas storage devices, and fast simulation of thermal-mechanical systems. This work builds on the Gauss-Newton with approximated tensors (GNAT) model reduction method that has generated exciting results on a wide variety of problems.

The first step of the project integrates the GNAT method within a robust predictive framework. Components include: 1) decreasing the number of required linear-system solves in a simulation, 2) error estimates, and 3) model-refinement capabilities.

The second step targets specific applications: uncertainty quantification and optimization. The above framework will be tailored to these applications.

The final step targets the aforementioned physical problems of interest to Sandia. The above framework will be specialized to the problem of interest within the application of interest. Preserving special problem structure will be of particular interest.

This research constitutes a major step towards shattering the barrier separating high-fidelity, physics-based numerical simulations from time-critical applications.

The Principal Investigator is a Truman Fellowship recipient.

Summary of Accomplishments:

We developed a technique that exploits time-domain data to forecast the solution at future time steps. The Newton solver employs this forecast as an accurate initial guess. This approach decreased simulation times by a factor of two with no loss in accuracy for reduced-order models (ROMs) of a truss-structure model.

We developed a ROM method that preserves Lagrangian structure and leads to efficiency in the presence of nonlinearities. The method significantly improved accuracy and stability over existing methods on a nonlinear structural-dynamics problem.

We developed ROMES, a statistics-based approach to quantify the epistemic uncertainty introduced by the ROM. This method enabled us to develop approaches to integrate experimental data with models via Bayesian inference. To achieve this, we combined importance sampling with ROMs equipped with ROMES error models.

We developed a methodology to refine a posteriori ROMs via an analogue to mesh-adaptive *h*-refinement. The method is the first to provide enrichment without requiring additional high-fidelity model simulations. On a hyperbolic problem, the method allowed ROMs to capture phenomena not present in training data and satisfy any error tolerance.

We developed methods to integrate ROM techniques for optimal, goal-oriented truncation with recycling Krylov subspaces in the context of solving sequences of sparse linear systems.

We applied the GNAT ROM method to a compressible Navier-Stokes simulation of a cavity-flow problem with over 1.2 million degrees of freedom. The method reduced the computational cost (cpu x time) by a factor of 232.

We investigated differences between discrete-optimal and continuous-optimal ROMs. We made a critical discovery: a larger time-step size can lead to less expensive and significantly more accurate discrete-optimal ROMs.

We developed a model-reduction interface to equip Trilinos-based simulation codes for nonlinear model reduction. The software significantly decreases the barrier to entry for implementing model-reduction methods in different Trilinos-based codes.

Significance:

The methods developed in this project form the groundwork for enabling rigorous, pervasive simulation across a range of national security applications. The *h*-refinement method provides a breakthrough in the field of model reduction: it enables ROMs to guarantee the satisfaction of any error tolerance regardless of the relevance of the training data. The ROMES method is also revolutionary, as it is the first method that enables surrogate models to be rigorously incorporated in uncertainty-quantification tasks. Finally, the GNAT experiments highlighted a promising avenue to allow nonlinear ROMs to make significant impact on large-scale computational fluid dynamics simulations that underlie many mission-critical analyses.

Refereed Communications:

K. Carlberg, “Adaptive *h*-Refinement for Reduced-Order Models,” to be published in the *International Journal for Numerical Methods in Engineering*.

K. Carlberg, “Adaptive *h*-Refinement for Reduced-Order Models with Application to Uncertainty Control,” presented at the *SIAM Conference on Uncertainty Quantification*, Savannah, GA, 2014.

Exploring Heterogeneous Multicore Architectures for Advanced Embedded Uncertainty Quantification

158792
Year 3 of 3
Principal Investigator: E. T. Phipps

Project Purpose:

In the near future, high performance computing will undergo dramatic changes as heterogeneous multicore nodes are incorporated into distributed memory architectures. Significant work is under way to exploit these new architectures for single-point forward simulations. However, critical to predictive simulation is the quantification of uncertainties in these simulations, for which propagation of uncertainties in simulation input data to simulation output quantities of interest is key. Since one avenue of forward uncertainty propagation relies solely on sampling a simulation code over the uncertain input space (so-called nonintrusive approaches), any improvement in the forward simulation enabled by multicore architectures will result in commensurate improvement in the forward uncertainty calculation. However, even with these improvements, there will be many problems of strategic interest where the computational requirements for accurate uncertainty propagation will still be too great. To address these challenges, it is critical to develop new architecture-aware uncertainty propagation algorithms that fully exploit the performance benefits of heterogeneous multicore architectures.

The purpose of this project was to create new embedded uncertainty quantification methods that fundamentally alter the structure of a simulation code to implement forward uncertainty propagation directly, leveraging high on-node core and thread counts, with the aim of achieving significant reductions in overall computational run times and increased scalability over nonintrusive methods. This required fundamental algorithmic, computer science, and software research to develop algorithms and approaches that leverage to the greatest extent possible the capabilities provided by these emerging architectures. Significant challenges were developing effective uncertainty-adapted solution strategies that scale to very high thread counts and software tools allowing these approaches to be incorporated in a diverse set of scientific simulation codes. The work was foundational across all Sandia scientific computing missions, and illuminated a path to exascale computing where uncertainty quantification, not single-point forward simulation, is the driving technology.

Summary of Accomplishments:

Through this project, we created embedded uncertainty quantification algorithms designed for Sandia scientific computing mission applications that propagate uncertainty information at the lowest levels of the simulation code. We demonstrated significantly improved performance for aggregate uncertainty quantification calculations on modern multicore and manycore computer architectures using these techniques. These performance improvements were achieved through improved memory access patterns, better utilization of fine-grained parallelism, improved cache reuse, reduced communication, and increased floating-point intensity. We also developed an approach for incorporating these techniques in diverse simulation codes that doesn't require the developers of these codes to explicitly manage the propagation of uncertainty, yet allows low-level fine-grained parallelism to be applied to the uncertainty discretization. These techniques were encapsulated in a set of software tools that are publicly released within the Trilinos software framework, making them immediately available to Sandia simulation codes. Furthermore, we developed a fully functioning proxy application that demonstrates how these techniques are used to solve uncertainty quantification problems as well as how to incorporate them into application codes.

Significance:

Uncertainty quantification is a critical component of rigorously justified predictive computational simulation, which in turn is a critical component of many national security mission areas. Emerging high performance computational architectures threaten our ability to achieve the requisite needed fidelity. This project developed a strategy for maintaining and improving performance of aggregate uncertainty quantification calculations on these architectures, as well as algorithms and software supporting the strategy, ensuring the predictive simulation needs of important mission applications can potentially be addressed on these emerging architectures.

Refereed Communications:

E. Phipps, "Uncertainty Quantification Challenges in High Performance Scientific Computing," presented (invited) at the *SIAM Conference on Uncertainty Quantification*, Savannah, Georgia, 2014.

Architecture- and Resource-Aware Partitioning and Mapping for Dynamic Applications

158793
Year 3 of 3
Principal Investigator: K. D. Devine

Project Purpose:

As computer systems grow in both size and complexity, the need for applications and run-time systems to adjust to their dynamic environment also grows. For decades, parallel computers were largely homogeneous; thus, prior work-distribution approaches did not account for heterogeneous hardware and data-access costs. Today's systems, however, feature network, processing, memory hierarchies, and nonuniform performance characteristics. Greater attention to architectural features and real-time system state is required to enable efficient and scalable application performance. Even the shear size of emerging systems (hundreds of thousands or millions of cores) challenges their effective use. Larger systems invite more users, increasing competition for shared resources like network bandwidth. In larger systems, the distance in the network across which a single job might be spread widens, thus increasing the cost of application communication. Larger, more complex systems also require greater amounts of power, increasing the overall cost of computing.

Our goal was to combine static architecture information and real-time system state with algorithms to conserve power, reduce communication costs, and avoid network contention. We developed new data collection and aggregation tools to extract static hardware information (e.g., node/core hierarchy, network routing) as well as real-time performance data (e.g., central processing unit [CPU] utilization, power consumption, memory bandwidth saturation, percentage of used bandwidth, and number of network stalls). We created application interfaces that allowed this data to be used easily by algorithms. Finally, we demonstrated the benefit of integrating system and application information for two use cases. The first used real-time power consumption and memory bandwidth saturation data to throttle concurrency to save power without increasing application execution time. The second used static or real-time network traffic information to reduce or avoid network congestion by remapping message passing interface (MPI) tasks to allocated processors.

Summary of Accomplishments:

We developed strategies to reduce power consumption within nodes by automatically reducing node-level concurrency (number of threads) when memory bandwidth is saturated. We demonstrated this technique both for single-node applications and for parallel multinode MPI+OpenMP applications. We demonstrated reductions in power consumption of 7.4% in the Lulesh parallel MPI+OpenMP application with no increase in application execution time.

We developed new data collection and aggregation tools in the lightweight distributed metric service (LDMS), as well as interfaces to deliver the data to algorithms for resource management. The data available includes both static routing information and network traffic data from Cray's Gemini routers. These new scalable data collection and aggregation strategies provided full system status snapshots within 0.25 seconds on a Cray system with 27648 nodes. Deployment on Cielo is in planning stages.

We examined architecture-aware geometric mapping algorithms based on geometric partitioning algorithms. These algorithms reduce application communication costs and execution time by reducing the distance messages travel in the network. Our new architecture-aware geometric mapping in Zoltan2 reduced application execution time by 31% on 64K cores of Cray Cielo for a finite-difference proxy application.

We used our new network performance-counter tools to verify that our mapping algorithms did, indeed, reduce network congestion. We also correlated real-time network data with application performance to identify effective metrics for mapping tasks to cores. We integrated our real-time performance collection tools with graph-based mapping tools to allow applications to avoid network contention from competing applications. Our resulting dynamic mapping using real-time network data recovered 49% of execution time lost to congestion in a sparse matrix-vector multiplication kernel on a shared computer system.

Our software is available in the open-source LDMS and Zoltan2 toolkits.

Significance:

With heterogeneous architectures, dynamic performance characteristics, and power constraints, exascale computers pose significant challenges to application developers. Our work enables both new applications and those written for homogeneous computing environments to perform well in increasingly heterogeneous and unpredictable environments. Our research also lays the groundwork for data collection, power management, and mapping strategies of potential benefit for new DOE platforms such as the Alliance for Computing at Extreme Scale (ACES) Trinity and the National Energy Research Scientific Computing Center (NERSC) Cori.

Refereed Communications:

J. Brandt, K. Devine, A. Gentile, and K. Pedretti, "Demonstrating Improved Application Performance using Dynamic Monitoring and Task Mapping," in *Proceedings of Workshop on Monitoring and Analysis for High Performance Computing Systems Plus Applications (HPCMASPA), IEEE Cluster*, 2014.

M. Showerman, J. Enos, J. Fullop, P. Cassella, N. Naksinehaboon, N. Taerat, T. Tucker, J. Brandt, A. Gentile, and B. Allan, "Large-Scale System Monitoring and Analysis on Blue Waters using OVIS," In *Proceedings of Cray User's Group (CUG)*, 2014.

V. Leung, D. Bunde, J. Ebbers, S. Feer, N. Price, Z. Rhodes, and M. Swank, "Task Mapping Stencil Computations for Non-Contiguous Allocations," in *Proceedings of ACM SIGPLAN Symposium Principles and Practice of Parallel Programming (PPoPP14)*, 2014.

A. Agelastos, B. Allan, J. Brandt, P. Cassella, J. Enos, J. Fullop, A. Gentile, S. Monk, N. Naksinehaboon, J. Ogden, M. Rajan, M. Showerman, J. Stevenson, N. Taerat, and T. Tucker, "Lightweight Distributed Metric Service: A Scalable Infrastructure for Continuous Monitoring of Large-Scale Computing Systems and Applications," in *Proceedings of SC14*, 2014.

M. Deveci, S. Rajamanickam, V. Leung, K. Pedretti, S. Olivier, D. Bunde, U. Catalyurek, and K. Devine, "Exploiting Geometric Partitioning in Task Mapping for Parallel Computers," in *Proceedings of IEEE International Parallel and Distributed Processing Symposium (IPDPS)*, 2014.

R. Grant, S. Olivier, J. Laros, R. Brightwell, and A. Porterfield, "Metrics for Evaluating Energy-Saving Techniques for Resilient HPC Systems," in *Proceedings of IEEE Workshop High Performance, Power-Aware Computing (HP-PAC)*, 2014.

E. Balzuweit, D. Bunde, V. Leung, A. Finley, and A. Lee, "Local Search to Improve Task Mapping," in *Proceedings of International Workshop on Parallel Programming Models and Systems Software for High-End Computing (P2S2)*, 2014.

Automated Algorithms for Achieving Quantum-Level Accuracy in Atomistic Simulations

158794
Year 3 of 3
Principal Investigator: A. P. Thompson

Project Purpose:

Molecular dynamics (MD) is a powerful materials science simulation tool for bridging between quantum mechanical (QM) systems with a few hundred atoms, and the length/time scales required to model entire microscale devices. However, the impact of MD is severely limited by the lack of suitably accurate interatomic potentials for many important materials. Examples include III-V semiconductor compounds indium phosphide (InP) and refractory metal alloys (Ta/W). Building traditional physics-based potentials is a time-consuming, high-risk endeavor, incompatible with time-sensitive, mission-critical projects. A recent breakthrough enables automated development of quantum-accurate potentials for metals and semiconductor compounds with systematically controllable accuracy. This game-changing capability for predictive materials modeling may enable timely MD simulation of materials of arbitrary chemical composition with unprecedented fidelity, limited only by the availability of relevant QM training data.

The Gaussian-approximation potential (GAP) approach of Bartok, et al., demonstrates that Gaussian process regression can produce accurate surrogates for QM models. The authors have demonstrated the accuracy of GAP for several metals and semiconductors. Building on the GAP formalism, we plan to build an in-house capability called SNAP (spectral neighbor analysis potential) for automated generation of potentials for arbitrary materials using existing DAKOTA regression tools coupled to the LAMMPS (large-scale atomic/molecular massively parallel simulator (molecular dynamic (MD) code. We will generate SNAP potentials for refractory metals and III-V semiconductors. We will also create a scalable parallel implementation of SNAP potentials in LAMMPS, suitable for use in large-scale simulations. The primary risk we anticipate is whether SNAP potentials can provide QM surrogates of sufficient accuracy for national security mission needs.

Summary of Accomplishments:

During the course of this project, we have developed an interatomic potential for solids and liquids called SNAP. The SNAP potential has a very general form and uses machine-learning techniques to reproduce the energies, forces, and stress tensors of a large set of small configurations of atoms, which are obtained using high-accuracy quantum electronic structure QM calculations. The local environment of each atom is characterized by a set of bi-spectrum components of the local neighbor density projected on to a basis of hyperspherical harmonics in four dimensions. The SNAP coefficients are determined using weighted least-squares linear regression against the full QM training set. This allows the SNAP potential to be fit in a robust, automated manner to large QM data sets using many bi-spectrum components. The calculation of the bi-spectrum components and the SNAP potential are implemented in the LAMMPS parallel MD code. Global optimization methods in the DAKOTA software package are used to seek out good choices of hyperparameters that define the overall structure of the SNAP potential. FitSnap.py, a Python-based software package interfacing to both LAMMPS and DAKOTA, is used to formulate the linear regression problem, solve it, and analyze the accuracy of the resultant SNAP potential. We developed SNAP potentials for InP and silica (SiO_2). We developed efficient algorithms for calculating SNAP forces and energies in molecular dynamics simulations using massively parallel computers and advanced processor architectures. We also implemented the multilevel summation method (MSM) for efficient calculation of electrostatic interactions on massively parallel computers.

Significance:

The SNAP software framework, including the FitSnap.py software, the LAMMPS implementation of SNAP, and the expertise accumulated around training set design, is now available for use in many Sandia materials modeling applications that are limited by the availability of suitably accurate interatomic potentials. These potentials are already being used, or being considered for use, in specific materials modeling projects. In addition, each of these potentials provides a starting point for chemically similar materials, such as refractory metals (Ta), III-V semiconductors (InP), and oxides (SiO_2).

The SNAP automated potential generation tool may benefit many materials modeling efforts critical to national security missions, as well as the many research programs at DOE laboratories and universities using LAMMPS to understand materials behavior.

Refereed Communications:

C.R. Trott, S.D. Hammond, and A.P. Thompson, "SNAP: Strong Scaling High-Fidelity Molecular Dynamics Simulations," in *Proceedings of the International Supercomputing Conference*, p.7905, 2014.

S.M. Foiles, A.P. Thompson, L.P. Swiler, G. Tucker, C.R. Trott, and C. Weinberger, "A New Approach for Interatomic Potentials: Application to Tantalum," presented at *TMS 2014*, San Diego, CA, 2014.

A.P. Thompson, "Large-Scale Atomistic Materials Simulation using Quantum-Accurate Interatomic Potentials," presented at the *Materials Research Society Spring Meeting*, San Francisco, CA, 2014.

S.G. Moore and P.S. Crozier, "Extension and Evaluation of the Multilevel Summation," *The Journal of Chemical Physics*, vol. 140, p. 234112, 2014.

Fault Survivability of Lightweight Operating Systems for Exascale

158802
Year 3 of 3
Principal Investigator: K. B. Ferreira

Project Purpose:

Concern is growing in the high performance computing (HPC) community regarding the reliability of proposed exascale systems. Research at Sandia has shown that the reliability requirements of these machines will greatly reduce their scalability. Current fault-tolerance techniques have focused on application faults and ignored the most critical software running on a node, the operating and runtime system.

We can think of the operating system (OS) on these machines as a single, scalable application that manages the available resources on a node. Today's OSs and runtime systems make many of the same assumptions about reliability that applications do. Many of these basic assumptions will need to be addressed to enable more reliable system software.

HPC system software needs to be able to continue running through faults if emergent application-level fault tolerance is to succeed. This is in contrast to current OSs, which are unable to recover from the vast majority of failures. We will examine the structure of modern HPC OSs with the goal of characterizing important reliability assumptions and determining alternative strategies for exascale systems. For example, errors in memory and logic can have different impacts on the OS and a cost/benefit model for different approaches to handling such errors will need to be developed and analyzed.

In contrast to current fault-tolerance methods that are focused on application faults, this work is focused on ensuring the operating and runtime systems can continue in the presence of faults. This is a much finer-grained and dynamic method of fault tolerance than the current, coarse-grained, application-centric methods. Handling faults at this level has the potential to greatly reduce overheads. Additionally, in contrast to much of the current work, this work focuses on more realistic fault models, for example, silent data corruption. Lastly, in this project, we investigate forward recovery methods rather than the expensive rollback methods of current work.

Summary of Accomplishments:

In this final fiscal year, we reached a number of key research and development milestones demonstrating the benefits of this approach. These milestones include:

- Development of an efficient resilience evaluation approach based on an analogy with OS jitter. This analogy allows for the use of lessons learned from OS jitter work here at Sandia to be utilized for resilience.
- Development of a highly scalable, accurate simulator for evaluating resilience approaches. This simulator, based on the existing LogGOPSim simulator, allowed for efficient simulation of resilience approaches by only simulating this activities impacting resilience.
- Demonstration of the benefits of this approach over competitive methods. For example, demonstrating the cost of uncoordinated checkpointing, suggested as a viable alternative for extreme scale systems.
- Analysis of the failure logs on a number of leadership-class systems, including Cielo, Hopper, and Jaguar. This analysis uncovered the importance of counting faults rather than counting errors as other work has done, demonstrated the static random-access memory (SRAM) failure on these machines in comparison to dynamic

random-access memory (DRAM), and demonstrated the inappropriateness of single error correcting and double error correcting (SEC-DED) error correction codes (ECC) in protecting future extreme scale systems.
- Demonstration of the benefit of the forward error recovery methods enabled by this project in comparison to current rollback methods.

Significance:

The results of this project have significant positive results. Resilience has been identified by DOE and DoD as a key fundamental challenge of extreme scale computing that must be overcome to enable effective predictive modeling and simulation. Performance of these simulation and modeling workloads is important for a wide variety of national security applications. The technology developed in this project will increase the scalability and fidelity of these workloads by enabling applications to roll forward through errors, with the OS isolating errors, as opposed to having to initiate a wasteful rollback/recovery, greatly reducing time-to-solution.

Refereed Communications:

B. Mills, T. Znati, R. Melhem, K.B. Ferreira, and R. Grant, "Energy Consumption of Resilience Mechanisms in Large-Scale Systems," presented at *the 21st Euromicro Conference on Parallel, Distributed and Network-Based Processing*," Los Alamitos, CA, 2014.

P. Widener, K.B. Ferreira, S. Levy, and T. Hoefler, "Exploring the Effect of Noise on the Performance Benefit of Non-Blocking MPI Allreduce," presented at the *21st European MPI Users' Group Meeting (EuroMPI/Asia)*, Kyoto, Japan, 2014.

K.B. Ferreira, S. Levy, P. Widener, D. Arnold, and T. Hoefler, "Understanding the Effects of Communication and Coordination on Checkpointing at Scale," in *Proceedings of the International Conference on High Performance Computing, Networking, Storage and Analysis (SC14)*, 2014.

S. Levy, B. Topp, K.B. Ferreira, D. Arnold, T. Hoefler, and P. Widener, "Using Simulation to Evaluate the Performance of Resilience Strategies at Scale," in *Proceedings of the 4th International Workshop on Performance Modeling, Benchmarking and Simulation of High Performance Computing Systems*, 2013.

B. Mills, R. Grant, K.B. Ferreira, and R. Riesen, "Evaluating Energy Savings for Checkpoint/Restart," in *Proceedings of the E2SC '13 1st International Workshop on Energy Efficient Supercomputing*, 2013.

D. Ibtesham, D. DeBonis, K.B. Ferreira, and D. Arnold, "Coarse-Grained Energy Modeling of Rollback/Recovery Mechanisms," presented at the *4th Fault Tolerance for HPC at eXtreme Scale*, Atlanta, GA, 2014.

Next-Generation Algorithms for Assessing Infrastructure Vulnerability and Optimizing System Resilience

158804
Year 3 of 3
Principal Investigator: C. A. Phillips

Project Purpose:

The US economy and way of life are increasingly dependent on complex, adaptive, networked systems. These systems arise in critical infrastructure (e.g., electricity and water systems, transportation, banking and finance), global trade, and supply chains, etc. Thus, understanding their behaviors under attack or disruption and increasing their resilience is an important national security challenge. A key component of these systems, which must be accounted for in vulnerability/resiliency analysis, is their intelligent management by human system operators. Under attack, these actions ideally mitigate (though sometimes exacerbate) the system's response and also influence the subsequent behavior of the attacker.

The theme of this research project involves bi-level discrete optimization problems for network design and security. Bi-level optimization problems involve two entities that make decisions in an uncooperative fashion, often involving one primary entity whose actions are opposed by an adversarial entity. While contemporary mathematical programming techniques have been studied for simple cases, the methods cannot yet be extended to complex adversary actions or arbitrarily deep chains of operator/adversary interactions. This research seeks to develop new mathematical theory and algorithms in these areas.

If the research is successful, it will greatly expand the class of bi-level optimization problems that can be addressed with modern computational tools and can be applied to varied national security mission areas including enhancing understanding of US critical infrastructure systems. As both foundational mathematical theories and practical implementations applicable to real-world problems do not yet exist, this project will create the scientific basis and demonstrate feasibility of an approach which could be differentiating to Sandia's national security missions and customers. This project is in collaboration with the University of Florida.

Summary of Accomplishments:

We applied mixed-integer programming, a general optimization technology, to the solution of multicommodity capacitated network design problems (MCND). The multicommodity flow problem optimizes the movement of products through networks such as transportation or telecommunications networks. Network design problems involve selecting the cheapest set of edges (transportation channels) to create a network capable of transporting a given set of demands for product movement. We formulated and studied the multicommodity variable upper bound flow model (MVF), a variant of MCND. We discovered a new mathematical constraint: hierarchical flow cover inequalities (HFCIs) that could allow solvers to find optimal flows faster. Our computational experiments suggest that HFCIs provide an advantage over previous flow-cover inequalities when solving MCND in a branch-and-cut algorithm.

We studied the directed edge-failure resilient network design problem (DRNDP). This is a variant of MCND to build a network capable of meeting some pre-specified proportion of demand even if any k links are destroyed, where k is a constant. DRNDP can be viewed as an uncooperative game, in which a designer attempts to minimize the cost of constructing a network while an opponent tries to maximize that same cost by destroying links. As such, it can be modeled as a bi-level discrete optimization problem. We created a mixed-integer program formulation of DRNDP and designed and implemented a branch-column-and-cut algorithm for solving the model. We tested the algorithm on a PC using randomly generated problem instances. We are also constructing a real world instance, based on the Florida highway network, which we plan to solve on a Sandia server.

Significance:

These results may have applications in building national-scale networks resilient to attack, either by an adversary or forces of nature. The work on directed network design extends previous Sandia research to designing networks with asymmetric channel capacities. The results provide better understanding of the structure of the space of solutions and provide better computational methods for finding optimal solutions to bi-level optimization problems. The data set is significantly larger than any currently available in public benchmark sets.

Refereed Communications:

D. Burchett, "Directed Edge Failure Resilient Network Design," presented (invited) *INFORMS Institute for Operations Research and the Management Sciences Conference*, Houston, TX, 2014.

D. Burchett, "Multicommodity Variable Upper Bound Flow Models," presented (invited) *INFORMS Institute for Operations Research and the Management Sciences annual meeting*, Minneapolis, MN, 2013.

Using High Performance Computing to Examine the Processes of Neurogenesis Underlying Pattern Separation/Completion of Episodic Information

158836
Year 3 of 3
Principal Investigator: J. B. Aimone

Project Purpose:

One of the most perplexing questions pertaining to our understanding of memory concerns how the brain distinguishes between patterns of related events that are separated in time. Understanding this question could have far-ranging impacts with regard to Sandia's ambition to establish next-generation memory processing and pattern classification systems. Studies have provided evidence that the dentate gyrus (DG) processes highly convergent information from cortical regions of the brain. This information is further processed and associated within the Cornu ammonis area 3 (CA3) subarea of the hippocampus to help distinguish patterns of events. Studies suggest this process is aided in the DG through neurogenesis. Neurogenesis may serve to support the process of discriminating (separating) patterns by reducing similarity between new and older event information. It may also support pattern completion by increasing associations between temporally similar events, which are then transmitted to the CA3 area of the hippocampus as sparse inputs. Unfortunately, little is known about how the underlying processes of these subareas work as a system. Also, the computational models that have been developed tend to have very reduced representations of the actual neural processes, greatly diminishing their generalizability to actual brain functioning. Accordingly, we will neurocognitively model the population dynamics of a fully representative, neurogenesis association system in order to examine how these subareas enable pattern separation and completion of information in memory across time as associated experiences. Fifteen years ago, most neuroscientists believed that the brain did not add new cells over the course of its lifetime. While initially controversial, it has been increasingly appreciated that neurogenesis occurs in certain regions of the brain, with debate having now turned to the functional role of neurogenesis. This research would place Sandia at the forefront of one of the most significant paradigm shifts in the history of neuroscience, which could have major ramifications for efforts to emulate neural processes in computer code.

Summary of Accomplishments:

Our research examined the computational function of neurogenesis from a number of different perspectives. We achieved human scale neuron number in simulations of the neurogenic DG region, which is among the first times this has been done in biologically realistic, hypothesis driven computational neuroscience research. These scaling studies showed a marked interaction of scale with neurogenesis function. We further developed a procedure for assessing the sensitivity and validity of large-scale neural models. Again, this application of uncertainty quantification (UQ) techniques to neuroscience is among the first demonstration of these methods to neuroscience. Finally, we developed novel metrics for assessing the information content of the neurons in our simulations. These ensemble-based information methods, which are based on compression theoretic approaches in computer science, have the potential to impact neuroscience broadly.

Significance:

The impact of this research on the neuroscience community is substantial. This is among the first human-scale neural circuit models that address a meaningful biological question, specifically the function of adult neurogenesis, which has been implicated in a number of cognitive tasks. Second, the UQ approach and novel metrics have broad potential relevance to the neuroscience community, both as potential tools in understanding neural function as well as possibly impacting government programs such as Intelligence Advanced Research Projects Activity (IARPA's) Machine Intelligence from Cortical Networks (MICrONs) Program. Finally, this work helped inspire a number of machine learning techniques that have potential impact in extending algorithmic pattern recognition capabilities.

Refereed Communications:

J.B. Aimone, W. Deng, and F.H. Gage, "Adult Neurogenesis in the Dentate Gyrus," *Space, Time, and Memory in the Hippocampal Formation*, Springer, ed., J. Knierim and D. Derdikman, 2014.

C.M. Vineyard, S.J. Verzi, and J.B. Aimone, "Quantification of Neural Computation," presented (invited) at *5th Annual International Conference on Biologically Inspired Cognitive Architectures*, Boston, MA, 2014.

J.B. Aimone, "Computational Modeling of Adult Neurogenesis," *Adult Neurogenesis*, Cold Spring Harbor Perspectives, ed., F.H. Gage, 2014.

J.B. Aimone, "Revisiting a Model: Continually Reassessing the Computational Role of Adult Neurogenesis," presented (invited) at *UC Irvine Center for Neurobiology of Learning and Memory 2014 Spring Meeting*, Irvine, CA, 2014.

J.B. Aimone, Y. Li, S.W. Lee, G.D. Clemenson, W. Dengand, F.H. Gage, "Regulation and Function of Adult Neurogenesis: from Genes to Cognition," *Physiological Reviews*, vol. 94, pp. 991-1026, October 2014.

J.B. Aimone, "Are New Neurons in Humans Important? How Scale Affects Neurogenesis Function," presented (invited) at *Keystone Meeting on Adult Neurogenesis*, Stockholm, Sweden, 2014.

A Cognitive and Economic Decision Theory for Examining Cyber Defense Strategies

161871
Year 3 of 3
Principal Investigator: A. B. Naugle

Project Purpose:

Cyber attacks pose a major threat to modern organizations. Little is known about the social aspects of decision making among organizations that face cyber threats, nor do we have empirically grounded models of the dynamics of cooperative behavior among vulnerable organizations. The effectiveness of cyber defense can likely be enhanced if information and resources are shared among organizations that face similar threats. Cyber defense teams must balance potential benefits from cooperation against motivations not to cooperate, such as potential for embarrassment, group inertia, or competitive strategy. Despite these risks, cooperation could mitigate a range of cyber-related vulnerabilities, including espionage, identity theft, and attacks on critical infrastructure. This research will develop a dynamic computational model to address these issues, leading to better scientific understanding of cognitive processes while simultaneously identifying critical gaps and potential improvements in cooperative cyber defense communication and strategy formation.

We plan to develop a computational model for researching the psychological, social, and economic factors that drive decision making about intra- and inter-group interactions in cyber defense. The model will incorporate cultural, cognitive, and institutional constraints and conditions to simulate how cognition and environmental circumstances determine cyber defense strategies and behaviors. The model will serve as a testbed for studying theories of cognition in cyber environments, potentially enhancing scientific knowledge of cognitive processes and improving our ability to model decision making in any context.

If successful, this project will result in the first psychological-socio-economic dynamic model designed for this type of analysis. Validation and uncertainty quantification will bolster confidence and enhance the utility of results. The model will enable better understanding and anticipation of cyber defenders' reactions to organizational strategies and priorities, giving insight into strategic policy design. It will be applicable to any set of organizations, creating flexibility in application while providing useful insight into cognitive processes in cyber defense and cooperation.

Summary of Accomplishments:

Through this project, we successfully assessed and simulated potential dynamics of a multi-organization cybersecurity information-sharing program. The computational models built for this project incorporated cultural, cognitive, and institutional constraints and conditions to simulate how cognition and environmental circumstances determine cyber defense strategies and behaviors.

The first model created through this project simulates a cooperative cybersecurity program between two organizations. This model provided insight into some of the potential dynamics that might be seen when organizations cooperate with each other. The second model simulates Tracer FIRE, a cybersecurity training program implemented by Sandia and Los Alamos National Laboratories, in which participants interact to solve problems. This model was used to understand cyber defense decision making in a controlled laboratory environment. Tracer FIRE provided substantial validation data, and model assessment helped to indicate potential Tracer FIRE changes to improve cooperation between participants. The third model simulates an information-sharing program between six organizations. Analysis of this model helped to indicate how free riding behavior might impact the success of a cooperative cybersecurity program.

The computational models developed were based on substantial data collection efforts. We collected environmental data at Tracer FIRE exercises and general cyber defense information. We conducted in-depth interviews with cybersecurity professionals at Sandia to describe decision-making processes.

Significance:

Cyber attacks pose direct and serious threats to national security, with potential for espionage, destruction of critical infrastructure, and other severe consequences. These attacks can have long-lasting negative impacts on the organizations they target, including DOE laboratories and other national security organizations. This project helped to improve cyber defense by identifying critical gaps in and potential improvements to strategies regarding organizational cooperation in cyber defense. Results from this project led to new strategies that leverage the human element of the cyber problem, creating potentially significant benefits for cyber defense in the DOE laboratories and other organizations.

Refereed Communications:

A. Bier, "Behavioral Influence Assessment for Organizational Cooperation in Cyber Security," presented at the *INFORMS Winter Simulation Conference*, Washington, DC, 2013.

A. Bier and M. Bernard, "Validating a Hybrid Cognitive-System Dynamics Model of Team Interaction," presented at the *5th International Conference on Applied Human Factors and Ergonomics,* Krakow, Poland, 2014.

Operationally Relevant Cyber Situational Awareness Tool Development

165611
Year 2 of 3
Principal Investigator: R. G. Abbott

Project Purpose:

The effectiveness of cybersecurity incident response team (CSIRT) members is a key component in the cyber security of organizations. When investigating an incident, CSIRT personnel must cope with large volumes of data that can be terabytes in size. From this mountain of network, system, and log data, analysts must extract the subtle, and often complex, patterns of adversary activity. The difficulty of extracting information from these large data sets has resulted in the development of sophisticated software tools to aid in this analysis. In turn, this has created an industry that aggressively markets these products to DOE, DoD, and other government agencies.

While enumerating the features of these software tools is easy, assessing the overall benefit to an analyst or an organization (i.e., the actual utility of the tool) is much harder. The result is that decisions regarding acquisition and use of these tools rely on subjective judgments. The goal of this research is to develop methods that accurately and objectively predict the utility of a tool to CSIRT members and an organization. Today, we do not even know what the appropriate measures of human performance might be. Furthermore, given that in the cyber domain, the defender often never knows ground truth, the cyber domain presents challenges that are unique to this domain, posing research questions regarding human situation awareness and decision making that has not been addressed within other domains.

Measuring performance is generally simple, such as determining false-positive rates or precision recall. However, measuring utility is more complex, often involving a trade-off between desirable features such as time savings and depth of coverage. There are risks arising from the lack of foundational research concerning the human-in-the-loop component of cyber and, therefore, a need to develop innovative experimental protocol for conducting valid studies of human performance within a simulated cyber operations environment.

Cognitive Computing for Security

165613
Year 2 of 3
Principal Investigator: E. Debenedictis

Project Purpose:

The goal of this project is to implement a brain-inspired computing method with memristors for the purpose of computing securely. Cognitive computing and artificial neural networks have been studied as ways for a computer to duplicate the brain's "smart thinking," but timely issues in cybersecurity suggest a different goal may be important as well. This other goal would be to think (process information) without revealing information (secrets) upon which that thinking is based, such as an encryptor, not revealing the key upon which the encryption is based. Artificial neural circuits duplicate to some extent the thinking in the brain; however, the security method for brains has a different basis than in electronics. The project will develop an artificial neural network based on a new nanoelectronic device called a memristor, establishing a new type of computing with a different basis for security.

This project is combining and reapplying activities from the fields of artificial intelligence and nanotechnology. Artificial neural networks have been studied mainly for the purpose of emulating the "smart thinking" of human brains. Most of this research has been done in simulation because neural networks are difficult to understand due to heavy intermixing of information. This project will target moderate complexity neural networks and will use the intermixing of information as a security advantage. Security advantages will be conferred both by the physical advantages of the memristor technology and the complexity of the neural circuits. A demonstration of physical security is essential in this project to both understand how practical implementations may be and to understand the difficulty an adversary would face if they tried to extract information.

HostWatch: Situational Awareness of Machine State for Cybersecurity

165614
Year 2 of 3
Principal Investigator: J. B. Ingram

Project Purpose:

There are two behaviors that are common to most malware (malicious software): persistence and communication. To date, most research and tool development for intrusion detection has been focused solely on communication, presumably because mature network traffic collection tools have existed for some time. Recently, tools to collect host state data have matured enough to allow large-scale collection. However, tools to analyze this voluminous data are very rudimentary.

The purpose of this project is to advance the state of the art of machine learning as applied to cybersecurity applications by analyzing host state data in order to detect the persistence of malware on a network. The successful application of machine learning to cybersecurity problems has been largely unproven, and to our knowledge, no other research has attempted a large-scale analysis of host state.

For this analysis, we use two types of machine learning algorithms: anomaly detection and supervised/semi-supervised learning. Anomaly detection is an unsupervised strategy, which means that the algorithm does not know if an instance is benign or malicious when generating the prediction model. It is used to identify potential unknown threats that cannot be found using searches. Supervised learning is used to detect known threats, which remain unidentified on the network.

Both strategies are necessary. Anomaly detection may identify new malware, but it may also identify unusual but harmless host artifacts. In other words, anomalous data is not always bad. Supervised learning, on the other hand, can differentiate good and bad software, but it may miss new malware, which is substantially different from that which has been previously encountered. Together the two approaches can highlight potentially new, previously unseen threats, as well as new instances of previously seen threats.

Sublinear Algorithms for In Situ and In-Transit Data Analysis at Exascale

165615
Year 2 of 3
Principal Investigator: J. C. Bennett

Project Purpose:

Post-Moore's law scaling is creating a disruptive shift in simulation workflows as saving the entirety of raw data to persistent storage becomes increasingly expensive. Consequently, we are shifting away from a post-process centric data analysis paradigm towards a concurrent analysis framework in which raw simulation data is processed as it is computed. This shift is introducing enormous research challenges for data analysis. Algorithms must adapt to machines with extreme concurrency, low communication bandwidth, and high memory latency, while operating within the time constraints prescribed by the simulation. Furthermore, input parameters are often data dependent and cannot always be prescribed.

The study of sublinear algorithms is a recent development in theoretical computer science and discrete mathematics that shows significant promise in its potential to provide solutions to some of these fundamental issues. These algorithms find small portions of the input that reveal information about global properties of the input. We intend to design sublinear algorithms that efficiently perform in situ and in-transit analysis at extreme scale. A concrete problem of focus is the sublinear computation of feature-based statistical summaries, a commonly used tool for applications like energy and climate.

Extreme scale scientific simulations are facing major roadblocks as compute capabilities are outpacing input/output capabilities. The approaches of sublinear algorithms address the fundamental mathematical problem of understanding global features of a data set using limited resources. These theoretical ideas are directly aligned with practical challenges of in situ and in-transit computation in which vast amounts of data must be processed under severe communication and memory constraints. The study of sublinear algorithms is a recent development and there is no precedent in applying these techniques to large-scale, physics-based simulations. Any success in applying sublinear approaches for a tool like feature-based statistical summaries would likely lead to algorithmic improvements for many scientific high performance computing problems.

Strong Local/Nonlocal Coupling for Integrated Fracture Modeling

165616
Year 2 of 3
Principal Investigator: D. J. Littlewood

Project Purpose:

Peridynamics, a nonlocal extension of continuum mechanics, is unique in its ability to capture pervasive material failure and fracture. Its use in the majority of system-level analyses carried out at Sandia, however, is severely limited due in large part to computational expense and the need for specialized finite element technology. Combined analyses in which peridynamics is employed only in regions susceptible to material failure are, therefore, highly desirable, yet the ability to couple classical finite elements and peridynamics remains limited. Recent work in the literature on local/nonlocal coupling has failed to address key issues, including determination of mathematical bounds on numerical artifacts at the local/nonlocal boundary and algorithm design compatible with production analysis codes. Resolution of these issues, and the subsequent deployment of a local/nonlocal coupling scheme, will provide an integrated fracture modeling capability.

We will develop a mathematically consistent formulation for local/nonlocal coupling that allows for full integration of peridynamics with classical finite element analysis. We will focus on two classes of coupling approaches. The first is comprised of blending methods. These are interface models that extend approaches currently employed for domain decomposition. The second class achieves local/nonlocal coupling in the context of a unified model by selective reduction of the peridynamic horizon. Coupling algorithms will be vetted in an open source, collaborative software framework. A primary risk is that formulations will not be amenable to implementation in a production code. Prototype construction via Trilinos agile components will mitigate this risk by providing a proving ground for algorithm development. Coupling schemes will be validated through comparison against the perforation experiments of Borvik, et al., and the spallation experiments of Dandekar. A single coupling scheme, selected through analysis of the prototype software, will be implemented in Sierra/SolidMechanics.

Efficient Probability of Failure Calculations for QMU using Computational Geometry

165617
Year 2 of 3
Principal Investigator: S. A. Mitchell

Project Purpose:

We consider the quantification of margins and uncertainties (QMU) problem of estimating probability-of-failure. These are ubiquitous safety and reliability calculations. To ensure the QMU methods we develop are useful, we consider test problems whose functional form is similar to analyzing electrical device and circuit failures induced by hostile radiation environments.

Calculating failure probabilities is much harder than computing means and variances over simulations. Challenges include large input uncertain parameter spaces (dimension > 10), small probabilities ($<10^{-6}$), high cost per model run (hours on hundreds of CPUs), nonlinearity, and discontinuities. Combining multiple functions to analyze a complicated and large system often creates nonsmooth and multimodal responses over 10-20 model parameters. Effective reliability methods must identify and characterize tiny critical subspaces in a vast parametric space, given highly restrictive simulation budgets.

We will pursue new methods for exploring high-dimensional parameter spaces, based on our prototype concrete algorithm that solves simple problems, including some single-mode failures. We enumerate research directions that have been vetted and have potential to generalize this to harder problems.

Our new approach uses computational geometry to cut off wide swaths of space requiring no further exploration, and geometry-guided exploration of the remainder. These swaths are spheres and slabs around sample darts, where the function estimate is either entirely above or below some threshold. Our second geometric innovation replaces single point samples (0d-darts), with a hierarchy of flat subspaces called k-d darts (e.g., lines for k=1). Flat exploration can be made more efficient by exploiting a surrogate function's analytic form, our third major innovation. Flats are very good at intersecting (detecting) long and thin failure regions. This shape is typical of reliability calculations because parameters differ in significance. But even for cubical failure regions, initial mathematical analysis indicates that failure probabilities converge faster for kd-darts than point-based Monte Carlo sampling.

The general parameter-space exploration capability could benefit the nuclear security mission, but extends more broadly (e.g. to nuclear regulatory and climate missions) and design problems.

A Universal Quantum Transport Computational Capability for Cross-Technology Comparisons of Beyond-CMOS Nanoelectronic Devices

165618
Year 2 of 2
Principal Investigator: D. Mamaluy

Project Purpose:

As industry and academicians work to increase the speed of transistors by shrinking their size to nanometer dimensions with the gate lengths of 10 nm or less, conventional theories used to predict device behavior are becoming obsolete because they fail to account for quantum effects. Existing semi-classical technology computer-aided design (TCAD) tools work only with conventional complementary metal-oxide-semiconductor (CMOS) devices and, while there is a significant effort in the computational nanoelectronics community to simulate a particular promising novel beyond-CMOS device, there is no common tool that would allow comparing the performance of different types of beyond-CMOS devices, such as ultra-scaled Si and III-V FinFETs, carbon nanotube field-effect transistors (FETs), graphene-based and other 2D material-based transistors, single-electron transistors or tunneling FETs. We plan to create a universal quantum transport simulator that will allow assessment and comparison, within a reasonable simulation time, of the performance of these different types of beyond-CMOS transistor technologies. The simulation tool will be based on a novel numerical method called contact block reduction (CBR) that we developed. The CBR method provides an efficient and accurate implementation of the nonequilibrium Green's function (NEGF) formalism for quantum transport simulation that turns out to be significantly faster than other existing methods, as identified by independent reviews. The planned universal, state-of-the-art computational tool will allow predicting performances of both already existing and not yet experimentally studied nanodevices, performing their geometry and material/doping optimization and process variation analysis, thus helping to select the best design options for each beyond-CMOS technology type. Furthermore, the simulator will greatly aid in identifying, characterizing, and comparing different novel nanodevice paradigms that can serve as the foundation for post-Moore's law computing. It may potentially contribute to design of exascale systems for scientific computing by helping to select the most suitable nanodevice paradigms for extreme scale computing systems.

Summary of Accomplishments:

1) We created a highly efficient, universal 3D quantum transport simulator. We demonstrated that it "scales linearly" — both with the problem size (N) and number of CPUs; this presents an important breakthrough in the field of computational nanoelectronics. It allowed us, for the first time, to accurately simulate and optimize a large number of realistic nanodevices within a short time frame; our demonstrated linear scaling can be compared to other methods/codes.
2) In order to determine the best in class for different beyond-CMOS paradigms, we performed rigorous device optimization for high-performance logic devices at 6, 5, and 4 nm gate lengths.
3) We have discovered that there exists a "fundamental down-scaling limit" for CMOS technology and other FETs. We have found that, at room temperatures, all FETs, "irrespectively of their channel material," will start experiencing an unacceptable level of thermally induced errors around 5 nm gate lengths. This effectively means the end of Moore's law for all FETs (including MuGFETs, nanowire transistors, TFETs, etc.), which would happen, according to the current International Technology Roadmap for Semiconductors (ITRS) projections, no later than 15 years from now.

Significance:

This project resulted in discovering a fundamental down scaling limit for CMOS and other FETs; this finding is of a high importance for beyond-CMOS computing systems research. We analyzed the industry possibilities after the thermal fluctuation limit is reached, and developed an intriguing prospect of extending single electron technology for scaling below the 5 nm gate length and beyond.

Refereed Communications:

D. Mamaluy, X. Gao, E. Nielsen, R.P. Muller, R.W. Young, N. Bishop, M. Lilly, and M.S. Carroll, "Efficient Charge Self-Consistent Quantum Transport Simulation in Complex Geometry Devices," presented at the *International Symposium on Advanced Nanodevices and Nanotechnology*, Poipu Beach, Kauai, 2013.

X. Gao, D. Mamaluy, E. Nielsen, R.W. Young, A. Shirkhorshidian, M. Lilly, N. Bishop, M.S. Carroll, and R.P. Muller, "Efficient Self-Consistent Quantum Transport Simulator for Quantum Devices," *Journal of Applied Physics*, vol. 115, p. 133707, 2014.

D. Mamaluy, X. Gao, and B.D. Tierney, "The End of FET Scaling is Near," presented at the *17th International Workshop on Computational Electronics*, Paris, France, 2014.

D. Mamaluy, X. Gao, and B. Tierney, "How Much Time Does FET Scaling have Left?" in *Proceedings in Computational Electronics IWCE*," 2014.

X. Gao and D. Mamaluy, "Quantum Transport Simulation and Optimization of Below-6-nm FinFETs with HfSiON/SiO_2 Gate Dielectrics," presented at the *International Conference on Superlattices, Nanostructures, and Nanodevices*, Austin, TX, 2014.

Adaptive Multimodel Simulation Infrastructure (AMSI)

166140
Year 2 of 3
Principal Investigator: M. W. Glass

Project Purpose:

The purpose of this research is to create a simulation infrastructure to facilitate both the incorporation of proven legacy components to build single simulation scale-tasks and implementation of multimodel adaptive simulations. This infrastructure will leverage high-level programming techniques and variations on component-based techniques to facilitate the easy integration of legacy software components for use in the infrastructure. It will also provide support for dynamic management of multiscale simulation execution on high performance computing (HPC) machines, both managing the execution of individual scales and scale-tasks and easing the transfer/communication of scale-coupling data between simulation scales.

Runtime adaptation of the parallel execution space discretization/scale-task assignment will be accomplished through control functions and user-defined control algorithms operating on user-defined simulation/scale metadata. The control functions will be decentralized —local/hierarchical — in nature in order to avoid collective blocking/synchronization of processes executing separate scale-tasks. Removing the requirement of low-level programming expertise in order to construct simulations, domain-specific experts and industry-level users will be able to reuse proven legacy software components in order to simulate the physical phenomena of importance to them. Further, the infrastructure aims to allow improved multiscale simulation performance through providing dynamic simulation-adaptation control functionalities.

The implementation of a massively parallel multiscale/multiphysics simulation requires expertise not only in the physical domain of interest, but also in parallel programming and software engineering. Incorporation of software components used in these simulations can require a great deal of expertise and effort. The successful development of this infrastructure will greatly reduce the efforts to implement massively parallel multiscale/multiphysics simulations and allow the reuse of legacy components.

This work is in collaboration with Rensselaer Polytechnic Institute (RPI).

Kernel and Meshless Methods for Partial Differential Equations

166141
Year 2 of 3
Principal Investigator: R. B. Lehoucq

Project Purpose:

The purpose of this project is to develop kernel and meshless methods for partial differential equations (PDEs). Efficient methods for solving PDEs and methods in image processing are at the core of a multitude of engineering and science problems, which are critical to national security missions. For example, simulations often use PDEs. In order to obtain high amounts of precision, the simulations can take an inordinate amount of time to compute. Improved methods for solving PDEs will allow for more timely and rapid simulations, which are critical to many projects.

We anticipate that our results will offer new methods to improve the computation of solutions to numerical PDEs. We further anticipate that our techniques can be applied to method of image interpolation, which might outperform some current methods in image processing.

This work is in collaboration with Texas A&M University.

Enabling Bidirectional Modality Transitions in Collaborative Virtual Environments

166537
Year 2 of 3
Principal Investigator: K. M. Mahrous

Project Purpose:

Due to the time and cost of manufacturing, nearly all items, from metal casings to weapons to buildings, are first designed virtually. Most collaborative engineering environments allow for the manipulation and visualization of these virtual designs through a 2D interface (e.g., computer monitor), which is an insufficient substitute for interacting with the model in 3D (regardless of scale). In a collaborative design process, this often makes it difficult to thoroughly review and discuss designs. This is exacerbated by geographically distributed teams.

This research aims to address this problem by enhancing the work done in collaborative virtual environments (CVEs). Current CVEs focus on visual (2D or 3D) interactions with the design; enhanced CVEs incorporate haptic feedback via devices such as force-feedback gloves. We will explore this research direction further but also take an entirely novel approach by introducing 3D materializers into the environment so that we can interact with cheap, quickly made, but still geometrically identical copies of objects. Furthermore, the ability of current CVEs to transform physical objects into virtual ones via 3D scanning algorithms will be extended to form a bidirectional pipeline that allows for a physical to virtual to physical sequence where the object can be modified in both forms; we deem this novel procedure the multimodal collaboration pipeline (MCP).

This work is in collaboration with the University of California at Davis.

Current CVEs only allow for 3D scanning to convert physical objects into virtual ones, which necessitates that the engineer do most of the work in one of the two domains. By closing the gap and allowing for bidirectional modality transitions between the physical and virtual domains, we are creating a cutting-edge CVE with the potential to reduce manufacturing costs and design time.

Simulation Capability and Computational Assessment of Memristors as Beyond-CMOS Logic and Memory Devices

173024
Year 1 of 3
Principal Investigator: D. Mamaluy

Project Purpose:

Transition metal oxide (TMO) memristors have recently attracted special attention from the semiconductor industry and academia. Memristors are one of the strongest candidates to replace flash, possibly dynamic random-access memory (DRAM) and static random-access memory (SRAM) in the near future. Moreover, memristors have a high potential to enable beyond-complementary metal-oxide semiconductor (CMOS) technology advances in novel architectures for high performance computing (HPC). Memristors utility has been demonstrated in reprogrammable logic (cross-bar switches), brain-inspired computing, and in non-CMOS complementary logic. This potential use of memristors as logic devices is especially important considering the inevitable end of CMOS technology scaling, anticipated by 2025. However, despite the spectacular progress in experimental demonstration and fabrication of TMO memristors, their microscopic transport theory, and even some key operational principles — essential to advance experimental progress — remain uncertain. In order to establish clear physical picture of resistance switching in TMO memristors, to aid in the ongoing Sandia memristor fabrication efforts, and perform a computational assessment of memristors' utility as potential "beyond Moore's law" logic devices, we are creating a memristor charge transport simulator.

The purpose of this project is to create a memristor charge transport simulator that will facilitate understanding of switching mechanisms, predict electrical characteristics, and aid Sandia experimentalists in device optimization for different applications. Switching in these devices involves a complex process of oxygen vacancy motion in the TMO film, governed by temporally and spatially intertwined thermally and electrically driven processes. Computational simulation of these phenomena requires a new method that captures effects of many species (ions/vacancies/electrons/holes) transport, changes in material composition, Fickian diffusion, thermophoresis, and field drift. The simulator will greatly assist in evaluating novel memristor-based designs and will potentially benefit high performance computing systems for scientific computing and informatics.

Coupling Computational Models: From Art to Science

173025
Year 1 of 3
Principal Investigator: P. B. Bochev

Project Purpose:

For many mission-critical DOE applications, the accurate and efficient coupling of trusted simulation codes could expand their scope and deliver new modeling capabilities for a fraction of the time and cost of new development. The main focus of this project is coupled computational models (CCM) for high-consequence analyses of impact fuzes and asset protection. Current state-of-the-art CCM poses the coupling as a “hard” constraint on the models. Mathematically correct implementation of such couplings can be difficult and is often substituted by simpler, ad hoc solutions. Such tactics, while expedient, are frequently mathematically questionable (e.g., regarding stability), physically inconsistent (e.g., regarding conservation), and sometimes computationally catastrophic (e.g., leading to clearly inadmissible results). We intend to significantly improve the robustness, accuracy, and physical fidelity of CCM by developing a new, mathematically rigorous, yet adaptable coupling strategy that casts the coupling into a constrained optimization problem.

Posing CCM as a constrained optimization problem — to minimize the mismatched “energy” between the states subject to physical constraints — enables a reversal of roles, where the coupling adapts to the physical models. This adaptable coupling strategy is a first-of-its-kind application of optimization ideas to CCM that aims to deliver an advanced simulation capability. In broad terms, the innovative application of optimization ideas to modeling and simulation fosters the development of cutting-edge science and engineering that enhance national security.

Towards Rigorous Multiphysics Shock-Hydro Capabilities for Predictive Computational Analysis

173026
Year 1 of 3
Principal Investigator: J. N. Shadid

Project Purpose:

A number of critical science and weapons applications at Sandia, DOE, and DoD require predictive analysis of complex shock-hydrodynamics of fluid/solid materials with possible electromagnetic interaction. The physical mechanisms include wave phenomena, material transport, diffusion, chemical reactions, and electromagnetics. Systems of interest include z-pinch experiments, electromagnetic launch, fuzes, power supplies, and exploding wires/foils for high explosives. The highly nonlinear multiple-time and length-scale response of these systems includes discontinuities formed from shocks, contact surfaces, and complex tabular equations of state (EOS). Current dominant computational solution strategies use ad hoc combinations of operator-splitting, semi-implicit, and explicit time-integration methods and decoupled nonlinear solvers. While these approaches have enabled progress in forward simulation, the inherited mathematical structure has not provided stability, accuracy, and efficiency to resolve all the dynamical time scales of interest, nor has it enabled integrated fast sensitivity analysis and uncertainty quantification (UQ).

Our goal is the development of a unique, modern, mathematical/computational approach for multiphysics shock-hydro that integrates efficient sensitivity and UQ analysis techniques for specific scientific quantities of interest (QoI) that are required outputs from the forward simulation. Our approach is to develop a well-structured, high-level mathematical model employing recent IMplicit-EXplicit (IMEX) time-integration methods and new robust arbitrary Lagrangian-Eulerian (ALE) spatial discretizations. This will enable development of fast adjoint-enhanced integrated sensitivity and UQ methods that focus directly on critical scientific QoI. Achieving this will require developing: 1) a new general space-time discretization algorithmic framework for stable, accurate, and efficient multiphysics shock-hydro forward solutions that provides for adjoint-enhanced sensitivity and UQ and 2) robust adjoint-based techniques (both discrete and continuous as appropriate) for sensitivity analysis, surrogate model creation for UQ, numerical error estimation, and methods to detect and handle discontinuities in QoI over parameter space. To guide and challenge this effort, the exploding wire will be our focus multiphysics shock-hydro application.

Analyst-to-Analyst Variability in Simulation-Based Prediction

173028
Year 1 of 3
Principal Investigator: M. R. Glickman

Project Purpose:

Despite the tremendous number of compute cycles devoted to computer-based simulation, the value of all this computation is only realized when coupled with a different kind of computational process that is performed by human beings seeking to refine their understanding and make predictions. Moreover, from informal observation and discussions with analysts, we have become aware that, even when provided the same problem, source data, simulation tools, and specific questions, it is unlikely that two analysts will arrive at precisely the same predictive judgments.

Analyst-to-analyst variability is an indicator of potential uncertainty in simulation-based assessment. What impact might such uncertainty have on our national security mission? Are there effective ways to mitigate associated risk and/or improve decision making? We don't know because there have been few, if any, formal studies of analyst-to-analyst variability in simulation-based assessment. In lieu of such studies, analyst judgment is developed through professional training and mentoring and subjected to peer review. Despite these wise practices, there remains a large disparity between our relatively intuitive approach to analyst judgment and our formal treatment of other stages of the simulation-based assessment pipeline such as hardware architectures and numerical algorithms. More alarmingly, psychological research continues to reveal consistent biases in human judgment and decision making, biases that were only divined via formal analysis.

We are conducting both: a) in situ observational studies of simulation-based judgment as practiced at Sandia and b) formal, controlled experiments in which subjects are given carefully chosen data and tools and asked to derive their best assessment. The goals of this project are to: 1) identify and document significant factors that underlie variability in simulation-based assessment and 2) begin investigating how this understanding might be leveraged to boost predictive performance. This novel project leverages psychological findings within the already highly interdisciplinary enterprise of predictive computer simulation of physical processes.

User-Accessible Unified Manycore Performance-Portable Programming Model

173029
Year 1 of 3
Principal Investigator: H. C. Edwards

Project Purpose:

To sustain scalability on emerging manycore computing architectures (terascale workstations, petascale clusters, and exascale supercomputers), analysis codes must exploit all opportunities for manycore parallelism. Migrating applications to manycore architectures currently requires scientists and engineers to have detailed knowledge of vendor-specific performance characteristics and constraints, obfuscate essential mathematics in their codes with parallel processing directives, and generate and maintain multiple versions of codes to meet vendor-specific performance requirements. Even vendor-neutral programming models (OpenMP, OpenACC, OpenCL) require architecture-specific knowledge to achieve acceptable performance and pollute mathematical code with parallel processing directives.

Two key Sandia R&D products are addressing independent facets of manycore parallelism. Qthreads addresses task parallelism with highly efficient task scheduling algorithms. Kokkos addresses data and vector parallelism through a performance-portable interface that minimizes users' exposure to architecture-specific details. We plan to integrate these R&D efforts to create a unified user-accessible manycore performance-portable programming model for the complete range of manycore parallelism: task, data, and vector. Our qualitative user accessibility goal is to allow scientists and engineers to program emerging manycore architectures with neither extensive architecture-specific knowledge nor ubiquitous parallel processing directives.

Merging these disparate and cutting-edge tracks of R&D into a unified and user-accessible and performance-portable manycore programming model is an extreme challenge that has not yet been met by numerous, multi-year R&D efforts. If successful, the new programming model will provide a clear and cost-effective path forward for our broad set of mission-critical analysis codes to meet the disruptive, ongoing manycore revolution in computer architectures.

APEX: Application Characterization for Exascale Systems

173031
Year 1 of 2
Principal Investigator: S. D. Hammond

Project Purpose:

Scalable parallel applications and computer architectures are a critical capability for Sandia's mission, the NNSA's Advanced Simulation and Computing Program, and many other national security related programs. As the community continues to pursue significant increases in the performance of supercomputers, we are very quickly finding that the mapping of existing algorithms and programming models to leading edge hardware is becoming highly strained. This is, in part, a result of the changing approach to delivering hardware performance — parallelism is offered instead of increased clock frequencies — as well as implicit assumptions regarding the behavior and structure of machines that no longer continue to hold. When combined with the challenges of lowering power consumption and reduced reliability of future hardware systems used at scale, the use of existing production codes on future supercomputers without modification now seems unlikely.

Application developers are, therefore, facing the prospect, for perhaps the first time in two decades, of needing to fundamentally re-architect, and in some cases rewrite, large sections of key production code. Whilst a full application rewrite may seem an appealing route, the cost and time associated with this activity alone means it cannot be undertaken for more than a handful of codes or libraries before it becomes prohibitive. An alternative approach is to evolve applications through the identification of key kernels and libraries addressing performance, power, and reliability concerns in a step-wise manner.

We are, therefore, creating a suite of binary analysis and instrumentation tools to support developers in characterizing their existing applications with a specific focus on identifying areas of concern relating to performance, data motion (power), and reliability. The output of these tools will relate program level objects such as data structures, functions, loops, or even code segments to specific program metrics of interest in exascale systems.

Advanced Uncertainty Quantification Methods for Circuit Simulation

173331
Year 1 of 3
Principal Investigator: E. R. Keiter

Project Purpose:

This research aims to develop reliability methods for analog circuit simulation, with the goal of mitigating the expense of large ensemble Xyce circuit calculations. The primary output will be discovery of a set of advanced methods to determine time-dependent failure probability of nuclear weapon (NW) circuits. Currently, NW circuit designers and analysts rely almost exclusively on brute-force nested sampling methods, requiring expensive numbers of Xyce simulations. Our research will extend reliability methods to handle two unaddressed topics which are critical to circuit analysis: time-dependent failure behavior and "physics-informed" correlations amongst input parameters calibrated from test devices. The successful development of this research will reduce the number of simulations required to assess NW circuit failure due to hostile radiation, and determine the probability of circuit failure, after radiation exposure. These effects include power-rail collapse and reduction of bipolar transistor gain.

We outlined two main focus areas for this research:

1) The development of uncertainty characterization approaches that will allow us to have "physics informed" correlations amongst calibrated input variables of compact models such as the Gummel-Poon or Virtual Bipolar Inter-Company (VBIC). The main algorithm of interest for this area is the backward propagation of variance approach which maps output uncertainties back to input uncertainties.
2) The capability to calculate time-dependent failure probabilities. This research area focuses on dimension reduction techniques that can incorporate the time dependency implicitly.

Active Learning in the Era of Big Data

173667
Year 1 of 3
Principal Investigator: W. L. Davis, IV

Project Purpose:

As the volume of data grows, so does the amount of computational power and the human ingenuity required to harness that power. Processing the data is not the problem. It is that, while the amount of data is growing, the time it takes a human to answer a question today is the same amount of time it will take to answer it tomorrow. And tomorrow, it will cost more. While many tasks have been automated (i.e., telephone operators), some tasks will always prefer to have a human in the loop. Such tasks may include sensitive high-risk applications, such as medical or security areas, but they also include areas that require more qualitative assessments of quality: the "I'll know it when I see it" quality that is difficult to automate.

This project aims to tackle the two major impediments to implementing active learning for big data in practice: 1) the logistics of query distribution and collection and 2) the lack of efficient algorithms with guarantees.

This research, in collaboration with the University of Wisconsin, will both extend the scalability of active learning approaches and expand the use of active learning techniques by lowering the barrier of complexity. In addition to these practical advancements, this research will advance the science of machine learning by enhancing the theoretical understanding of active learning constraints and guarantees.

A Framework for Wind Turbine Design under Uncertainty

173867
Year 1 of 3
Principal Investigator: M. S. Eldred

Project Purpose:

Wind energy is an increasingly vital component of the electricity generation system in the US. In 2009, over 3% of the nation's total electricity generation came from wind, and a report by the DOE outlines plans to satisfy 20% of the national energy budget with wind power by the year 2030. The DOE estimates that as much as a 35% increase in annual wind energy production can be obtained from improvements in the aerodynamics of wind turbines. Achieving these gains in performance will only be possible by using higher fidelity methods such as computational fluid dynamics (CFD) to model the aerodynamics. Therefore, a new framework for wind turbine design under uncertainty that makes effective use of high-fidelity tools will be developed to design these improved wind turbines. The ability to accurately assess the effect of all sources of uncertainty using predictive high-fidelity models will enable businesses to effectively estimate the investment risk in wind energy solutions and hopefully promote growth in the sector to the levels outlined in the DOE's plan.

Currently, wind turbines are analyzed and designed by low-fidelity tools with an inflow wind model that accounts for the stochastic nature of the wind. Current wind turbine manufacturers use low-fidelity tools because they are computationally inexpensive, allowing evaluation of thousands of design cases to determine ranges for quantities of interest (QoI), such as the average power output of the turbine or the maximum load it experiences. For newer, more aerodynamically aggressive wind turbine designs, there is little hope of obtaining accurate QoI ranges using the simple low-fidelity models.

This work is collaborative with Stanford University.

Reducing Computation and Communication in Scientific Computing: Connecting Theory to Practice

173882
Year 1 of 3
Principal Investigator: G. Ballard

Project Purpose:

The gap between the peak capabilities of computer hardware and the achieved performance of numerical computations is caused in large part by the high cost of communication (i.e., the movement of data between processors and throughout the memory hierarchy of a single processor). "Standard" $O(n^3)$ matrix multiplication is the most fundamental dense matrix computation, and communication-optimal algorithms exist that have been heavily tuned on most architectures to attain high performance. "Fast" $O(n^{2.81})$ matrix multiplication algorithms have been identified for over 40 years and are starting to become practical as communication costs dominate. The primary objective of this research, which is being conducted by a Truman Fellow, is to use computer-aided search to find a matrix multiplication algorithm that is both theoretically and experimentally faster than current implementations (i.e., $O(n^p)$ with $p < 2.81$). The secondary objective is to pursue several complementary tasks that involve developing other communication-optimal algorithms.

The theoretical computer science community has long been interested in the complexity of matrix multiplication. Strassen proposed the first fast algorithm in 1969, and since then, many improvements have been made (Williams 2012). Our goal is to use computer-aided search to discover an improved method. However, one of the main reasons for the difficulty in using computer-aided search is that the problem to solve is (nondeterministic polynomial time) NP-complete.

If the project is successful, the immediate reward will be improvement in applications like the coupled cluster method, a quantum chemistry computation where nearly all the computational time is spent in dense matrix multiplication. In addition, many efficient numerical linear algebra and combinatorial algorithms have been reduced to fast matrix multiplication, thereby inheriting the best-known complexity. By delivering a fast, practical matrix multiplication algorithm, we can connect all those theoretical results to practical implementations.

Scaling up Semiconductor Quantum Computers through Multiscale Analysis

173883
Year 1 of 3
Principal Investigator: J. K. Gamble, IV

Project Purpose:

Quantum computers have the capability to revolutionize the computation landscape in ways that incremental improvements to conventional computers cannot achieve. Although researchers have had recent success with small-scale devices in many architectures, the largest universal quantum computer demonstrated to date consists of 14 qubits, compared to the billions of bits found in classical computers. It is clear that for quantum computers to have an impact, they must be massively scaled up.

Barriers to achieving this breakthrough are essentially the same across all architectures: disorder and imperfections in real physical systems ruin the idealized proposals to build a scalable quantum computer. In semiconducting architectures, due to the huge amount of infrastructure support, working around or eliminating this disorder is the only main roadblock to scalable systems. Therefore, it is vitally important to thoroughly understand disorder in semiconductor systems.

In this project, which is being conducted by a Truman Fellow, a plan for scalable quantum computation in semiconductor systems has been put forth. By completing this course of research, Si-based quantum computing technologies will be brought closer to the level of gallium arsenide (GaAs) in terms of device reliability, while sidestepping the decoherence problems intrinsic to GaAs. To do this, first we will use the numerical and analytical building blocks developed in prior work to construct a clear picture of disorder in semiconductor quantum computers. We then will integrate this picture of disorder into realistic device solvers so that the entire system can be studied efficiently while not sacrificing accuracy. Finally, we will use this modeling capability to study the impact of disorder on realistic device operation. We will use this knowledge gained to optimize device designs to mitigate the role of disorder, helping to overcome one of the major obstacles to scalable quantum computing.

Game Theory for Proactive Dynamic Defense and Attack Mitigation in Cyber-Physical Systems

177965
Year 1 of 3
Principal Investigator: J. Letchford

Project Purpose:

Malicious attacks on cyber-physical systems, such as nuclear weapon (NW) systems or the electric power grid, are orchestrated by human attackers whose decisions are influenced by personal incentives. Current systems take into account that the value of a security system or policy is not only in the attacks that it successfully foils, but also in the way that potential attackers actions are changed. However, there are many other (unaccounted) decisions already being made in these systems that also have the potential for deterring attacks. For example, strategies for mitigating the extent of system failure or backup systems ignore this deterrence effect, and are not included in current security models. When our security and resilience models ignore the changes in attacker incentives due to investment in other areas, we are less effective in allocating our limited resources. Our goal is to develop models and algorithms that manage the computational issues that arise when we consider a wide range of potential deterrence effects and enable more efficient planning for investments in security, resiliency and mitigation, both exploiting potential synergies and avoiding costly redundant investments.

We will use adversarial game theoretic analysis to develop new models and algorithms for cyber-physical systems that characterize the deterrence factor of not only infrastructure investments that make attacks impossible, but also of factors that reduce the impact of system failures (including attacks) in a variety of ways. Additionally, we will be developing the first models that take into account the interconnected nature of many of these factors, to increase our understanding of when security is necessary and when other disincentives are more efficient.

Modeling Information Multiplexing in the Hippocampus

178470
Year 1 of 3
Principal Investigator: F. S. Chance

Project Purpose:

The purpose of this project is to develop and test a novel hypothesis that neurons multiplex multiple modalities of information in their output spiking. We have chosen to study neuronal multiplexing of information in CA1 (Cornu ammonis area 1) of the hippocampus, and have constructed a model in which sensory information from entorhinal cortex and memory information from CA3 (Cornu ammonis area 3) are multiplex in the spiking output of CA1 place cells. To validate this model, we are leveraging natural degradations in the one input pathway that occur with aging to examine the impact of input manipulation on CA1 neural activity patterns. This research will produce new insights into how neural circuits operate and may inspire development of new brain-inspired algorithms and computing devices, for example hardware that adaptively processes and communicates signals.

Integrated IO Services for Trilinos Data Structures

179754
Year 1 of 1
Principal Investigator: G. F. Lofstead

Project Purpose:

The Trilinos project offers algorithms and enabling technologies for the solution of large-scale, complex multiphysics engineering and scientific problems. While the project has succeeded at this broad goal, a current gap relates to input/output (IO) services. Trilinos currently supports various distributed data structures, but offers no standardized support for persisting and reloading any of these data structures for both checkpoint/restart and for analytics. This project seeks to investigate how to incorporate native IO services aware of the Trilinos data structures for interfacing with standard IO libraries. The Trios package within Trilinos has some support for IO services, but there is no integration with these services and the Trilinos data structures. This means that the end user must determine how to serialize their distributed data structures in order to interface with standard IO libraries.

Summary of Accomplishments:

We worked through the various Trilinos examples in isolation in an attempt to understand how to manipulate the data structures from a computer science rather than math perspective. In the process, we exposed several errors in the examples and documentation as well as identified several places where the documentation and even the Trilinos library could be improved to aid clarity.

We were able to understand how to create a simple distributed vector with local maps, write out elements, read them back in, and convert to a different distribution using a new map. Numerous conceptual difficulties had to be overcome. The most prominent of these is the idea of "ownership." For Trilinos, multiple processes can "own" a single element with the understanding that some reduction operator will combine these various "owned" portions into a single element. While this does not mean "ownership" for people less familiar with the library, it does introduce complexities any IO library will have to address.

There are also small, but important, documentation oversights discovered. For example, the different Trilinos application programmer interface (API) calls do not list if they require collective communication or can be done independently. Considering the profound performance impact collective communication can have, this should be added.

Significance:

While Trilinos addresses the need for a math library to aid science simulation creation, it has gaps that cause confusion for non-mathematicians and/or those with Trilinos expertise. These gaps should be filled to make the library use more robust and offer predictable performance for users. The ultimate goal of providing an IO library that can natively operate on Trilinos data structures can now be addressed. Sufficient knowledge of how Trilinos works and what to do to get both read and write access to elements is clear. The side benefit is improving documentation and examples. The outcomes of this project may benefit DOE's supercomputing mission.

Numerical Continuation Methods for Intrusive Uncertainty Quantification Studies

180132
Year 1 of 1
Principal Investigator: C. Safta

Project Purpose:

Rigorous modeling of engineering systems relies on efficient propagation of uncertainty from input parameters to model outputs. In recent years, there has been substantial development of probabilistic polynomial chaos (PC) uncertainty quantification (UQ) methods, enabling studies in expensive computational models. One approach, termed "intrusive," involving reformulation of the governing equations, has been found to have superior computational performance compared to nonintrusive sampling-based methods in relevant large-scale problems, particularly in the context of emerging architectures. However, the utility of intrusive methods has been severely limited due to detrimental numerical instabilities associated with strong nonlinear physics. Previous methods for stabilizing these constructions tend to add unacceptably high computational costs, particularly in problems with many uncertain parameters. In order to address these challenges, we plan to adapt and improve numerical continuation methods for the robust time integration of intrusive PC system dynamics. We will use adaptive methods, starting with a small uncertainty for which the model has stable behavior and gradually moving to larger uncertainty where the instabilities are rampant, in a manner that provides a suitable solution.

Summary of Accomplishments:

We investigated numerical algorithms aimed at providing robust solutions to initial value problem ordinary differential equations (ODEs) that are unstable for certain model parameters. For this study, we employed a two-equation ODE system that models an ignition process. We outlined a numerical continuation approach augmented with a solution constraint at long time horizons, designed to prevent the solution from 'blowing-up.' We proceeded to test the numerical continuation algorithm on a model elliptic problem, followed by the deterministic version of the ODE system. While these tests were successful, applying the same approach to the uncertain ODE system proved to be more difficult. Currently, the implicit approach requires significant damping, resulting in very poor convergence properties for the numerical continuation approach. Future efforts may work to identify the algorithmic advances necessary to overcome the poor convergence properties.

Significance:

This work represents a preliminary study on numerical methods for intrusive approaches for uncertain ODE systems. Current results, while promising, suggest that more algorithmic work is necessary to improve the convergence properties and remove some of the limitations we currently encounter. The successful future development of new algorithms could enable pervasive intrusive UQ in computationally expensive applications.

Noise, Decoherence, and Errors from Entanglement-Function Theory for Quantum Computing

180134
Year 1 of 1
Principal Investigator: R. J. Magyar

Project Purpose:

A significant problem in quantum computing is the development of physical realizations of algorithms that are robust against noise. One way to examine and mitigate noise would be to simulate large sets of qubits coupling to the external environment on classical computers. This is extremely challenging as quantum information processing is, in some sense, tied to computing resources that scale exponentially with the number of computing elements (qubits).

In this project, we set the foundation for a computational framework potentially allowing simulations of 1000s of qubits. Exact wave-function-based methods demand exponentially increasing resources with system size. Our methodology, using entanglement-functional theory (EFT), requires vastly fewer resources. The crucial step is to map the information contained in the wave functions into a simpler object with associated: 1) auxiliary gate operations and 2) entanglement functionals of this object. This is similar to the time-dependent density functional theory (TDDFT) approach that has revolutionized chemistry and materials science. Instead of dealing with the exponentially large wave function, EFT works with a polynomially large set of projections (the density) that are easily manipulated through unitary operations. For a given set of quantum gates, an isomorphism exists that relates the sequence of events to the time-dependent density. A system of entangled qubits can be simulated at drastically reduced cost relative to existing state-of-the-art vector-state simulation codes.

Once mature, this approach may enable 1000 qubit simulations with an explicit treatment of environmental effects. While the method under investigation is currently restricted to closed systems (i.e., strictly unitary evolution), we anticipate being able to generalize our approach to more general open systems. This approach will be possible once reasonably accurate density functionals have been identified and massive simulations can be done. The study of noise and decoherence is crucial for testing proposed noise tolerant algorithms and for assessing their feasibility in physical devices.

Summary of Accomplishments:

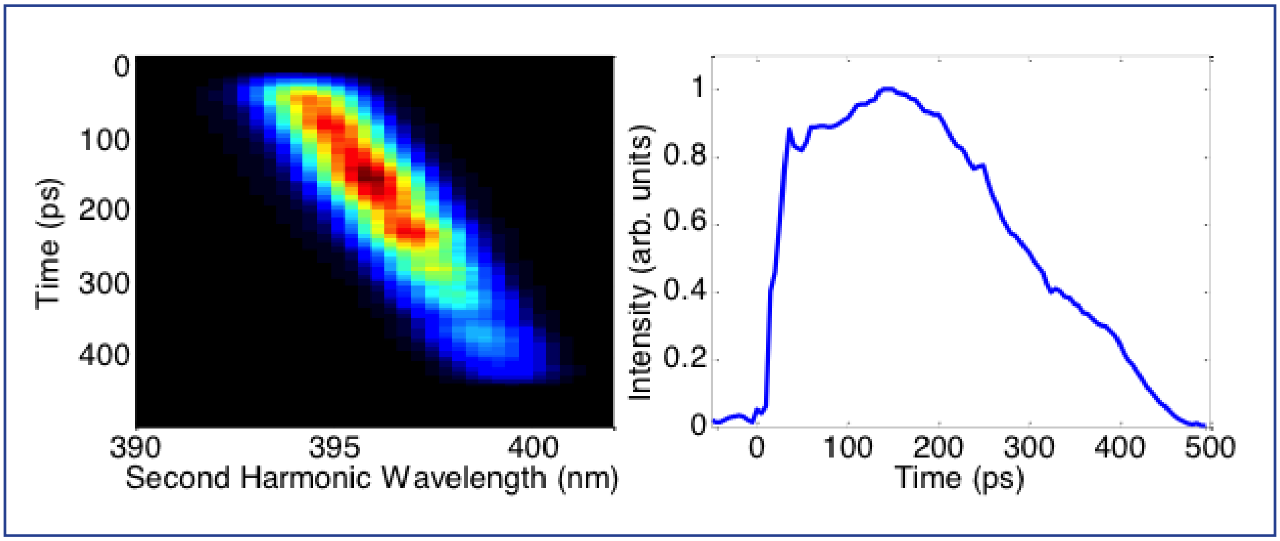
We discovered that EFT is possible for qubits by explicitly inverting exact solutions of the Heisenberg model, an exemplary time-dependent Hamiltonian capable of universal quantum computation. This work builds upon the success of TDDFT for Hamiltonians of interest in materials physics. To demonstrate that useful algorithms may be performed within this framework, we applied a series of multiqubit pulses on a Heisenberg model reproducing the Grover algorithm and created a simple Kohn-Sham (KS)-like representation through noninteracting qubits. Independently, we implemented an algorithm for an arbitrary number of qubits demonstrating that we can scale to more qubits than previously reported using an XY model system as a KS system. We developed pulses that achieve the desired unitary operations on qubits for the always-on Heisenberg model but discuss limitations due to being restricted to a degenerate subspace of the model. We also considered approaches to approximate functional design. While two KS systems with associated local density approximation (LDA)-type functionals have been considered in a different context, more investigations are needed in order to evaluate the applicability for quantum computing. While the first classical spin KS approach might be limited by the need to include all quantum coherence into the functional, the second XY model KS approach might be limited in its ability to treat larger spins and spin impurities and also by its much larger computational cost. It is likely that in both cases improved functionals are needed. It is desirable to also investigate if other KS systems can be found — perhaps among integrable systems that can be studied more easily than the full manybody problems. The challenge of history dependence can be addressed by developing memory-enabled potentials from exact solutions of the Heisenberg model or by converting time evolution into ground-state problem for a larger system of qubits.

Significance:

This work advances the frontiers by taking ideas that have been very successful in materials physics into a new field. The fundamental governing equations are similar in quantum information and Schrodinger equation based simulations. This work enhances the vitality of the workforce by encouraging interactions between experts in different fields, stressing the capabilities of a method to its extreme, and forcing innovation by changing the requirements of the theory. Continued work along these lines is likely to develop a simulation capability that could significant increase our ability to model quantum computers on classical systems.

ENGINEERING SCIENCES

The Engineering Sciences Research Foundation (ESRF) drives understanding and innovation by integrating theory, computational simulation, and experimental discovery and validation to understand and predict the behavior of complex physical phenomena and systems. The ESRF Investment Area supports innovative, leading-edge R&D that 1) advances the scientific understanding of physical phenomena underlying problems of interest to Sandia, 2) drives innovation and broad usage of state-of-the-art, validated computational modeling and simulation tools, and 3) accelerates the development of experimental diagnostics for discovery, model validation, and enhancement of our test and evaluation capabilities.



Extreme, picosecond-scale time resolution is achieved using Ultrafast Time Domain Interferometry measurements, a laser diagnostics tool. A second-harmonic Frequency Resolved Optical Gate trace showing the time dependence of the laser wavelength that encodes time into the spectral domain (left). Extracted laser pulse shape with rapid ~25 ps rise (right). (Project 158801)

ENGINEERING SCIENCES

Electromagnetic Extended Finite Elements for High-Fidelity Multimaterial Problems

158795
Year 3 of 3
Principal Investigator: C. Siefert

Project Purpose:

Surface effects are critical to the accurate simulation of electromagnetics (EM), as current tends to concentrate near material surfaces. Sandia EM applications include lightning blastthrough for weapon safety, electromagnetic armor, and magnetic flux compression generators for various NNSA and DoD applications. Sandia EM applications operate in a large deformation regime, where body-fitted meshes are impractical and multimaterial elements are the only feasible option. State-of-the-art methods use various mixture models to approximate the multiphysics of these elements. The empirical nature of these models can significantly compromise the accuracy of the simulation in this very important surface region. We plan to substantially improve the predictive capability of electromagnetic simulations by removing the need for empirical mixture models at material surfaces.

Highly accurate, edge-based (compatible) discretizations form the basis for EM simulations at the NNSA labs, as they correctly respect the underlying physics. Unfortunately, there is no edge-based method that allows for resolution of sub-element material interfaces. Our goal is to build a physically realistic EM scheme that resolves these critical sub-element material surfaces. We will adapt ideas from the extended finite element method (XFEM) to edge-based discretizations. The XFEM makes discontinuities at a sub-element level possible, but has only been developed for nodal discretizations. Realizing our goal requires the development of: 1) a novel edge-based technique to enforce the appropriate continuity conditions across material boundaries within an element, 2) implementation of the technique, 3) a novel, fully implicit linear solver capability to solve the resulting equations, and 4) a novel way to preserve XFEM quantities through large deformations (remap). Sandia has the necessary expertise in XFEM, edge-based discretizations, and solvers.

Summary of Accomplishments:

Many important physics problems have solutions that are strongly influenced by the effects of material interfaces. Electromagnetics, the accurate simulation of which requires compatible discretizations, provided our primary motivating examples. For applications with large deformations, maintaining a body-fitted interface-conforming mesh is untenable, leading to a loss of simulation accuracy in many cases. In response, we have developed variants of the XFEM and conformal decomposition finite element method (CDFEM) that restore effective interface conformity. The former enriches the solution space with the addition of interface-conforming basis functions, and the latter does so by cutting elements into interface-conforming sub-elements.

We proved the optimality of the XFEM using algebraic constraints (XFEM-AC) to enforce continuity, which allows us to sidestep the issue of stability and still maintain optimal convergence. We did this by proving the formal equivalence of XFEM-AC to CDFEM. We proved this equivalence in 2D and 3D for node, edge and face elements, allowing us to correctly capture the physics of electromagnetics. We also verified, over a variety of problems with analytical solutions, that optimal convergence is attained in practice. We contrasted that with the suboptimal performance attained by current methods that do not preserve interface conformity.

Finally, we began development of a remap or solution transfer scheme (i.e., the mapping of fields from one mesh to a second mesh). This is necessary for the application of our methods in operator-split Lagrange-remap codes like Sandia's ALEGRA code. Here we generalize the approach of Bochev and Shashkov (2005) to the remap problem for CDFEM discretizations. We demonstrated excellent results on 2D nodal fields and very good results for 2D edge fields. We hope this work will lay a solid foundation for further work in 3D in the future.

Significance:

Sandia has a long-term interest in accurate physical modeling of EM phenomena for national security applications. These problems include lightning blastthrough, electromagnetic armor, and magnetic flux compression generators. Solutions to EM problems are strongly influenced by surface effects, which make correct resolution of material surfaces critical. We have demonstrated two methods for resolving interface physics for magnetic diffusion in 2D and 3D, advancing our technical leadership in the development of enriched finite element methods.

Refereed Communications:

R.M.J. Kramer, P.B. Bochev, C.M. Siefert, and T.E. Voth, “Algebraically Constrained Extended Edge Element Method (eXFEM-AC) for Resolution of Multi-Material Cells,” *Journal of Computational Physics*, vol. 276, pp. 596-612, November 2014.

Ultrafast Laser Diagnostics for Energetic Material Ignition Mechanisms: Tools for Physics-Based Model Development

158801
Year 3 of 3
Principal Investigator: S. P. Kearney

Project Purpose:

Despite its importance, a fundamental description of initiation in energetic materials has eluded researchers for decades, in large part because ignition results from mechanical and thermochemical mechanisms that are tightly coupled at extreme spatial and temporal scales in the order of microns and picoseconds. Access to these extreme time and length scales under dynamic loading conditions has, until recently, been restricted to simulations, and experiments to underpin the relevant physics are sorely needed to provide model developers with an appropriate physical foundation. The recent availability of femtosecond laser sources has opened the door to fundamental experiments with the required extreme resolution and well-controlled measurements on the early time effects of shock drive have been reported. These experiments have largely been limited to homogeneous materials, while the majority of explosives of interest — both ideal and improvised — are heterogeneous in composition, with material microstructure effects that are absent in homogeneous samples, but which can dominate the response in many real explosives.

We will develop new capabilities for controlled small-scale, shock-drive experiments on heterogeneous samples. Extension to these more challenging materials will additionally require us to develop state-of-the-art ultrafast laser diagnostic approaches for spatially correlated imaging and spectroscopy on a single-laser-shot basis with extreme picosecond- and micron-scale resolutions. We will advance the science of ultrafast imaging and spectroscopy for elucidation of the mechanical and thermochemical response of energetics to shock drive in well-controlled experiments on dynamically loaded heterogeneous materials. The measurements will provide new physical insight into the initiation process and provide fundamental data of interest to molecular dynamics and mesoscale modelers. More significantly, the capabilities developed here will yield the first resolved-scale measurements of mesoscale phenomena to enable breakthroughs in modeling of shock-induced ignition of abundant heterogeneous explosives.

Summary of Accomplishments:

We have constructed an ultrafast time-domain interferometer (UDTI) system for the characterization of laser-driven shock waves in thin films of energetic materials. The UDTI system has been applied to inert polystyrene as well as explosive film samples. UDTI traces can be utilized to extract shock-Hugoniot data. Results obtained with the Sandia UDTI setup generally lay 10% above gas-gun results for inert pentaerythritol tetranitrate (PETN, a polymer) and the explosive hexanitroazobenzene (HNAB). Collaboration was formed with researchers at Lawrence Livermore National Laboratory (LLNL) and Sandia-fabricated UDTI samples were sent to LLNL for UDTI measurements. The Livermore data are in good agreement with historical gas-gun data for both PETN and HNAB, which reveals that UDTI is a valid diagnostic tool for shock wave characterization. We have additionally developed stimulated Raman spectroscopy (SRS) and transient absorption (TA) setups to characterize temperature, chemistry and electronic energy surfaces of materials under shock loading. The temperature response of the SRS system has been calibrated under static conditions in a cryostat. Further work is needed to extend this approach to high-temperature conditions, and this presents an extreme challenge to the energetic materials community. The TA diagnostic was additionally demonstrated on static inert and explosive films. A second UDTI system has been combined with the TA setup for fully characterized shock measurements.

Significance:

This work addresses the initiation of explosives at its most fundamental level, a problem which has been identified as an NNSA scientific grand challenge in national security. Explosives science and engineering has obvious and ubiquitous applications to weapons and threat reduction for not only the DOE but to the DoD and DHS. The work completed on this project represents an investment by Sandia in state-of-the-art experimental capabilities to address this problem in coming years.

Refereed Communications:

I. Kohl, B. Jilek, D. Farrow, J. Urayama, and S. Kearney, "Development of Spectral Interferometry for Shock Characterization in Energetic Materials," in *Proceedings of the Journal of Physics, Conference Series 500*, p. 022005, 2014.

B. Jilet, et al., "Unreacted Equations of State of Sylgard and Hexanitroazobenzne (HNAB)," presented at the *International Detonation Symposium*, San Francisco, CA, 2014.

Effect of Varying Convection on Dendrite Morphology and Macrosegregation

158803
Year 3 of 3
Principal Investigator: J. D. Madison

Project Purpose:

This work is an on-going collaboration with the University of Arizona as well as Cleveland State University to: 1) understand the effects of melt convection and shrinkage flow on dendritic microstructure and 2) examine and model alloy macrosegregation during directional solidification in Al-Si and Al-Cu alloys. Microstructural morphology determines important macroscopic properties, therefore, enhanced control of microstructures are of economic importance in directionally solidified castings used in aerospace, power generation, and other industries. In this project, research has examined microstructural changes caused by varying thermal gradients and differing solidification rates under both microgravity and normal gravitational conditions. It is anticipated that samples solidified under microgravity will produce microstructures practically free from the influences of convection, providing control cases in which the influence of convection can be reduced, if not eliminated, experimentally and subsequently modeled. Effects of changing cross sectional areas and the resulting changes in convection, shrinkage flows, and microstructural morphologies have also been investigated. These experiments were carried out under normal gravitational conditions and in microgravity. The novel approach here is in the attempt to grow relatively large samples of dendritic alloy, free from the effects of convection with minimized shrinkage flows for comparison against gravitationally processed samples. In addition to characterization, experimental results will be compared to established solidification models with and without convective effects. This work has been additionally innovative in that tools were developed for the automated extraction of composition and morphology from micrograph images, direct comparison of solidification models with experiment, extraction of convection and shrinkage induced melt velocities as well as quantifying and isolating certain convective effects.

Summary of Accomplishments:

Microgravity experiments were performed aboard the International Space Station while terrestrial experiments were carried out at Cleveland State University. Predictive models of macrosegregation were then developed and evaluated at the University of Arizona against said experiments.

While analyzing the samples from these various experiments, it was found that significant macrosegregation of solute can occur during both the melting and the solidification period. As a result, it was confirmed that it is rather intractable to treat both melting and solidification with a single model due to asymmetries between the two processes. In microgravity, large-scale elemental partitioning during melting was determined to be the predominant cause of macrosegregation and was examined first. Within terrestrially solidified samples, it is anticipated that macrosegregation would also occur during melting, but convection due to gravity would most likely be a rather significant factor making the treatment of macrosegregation in an isolated fashion a much more challenging problem to model using terrestrially solidified experimental data alone.

The primary technical accomplishment from this work has been the creation and validation of three models: a melting model, a straight-walled solidification model, and a changing cross section solidification model. Experimental validation has shown that the melting model provides an accurate description of macrosegregation caused by thermal gradients in the mushy zone. While this model slightly under-predicts macrosegregation in the vicinity of dendrite tips, the model captures the major redistribution of solute during temperature gradient zone melting. The straight-walled solidification model provides a good estimate of further macrosegregation in steepled castings while the changing cross section solidification model successfully incorporates varying mold type, demonstrating the importance of including mold thermal diffusivities and geometry in numerical simulations of solidification.

Significance:

There is a growing interest in additive manufacturing processes at DOE. As such, there is a growing need for more advanced and further developed models and simulation tools for solidification under a variety of conditions and among various constraints. This effort is a contribution to this growing knowledge base and overarching effort of building fundamental understanding and tools relative to solidification. As such, this work advances the science, technology, and engineering competencies that are the foundation of the NNSA mission.

Refereed Communications:

M.A. Lauer, D.R. Poirier, R.G. Erdmann, L. Johnson, and S.N. Tewari, "Simulations of the Effects of Mold Properties on Directional Solidification," in *Proceedings of ASME 2013 International Mechanical Engineering Congress and Exposition*, p. V02BT02A002, San Diego, CA, 2013.

Next-Generation Suspension Dynamics Algorithms

158805
Year 3 of 3
Principal Investigator: P. R. Schunk

Project Purpose:

The goal of this project is to develop, refine, and apply next-generation algorithms for the simulation of dense suspensions of colloidal particles from the nanoscale through micron size particles. The challenge is to conduct mesoscale simulations for tracking the motion and self-assembly of individual nanoparticles while accurately accounting for hydrodynamic interactions, stochastic Brownian forces, and interparticle forces associated with interparticle potentials. The algorithms must be scalable with O(Np) operations to facilitate simulations with several thousand particles and must be sufficiently fast to resolve the time scales associated with colloidal diffusion, self-assembly, and phases changes. The need for long time evolution on time scales from seconds to hundreds of seconds requires the efficiency of the mesoscale simulation algorithms. Similarly, the need to investigate self-assembly and phase changes requires large system sizes in terms of particle number. To resolve the relevant physics, suspensions of spheres require large particle counts O(1000), while suspensions of anisotropic particles require significant larger systems owing to orientation effects and the creation of more complex phase behavior and self-assembly. To meet these needs, we have developed the FLD (fast lubrication dynamics) algorithm, which has shown excellent predictions of physical phenomena while offering superior computational speed relative to competitive algorithms such as ASD (accelerated Stokesian dynamics), DPD (dissipative particle dynamics), and SRD (stochastic rotation dynamics). The work is in collaboration with University of Illinois at Urbana-Champaign.

Summary of Accomplishments:

A major focus of this project has been on extension to simulations of densification processes. In prior years, we developed hybrid OpenMP (multi-processing) formulations with pre-computed data structures over near neighbor loops and summation loops over global particle number to maximize parallel efficiency.

Algorithmic advances in FY 2014 have focused on the application of fast lubrication dynamics (FLD) to modeling of high throughput manufacturing processes. Prior implementations of FLD considered particle motion in two distinct base flows — quiescent systems (diffusivity calculations) and 1D simple shear flow (viscosity and rheometers). Both FLD and more expensive Stokesian dynamics perform well on these systems because of the dominance of lubrication forces in flows with strong relative particle motion. FLD includes a calibrated isotropic resistance, which yields good mean diffusivities, while the theory-based lubrication terms account for relative particle motion and assure good diffusivity prediction independent of local particle microstructure.

Densification flows in high throughput manufacturing processes require new classes of base flows including both 1D and 3D extensional flows as well as improved treatment of constant flow (e.g., sedimentation or permeability calculation). It is well known that FLD and even full expensive Stokesian dynamics simulations predict permeability of a fixed bed of particles poorly; the reasons are that there are no relative particle motions on a local scale, lubrication forces are negligible, and longer range interactions become more important. We have shown how the FLD approach can be extended to include one additional resistance term, which allows for accurate computation of both permeability and particle resistance in extensional densification flows. The inclusion of three resistance forms (isotropic, lubrication, and mean far field) involves negligible increase in computational effort but guarantees excellent accuracy for densification flows.

Significance:

The extension of the FLD algorithm to modeling of densification flows allows a significant increase in the breadth of its application to high throughput manufacturing processes, thus improving our understanding of the development of particle microstructure in materials arising from the processing of both monodisperse and polydisperse particle suspensions. This facilitates production of novel synthetic materials from disparate chemical constituents for applications such as electrodes, batteries, energetic materials, and novel smart materials. These materials are central to many energy and national security missions.

Multi-Scale Modeling of Brittle Heterogeneous Materials

158806
Year 3 of 3
Principal Investigator: T. Vogler

Project Purpose:

Heterogeneities and deformation mechanisms in engineering materials exist at length scales finer than the engineering scale. Concrete, for example, possesses heterogeneities on multiple length scales while engineering structures are on the scale of meters. Modeling at the scale of reinforcing phases, or mesoscale, is a methodology for understanding the role of microstructure during deformation, fracture, and failure. This scale is of particular interest due to the interfacial transition zone that exists between the cementitious matrix and reinforcing constituents, and typically acts as a crack nucleation point.

Peridynamics is used to capture plasticity and fracture of concrete at multiple length scales. Peridynamics offers several distinct advantages over classical continuum models. It does not rely on derivatives of the displacement field; thus, the discontinuities inherent to cracks can be included in a mathematically consistent manner. Furthermore, the nucleation and propagation of cracks are governed by the constitutive equations of the material as opposed to external laws. As a nonlocal theory, it is also well suited to problems involving localization of plastic deformation and strain softening.

In collaboration with Georgia Tech, we are studying the dynamic behavior and failure of high performance concrete (HPC). A pressure-dependent peridynamic plasticity model is developed to capture inelastic behavior. A dissipation bond failure criterion is coupled to the model to capture nonlinear fracture. A multiscale approach is implemented. Fine-scale structure and deformation mechanisms are modeled and effective properties are calculated and integrated into engineering-scale models to produce more accurate computations. The effect of reinforcement size and volume fraction will be determined and optimal material configurations determined. The work will serve as a basis for the development of new modeling and multiscale materials design approaches in the future. This problem has not been solved by current S&T due to both the computational demand and lack of appropriate constitutive theories to accurately address the problem.

Summary of Accomplishments:

A pressure-dependent peridynamic plasticity model was formulated. The yield surface was derived in force state space and the corresponding flow rule was assigned. Linearization and thermodynamic admissibility were derived. The parameters of the model were proven to be related to the parameters of the continuum Drucker-Prager model. An implicit integration was formulated to numerically calculate the force state and accumulated plastic bond extension. The model was validated on two peridynamic material points loaded in tension, compression, and shear along with a cylinder subjected to compression, splitting, and dynamic impact with spall.

A multiscale modeling methodology has been produced. Spherical, unstructured, mesoscale models of HPC are instantiated using a specially developed code and Cubit. The size of the mesoscale model corresponds with the peridynamic horizon at the engineering scale. The relationship between the kinematics at each scale has been established. The pressure-dependent peridynamic plasticity model is used to simulate the behavior of the matrix and reinforcing phases. A procedure for determining the effective values of the pressure-dependent plasticity model parameters at the engineering scale, by loading the models in tension, compression, and shear, has been formulated. The mesoscale models capture the nucleation, propagation, and interaction of multiple fracture process zones.

Significance:

The research supports the experimental characterization of the dynamic failure of cementitious, geological, and granular materials used in a wide range of applications relevant to national security. These materials are pressure-dependent and possess fine-scale deformation mechanisms that govern engineering-scale behavior. Our ability to simulate the behavior of these materials and, thus, design articles utilizing them depends upon our ability to simulate their behavior accurately. The modeling methodology can be extended to applications in planetary science, powder forming and consolidation, impact and penetration, and the initiation of energetic materials. Additionally, the work expands the modeling capability of the peridynamic theory developed at Sandia.

A Micro to Macro Approach to Polymer Matrix Composites Damage Modeling

161865
Year 3 of 3
Principal Investigator: S. A. English

Project Purpose:

Traditionally, polymer matrix composites (PMC) damage is assessed on the lamina scale in which distributed loads among the constituents exceed some failure criteria and lead to a reduction in laminate stiffness. An array of methodologies has been proposed to simulate this phenomenon. No consensus yet exists on the correct method to model damage and failure in composites. A micromechanical approach uses fiber and matrix properties to define decomposed constituent-level damage evolution and failure and, thus, may be extended to more complex compositions. Similarly, mesoscale (yarn) models can be used to directly assess damage evolution and failure in woven PMCs. The main challenge is to develop and implement a composites damage material model and characterization methodologies that utilize a micro and mesomechanical approach to determine homogenized macroscopic material response for varying levels of constituent complexity. Intermediate challenges include: 1) implementation and evaluation of multiple material models, 2) development of methodologies and length scale estimations for micro and mesomechanical modeling, 3) comparison with existing models (analytical and empirical), and 4) experimental validation for simplified cases with materials of interest. Sandia's high performance computational capabilities allow for a detailed analysis of the microstructure, iterative optimization of material parameter selection, and other tasks not generally suited for industry.

Summary of Accomplishments:

A series of constitutive responses are obtained using material and geometric measurements with representative volume elements (RVE). The geometrically accurate RVEs are used for determining elastic properties and damage initiation and propagation analysis in order to characterize a novel composites damage evolution and failure model. Finite element modeling of the mesostructure over the distribution of characterizing measurements is automated and various boundary conditions are applied. Plain and harness weave composites are implemented. Continuum yarn damage, softening behavior, and an elastic-plastic matrix are combined with known materials and geometries in order to estimate the macroscopic response as characterized by a set of orthotropic material parameters. Damage mechanics and coupling effects are investigated and macroscopic material models are demonstrated and discussed. The micro and mesomechanical approach to elastic property estimation produces excellent results and can be implemented for material selection and design scoping exercises. Furthermore, this study provides a verified toolset for elastic and damage property predictions for a wide range of composite materials and, with proper calibration and model enhancement, these models supplement experimental data and can be used in the design process.

Significance:

This study utilizes applied science for engineering applications in order to provide a basis for material parameter estimation using a statistical RVE approach. The end user can estimate an array of parameters for design and material scoping exercises with minimal experimental effort. Utilizing tools developed in this project will enable the assessment of more complex loading conditions to establish physical bases in macroscopic constitutive models.

Digital Holography for Quantification of Fragment Size and Velocity from High Weber Number Impacts

161867
Year 3 of 3
Principal Investigator: D. R. Guildenbecher

Project Purpose:

In transportation accidents, tanks containing flammable or hazardous liquids may impact rigid surfaces at high velocity. This can lead to liquid dispersion throughout large volumes. In these situations, knowledge of the initial fragment sizes and velocities is needed to elucidate the fundamental physics and provide boundary conditions for predictive models of dispersion (e.g., Brown and Jepsen, 2009). Previous attempts to acquire such data were unsuccessful due to the spatial limitations of phase Doppler anemometry, which records droplets at a point, and particle tracking velocimetry, which records droplets in a 2D plane. To enable measurement of droplet statistics, innovative new methods are required to probe a large 3D domain in single-shot, short-duration experiments.

Significant advancement of the state of the art is planned through the optimization of digital holography for quantification of the size, morphology, and velocity of liquid structures within a 3D measurement domain. The viability of digital holography has recently been established by a few proof-of-concept investigations, and we anticipate three significant leaps forward for diagnostics for high-velocity droplet fields. First, we will greatly improve temporal resolution through the use of nano- and pico-second laser pulses. Second, we will develop advanced algorithms to detect individual droplets and track them through multiple exposures. Finally, we will explore tomographic methods to improve the out-of-plane resolution of large-scale flow fields. Application of these techniques to high Weber number impacts will provide new physical insights into the governing mechanisms and fundamental data of interest to multiphase flow modelers. This data will enable significant breakthroughs in the development and validation of liquid dispersion simulations, such as Brown and Jepsen (2009). Finally, once perfected this technique could be extended to many other systems where index of refraction variation leads to light scattering. Consequently, the future application of digital holography may prove game changing for diagnostics of complex, 3D phenomena.

Summary of Accomplishments:

This work resulted in a number of important developments in digital in-line holography (DIH) for applications to particle field measurements. Through a partnership with collaborators at Purdue University, new algorithms were developed which automatically extract 3D particle position and morphology from recorded in-line holograms. Simulations and fundamental experiments showed that the accuracy of the measured positions was improved by an order of magnitude compared to previous literature results. This capability enabled a number of new applications to challenging flow fields including liquid dispersion via high Weber number impacts and breakup of liquids in aerodynamic flow fields. These experiments proved DIH's unique capability to quantify a statistically significant number of particles with limited experimental repetition, and the fundamental size and velocity distributions obtained are enabling new model development and validation.

In addition, these positive developments were applied to other challenging, 3D phenomena. For example, we completed the first ever measurement of high Mach number particles using single view DIH, proving viability of this technique in environments containing shock waves and other flow disturbances. Furthermore, DIH was applied to quantify the size distribution of aluminum drops ejected from a burning aluminized propellant, proving viability in a reacting environment. These developments are expected to expand applications of DIH to challenging environments well beyond the low speed multiphase flows typically found in the literature.

Significance:

This project developed distinguishing new measurement capabilities at Sandia. By quantifying all particles along a 3D line-of-sight, DIH is beneficial for rapid measurement of particle statistics with little need for experimental repetition. This is particularly advantageous for national security applications, such as propellant fires, and high-velocity impacts where experimental repetition is costly. Furthermore, by improving measurement accuracy and demonstrating viability in high-velocity and reacting environments, this project has advanced the frontiers of engineering.

Refereed Communications:

J. Gao, D.R. Guildenbecher, L. Engvall, P.L. Reu, and J. Chen, "Refinement of Particle Detection by the Hybrid Method in Digital In-Line Holography," *Applied Optics*, vol. 53, pp. G130-G138, September 2014.

J. Gao, D.R. Guildenbecher, P.L. Reu, and J. Chen, "Uncertainty Characterization of Particle Depth Measurement using Digital In-Line Holography and the Hybrid Method," *Optics Express*, vol. 21, pp. 26432-26449, November 2014.

D.R. Guildenbecher, M.A. Cooper, W. Gill, H.L. Stauffacher, M.S. Oliver, and T.W. Grasser, "Quantitative, Three-Dimensional Imaging of Aluminum Drop Combustion in Solid Propellant Plumes via Digital In-Line Holography," *Optics Letters*, vol. 39, pp. 5126-5129, September 2014.

D.R. Guildenbecher, L. Engvall, J. Gao, T.W. Grasser, P.L. Reu, and J. Chen, "Digital In-Line Holography to Quantify Secondary Droplets from the Impact of a Single Drop on a Thin Film," *Experiments in Fluids*, vol. 55, p.1670, March 2014.

D.R. Guildenbecher, "Digital In-Line Holography (DIH) for 3D Imaging of Aluminum Drop Combustion in Propellant Plumes," presented at *Laser Applications to Chemical, Security and Environmental Analysis (LACSEA)*, Seattle, WA, 2014.

Advanced Diagnostics for High-Pressure Spray Combustion

164668
Year 3 of 3
Principal Investigator: S. A. Skeen

Project Purpose:

Predictive high-pressure spray combustion simulations under development at Sandia will enable more rapid and cost-effective engine design that leverages fundamental physical and chemical information to reduce pollutant emissions and maximize efficiency. Anticipated advancements are crucial to the transportation sector as more stringent emissions regulations are imposed and new synthetic and bio-derived fuels with varying properties find greater usage. Development of a predictive simulation capability requires experimental data to both inform and validate the models, but very limited information is presently available about the chemical structure of high-pressure spray flames under engine-relevant conditions. Probing such flames for chemical information using nonintrusive optical methods or intrusive sampling techniques, however, is challenging because of the physical and optical harshness of the environment. For example, such flames are characterized by high velocities, temperatures, and pressures that make intrusive probing difficult. Further, beam steering effects caused by refractive index gradients are exacerbated at high pressure, complicating optical diagnostics. And finally, engine-relevant injection times are only a few milliseconds resulting in very small time windows for measurements under quasi-steady conditions.

This experimental project addresses the need for quantitative information from high-pressure spray flames under engine relevant conditions by developing and applying a suite of diagnostics to the constant volume high-pressure spray flame chamber at Sandia's Combustion Research Facility (CRF). A cutting-edge component of the work lies in the development of a 2D, high-speed, multiwavelength extinction diagnostic for quantitative soot volume fraction measurements and a first of its kind high-speed intrusive sampling technique to investigate the chemical structure of high-pressure spray flames under conditions previously unexplored by these methods. The potential exists to acquire high-impact, quantitative data; however, there are many risks and challenges associated with the proposed diagnostics at high pressure.

Summary of Accomplishments:

The present work leveraged the physical and optical access available in a pre-burn spray vessel, which simulates the thermodynamic conditions of modern diesel engines, to develop and apply sampling and optical diagnostics for the characterization of pre-burn reactant and product gases, gas-phase species within the lift-off region, and the temporal evolution of soot formation in n-dodecane spray flames. Prior to the present work, measurements of the minor gas-phase species following the pre-burn event have not been made. In this work, the pre-burn products were sampled and investigated in an off-line time-of-flight mass spectrometer (ToF-MS) to determine which minor species can be identified and potentially quantified. Further, gas-phase species were also extracted from the lift-off region of an n-dodecane spray flame for identification and quantification. We addressed the need to identify and quantify soot precursor species within the lift-off region and in the early stages of soot formation in a high-pressure n-dodecane spray flame. These measurements were the first of this kind. The high-speed soot extinction imaging diagnostic was developed to overcome limitations of laser-induced incandescence (LII). In general, high-speed LII imaging systems are rare and prohibitively expensive. LII can also be challenging in flames with high optical thickness. Quantification of LII also generally requires extinction measurements for calibration. The high-speed multiwavelength extinction imaging component of this work yielded novel information on the temporal progression of soot in a spray flame, quantified the quasi-steady soot field for a variety of ambient conditions including flames with high soot volume fraction (optically thick), and showed promise for determining changes in optical properties of soot particles as a function of spatial location.

Significance:

The development of cleaner and more fuel-efficient engines is a key objective toward the pursuit of energy security and environmental sustainability in the US. The development and application of the advanced high-pressure spray diagnostics in the present work has enhanced the understanding of soot formation in spray flames and has provided new benchmarks for modeling efforts focused on the design of advanced engines. The multiwavelength extinction imaging diagnostic and the high-pressure sampling system benefits the objectives of DOE's energy security mission.

Refereed Communications:

S.A. Skeen, J. Manin, and L.M. Pickett, "Simultaneous Formaldehyde PLIF and High-Speed Schlieren Imaging for Ignition Visualization in High-Pressure Spray Flames," in *Proceedings of the Combustion Institute 35*, San Francisco, CA, 2014.

J. Manin, S.A. Skeen, L.M. Pickett, E. Kurtz, and J.E. Anderson, "Effects of Oxygenated Fuels on Combustion and Soot Formation/Oxidation Processes," *SAE International Journal of Fuels and Lubricants,* vol. 7, pp. 704-717, October 2014.

S.A. Skeen, J. Manin, K. Dalen, A. Ivarsson, and L.M. Pickett, "Quantitative Spatially Resolved Measurements of Total Radiation in High-Pressure Spray Flames," SAE Technical Paper 2014-01-1252, April 2014.

J. Manin, S.A. Skeen, and L.M. Pickett, "Understanding Soot Optical Properties through Dual-Wavelength Diffused Back-Illumination Imaging," presented at *Thiesel 2014*, Valencia, Spain, 2014.

Reduced Order Modeling for Prediction and Control of Large-Scale Systems

164678
Year 3 of 3
Principal Investigator: I. Kalashnikova

Project Purpose:

Numerous engineering problems that Sandia is tasked with solving require the simulation of complex systems possessing many unknowns. The continuing push to incorporate into modeling efforts the quantification of uncertainties, critical to many Sandia applications, can present an intractable computational burden due to the high-dimensional systems that arise.

This research aims to enable real-time simulations of complex systems for on-the-spot decision making, probabilistic analysis, and control through the development of stable and efficient reduced order models (ROMs): models derived from a few high-fidelity simulations that capture the essential physics of interest at a low computational cost. For many ROM approaches, general results regarding the models' fundamental mathematical properties are lacking, or the reduction is computationally intractable for large-scale problems. This research will employ a provably stable and computationally tractable ROM technique we developed as a starting point to explore methods for developing stable and efficient ROMs for the control of large-scale systems. The work can be seen as the first step towards the development of an effective model reduction technique to support decision making under uncertainty. Targeted applications include the quantification of the captive-carry environment for the design of nuclear weapons (NW) systems.

For a ROM to serve as a useful predictive tool, the model should preserve the dynamical properties of the modeled system and be cost effective for large problems. As most ROM techniques are either computationally intractable for large-scale systems or lack an a priori stability guarantee, there is a critical need to explore new theoretically sound and computationally efficient techniques for building ROMs.

Summary of Accomplishments:

There were two primary goals of the proposed R&D for FY 2014:

1) Theoretical: Novel algorithm development of stability preserving model reduction approaches based on the POD/Galerkin method.

2) Implementation: Continue development of parallel C++/Trilinos (proper orthogonal decomposition) POD/Galerkin reduced order model (ROM) code ("Spirit") for compressible fluid problems (of interest to Sandia for the quantification of the captive-carry environment for the design of NW components) that would allow testing new approaches developed as part of (1).

Towards the first milestone, we have developed a new stability-preserving inner product for building provably stable projection-based ROMs for nonlinear compressible flow, termed the "total energy inner product." We have also been working in collaboration with Stanford and Duke Universities to develop a new approach for stabilizing and fine tuning projection-based ROMs for compressible flow. The key idea of this approach is to account for truncated POD modes a priori via a minimal rotation of the projection subspace.

Towards the second milestone, we have continued the development of the "Spirit" code, implementing in this code ROMs for nonlinear compressible flow constructed in the total energy inner product, and some energy inner products for the isentropic compressible flow. We tested the ROMs on some cavity flow problems that were simulated in the flow solver SIGMA computational fluid dynamics (CFD), with promising results. We also studied the effect of boundary conditions on ROM accuracy, and the ROMs performance for long-time simulations. Also towards the second milestone, we have been testing the approach on compressible cavity problems.

Significance:

This project was a necessary first step towards providing a mission-critical capability, namely the ability to do real-time analysis for compressible captive-carry flows for the design of NW components. Much was learned about the viability of energy-based ROM methods when applied to problems of interest in this application. The theory developed as a part of this project (total energy inner product, projection subspace rotation for ROM stabilization/fine-tuning) will benefit the broader scientific and engineering community, as it can be applied to compressible flow problems arising in other applications.

Refereed Communications:

I. Kalashnikova, J.A. Fike, M.F. Barone, S. Arunajatesan, and B.G. van Bloemen Waanders, "Energy-Stable Galerkin Reduced Order Models for Nonlinear Compressible Flow," presented at the *World Congress on Computational Mechanics (WCCM XI)*, Barcelona, Spain, 2014.

I. Kalashnikova, B.G. van Bloemen Waanders, S. Arunajatesan, and M.F. Barone, "Stabilized Projection-Based Reduced Order Models for Uncertainty Quantification," presented at the *SIAM Conference on Uncertainty Quantification (SIAM UQ14)*, Savannah, GA, 2014.

I. Kalashnikova, B.G. van Bloemen Waanders, S. Arunajatesan, and M.F. Barone, "Stabilization of Projection-Based Reduced Order Models for Linear Time-Invariant Systems via Optimization-Based Eigenvalue Reassignment," *Computer Methods in Applied Mechanics and Engineering*, vol. 272, pp. 251-270, April 2014.

Quantitative Imaging of Turbulent Mixing Dynamics in High-Pressure Fuel Injection to Enable Predictive Simulations of Engine Combustion

165646
Year 2 of 3
Principal Investigator: J. H. Frank

Project Purpose:

The purpose of this project is to develop a capability for quantitative imaging measurements of high-pressure fuel injection dynamics that will transform our understanding of turbulent mixing in transcritical flows, ignition, and flame stabilization mechanisms, and will provide essential validation data for developing predictive tools for engine combustion simulations. Advanced, fuel-efficient engine technologies rely on fuel injection into a high-pressure, high-temperature environment for mixture preparation and combustion. However, the dynamics of fuel mixing and combustion are not well understood and cannot be accurately predicted. Quantitative measurements for model validation are lacking because spatially and temporally resolved measurements of turbulent mixing and combustion dynamics in multiphase, high-pressure, high-temperature flows pose significant diagnostic challenges. Advanced diagnostics development at engine pressures and temperatures are needed to enable quantitative high-resolution measurements of the temporal evolution of fuel injection. The planned high-fidelity measurements will transform our understanding of fuel injection dynamics, which affect engine combustion processes such as flame lift-off, soot formation, and cycle-to-cycle variations. These quantitative data will be used for testing turbulent mixing models that are central to Sandia's efforts to develop predictive simulations of fuel injection.

The development and application of high-fidelity imaging diagnostics for understanding fuel injection dynamics is ambitious considering the complexity of the experiments and the demanding temporal and spatial resolution requirements. Quantitative interpretation of high-speed imaging data at high pressure and temperature are addressed by a detailed and innovative treatment of laser-based imaging measurements. To attain the extremely high data rates needed for tracking the motion of turbulent mixing (~100 kHz), we are developing a pulse-burst laser system that will enable high-speed planar laser imaging of fuel vapor mixing, velocity, and ignition. This unique diagnostic capability will be compact, robust, and mobile, enabling broad applicability for high-repetition rate imaging of motion in many areas of interest to Sandia.

A Process and Environment Aware Sierra/SM Cohesive Zone Modeling Capability for Polymer/Solid Interfaces

165649
Year 2 of 3
Principal Investigator: E. D. Reedy, Jr.

Project Purpose:

The performance and reliability of many Sandia components (e.g., neutron generators and firing sets) depend on the integrity of interfaces between dissimilar materials. Unfortunately, our ability to predict the performance of critical polymer/solid interfaces is limited. We will address this by combining Sandia's cutting-edge nonlinear viscoelastic polymer modeling capability with recent advances in finite element cohesive zone fracture modeling theory to create a significantly improved method for predicting interfacial failure. The anticipated outcome of this effort will be a unique capability that will enable Sandia's Sierra/SM finite element code to predict how variations in processing, environment, geometry, and loading affect the performance and reliability of polymer/solid interfaces. This effort must address several fundamental issues to succeed. For example, a physically based polymer constitutive model is essential since polymers undergo highly nonlinear relaxations during processing, aging, and mechanical loading. This is most strongly manifested in the highly stressed regions where failure usually initiates (e.g., sharp corners). However, it is unclear how to define and measure the primary parameters that define a cohesive zone interfacial fracture model (i.e., interfacial strength and the work of separation) when nonlinear energy dissipation in the bulk polymer dominates. One cannot simply define the cohesive zone model in terms of the molecular bonding between the joined materials since this would be analogous to modeling engineering components on the same nanometer scale as the molecular interactions. Likewise, it is not clear how one should incorporate the well-known increase in apparent interfacial toughness with increasing crack-tip shear deformation. We will use molecular dynamics simulations, detailed finite element fracture analyses, and key interfacial fracture tests to resolve such issues. Tests of component-scale adhesively bonded joints will also allow us to validate our work and to further establish the sensitivity of interfacial fracture to variations in processing and environment.

Prediction of Spark Discharge Paths and Voltages

165652
Year 2 of 3
Principal Investigator: L. K. Warne

Project Purpose:

A fundamental problem we repeatedly encounter is how a spark discharge path selects among candidate conductors that are in proximity to an electrode (or plasma) at high voltage and the statistics associated with such spark attachments. This determines whether penetrant energy is diverted to chassis or leads to difficulties. This problem pertains to penetrations associated with metallic burnthrough by lightning continuing current, to phenolic blastthrough events driven by lightning return strokes, and to other penetrations.

A previously proposed semi-empirical static breakdown criterion will not answer fundamental technical challenges arising from the transient development of the spark, particularly:

- Discharge timing (lightning-driven voltages are time limited)
- Conductor impedance (floating electrodes and dielectrics)
- Probability of path and statistics of attachment
- Effect of presence of excited gas species, which may exist after penetrations

There is a large body of work on sparkover, but the majority is empirical and not easily generalized to geometries and conditions (impedance, drive waveform, etc.) of interest to Sandia.

Our objective is to develop rigorous tools for determining dynamical criteria for sparkover and discharge path in arbitrary gap geometries, having applications to components subjected to high voltage in gaseous environments.

Although there are models and experiments in the literature addressing sparkover development, there is no clear picture of how this event occurs. Our new insight is that the intermediate stage of spark development, bridging the initial gas ionization stage with the final heating stage and involving interactions of the discharge with the electrodes, sets the sparking condition. This has been somewhat ignored in the literature. If successful in understanding how this occurs, our first-principles model will be a major advance and essential for addressing the project's technical challenges.

Time-Resolved Optical Measurements of Shock-Induced Chemistry in Energetic Materials

165656
Year 2 of 3
Principal Investigator: R. R. Wixom

Project Purpose:

State-of-the-art models for shock initiation of explosives are not predictive and thus have limited utility for engineering design, analysis, and quantification of margins and uncertainty (QMU) for energetic components. The development of physically based predictive tools is severely limited by a lack of knowledge of the reaction chemistry and a poor understanding of the physics of chemical energy release at hotspots. The reactive processes occurring during shock initiation are poorly understood due to the inherent difficulty of making measurements on the very fast timescales, short length scales, and extreme conditions which are typically encountered.

Direct observation of thermodynamic states and shock-induced reactions in heterogeneous, condensed-phase solids is difficult due to the technical challenge of obtaining sufficient signal/noise ratio while maintaining sufficiently high temporal and spatial resolution. When resolution is sacrificed, the measurements become averaged over time or space in the heterogeneous material and the observation of local nonequilibrium phenomena is compromised. However, newly available optically thin, homogeneous samples may allow us to probe reactions occurring within the material during shock initiation.

Vapor deposited films of certain explosives, including hexanitrostilbene (HNS), are relatively transparent, allowing measurement of optical emission from within the shocked material. The emission spectrum can be used to determine both temperature of the sample and the presence of chemical species which evolve over time — information that will validate equation of state (EOS) predictions and provide insight into the reactive processes. The ultimate goal of this project is to develop a fundamental understanding of reaction mechanisms and kinetics, and their relationship to the local thermodynamic state of the material. If successful, these experiments will revolutionize our understanding of initiation and we will be positioned to fill a major knowledge gap that is preventing the explosives community from developing predictive shock-initiation models.

Determining Constitutive Material Properties from Full-Field Experiments using the Virtual Fields Method

165667
Year 2 of 2
Principal Investigator: S. L. Kramer

Project Purpose:

Determination of parameters for constitutive material models is a vital capability for solid mechanics computational analysis. The standard practice is to extrapolate material properties from simple tests with closed-form solutions; but, this practice cannot reliably characterize complex loading responses, failure, anisotropies, or heterogeneous behaviors, requiring several experimental test configurations that can be cost prohibitive. With the maturation of full-field experimental methods that provide millions of data points from a single experiment, the constitutive parameter identification inverse problem need no longer rely on simple closed-form solution experiments. With constitutive models calibrated by deformations representative of real system behavior, predictive simulations should have reduced error and uncertainty. The remaining hurdle for this improved calibration process is robust numerical methods for solving this inverse problem using full-field experimental data. One promising inverse method recently developed is the virtual fields method (VFM), based on the principle of virtual work from continuum mechanics, requiring as little as one experiment with heterogeneous deformation fields to populate a complex model. VFM has been applied mainly to isotropic and anisotropic elasticity with limited work in plasticity; further research is required for reliable parameter identification for material models that capture large plastic deformations and material failure. This project specifically aims to extend VFM for common plasticity models at Sandia, not previously addressed in literature, to improve modeling behavior of finite-deformation plasticity, aided by newly developed numerical methods for designing optimal specimen geometries for the VFM identification. The primary goal is to demonstrate this new capability for a well-characterized material, 304L stainless steel sheets, in order to compare VFM to the standard practice of constitutive parameter identification.

Summary of Accomplishments:

We demonstrated the VFM for parameter identification for finite-deformation plasticity constitutive models. We implemented VFM in MATLAB (matrix laboratory) using the principle of virtual power, exploiting finite element model (FEM) kinematics and meshing methods, in conjunction with nonlinear optimization methods to perform the identification of finite-deformation plasticity constitutive models that have a nonlinear behavior over time. To verify the numerical implementation approach, we used simulated FEM data, for a given specimen geometry and nominal constitutive model parameters, as input to the VFM identification process, attempting to return the nominal constitutive model parameters. Once the VFM MATLAB code was verified with FEM data without any experimental noise issues, we then evaluated the quality of the VFM parameter identification process with more realistic data inputs. Inverse problem methodologies such as VFM rely on full-field experimental measurements from optical methods with experimental errors that can lead to large uncertainties in the identified parameters. The complete VFM inverse problem methodology was simulated using computationally derived displacements with superimposed measurement uncertainties, which were quantified for representative digital image correlation (DIC) experimental setups, as inputs to the identification algorithm. The simulated VFM process that incorporated measurement errors allowed for characterizing the impact of DIC uncertainties based on realistic experimental parameters without requiring cost-prohibitive iterative experimental investigations of the full VFM process. VFM was able to identify constitutive model parameters for the Bammann-Chiesa-Johnson (BCJ) plasticity model even in the presence of simulated DIC noise. We were able to investigate the influence of experimental noise, specimen geometry, and experimental data density on the quality of the parameter identification; this helps us to design better specimen geometries, experimental setup parameters, and aspects of VFM that will improve the parameter identification. Overall, this study demonstrated that VFM is a viable technique for constitutive model parameter identification when using full-field DIC data.

Significance:

Sandia requires reliable predictive capabilities for both safety and design of their systems for a variety of demanding environments. One area for improvement in predictive capabilities is more robust material modeling, which requires advancement in selection and calibration of constitutive models. This project implemented and evaluated the promising inverse method VFM for constitutive model parameter identification, specifically for ductile plasticity. We determined that VFM is a viable approach for this purpose, characterizing its merits and deficiencies, thus advancing the research area of inverse methods for material modeling, which ultimately will improve our predictive capabilities. This research benefits NNSA's nuclear security mission.

High Precision Testing and Structural Analysis of Li-Ion Batteries

166152
Year 2 of 3
Principal Investigator: S. R. Ferreira

Project Purpose:

In collaboration with the University of New Mexico, the purpose of this project is to understand high precision testing combined with materials characterization of battery cells to advance capabilities in screening of materials and in improving prognostics in lifecycle expectancy. Advances with current testing techniques and methodologies are becoming crucial, as the market for energy storage is moving beyond one- to two-year batteries for consumer goods, such as laptops and cellphones, into large-scale, long-term advanced technologies for electric vehicle and stationary storage applications. Current battery testing methods use low precision testers. Long-term cycling is currently the only reliable way to determine life. Long-term validation testing far exceeds the development cycle for battery technologies and is prohibitively expensive. A transformative way of quickly and reliably validating battery materials and battery life is critical to enabling advances in stationary storage technology. In this project, rapid, reliable battery evaluation, facilitated by high precision testing, will be coupled with materials characterization techniques. These will be used to understand and predict battery performance and life, to better enable their adoption for stationary storage applications.

Extensive previous efforts to rapidly validate battery life have been largely unsuccessful, especially using accelerated testing. An increase in the precision and accuracy of measurements may provide sufficient data for prognostication of battery life, decreasing the duration of testing to weeks or months rather than years. Our university researchers have tested the concept of high precision testing with positive preliminary results. We will expand on this work by evaluating battery cells before formation, at beginning-of-life (BOL), and at intervals in state of health through the end-of-life (EOL). These will be coupled with material characterization techniques, including scanning electron microscopy and surface area measurements of battery electrodes. Through a variety of analytical techniques, we will identify statistical structure-to-property relationships between the cycling and characterization data.

Upscaling Ab-Initio Quantum Chemistry Models for Nonequilibrium Reacting Flow Simulations

166153
Year 2 of 3
Principal Investigator: D. J. Rader

Project Purpose:

In collaboration with Purdue University, the purpose of the project is to create a state-specific air chemistry model by performing quasi-classical trajectory (QCT) simulations on potential energy surfaces (PES) obtained from ab-initio quantum chemistry calculations. This methodology allows construction of nonequilibrium collision, energy exchange, and reaction models for systems for which little or no experimental data exist. These models will then be used in rarefied-flow simulations to more accurately predict gas drag and thermal load to reentry vehicles. In particular, this work focuses on reactive oxygen processes that can affect high-speed flow-field structures and surface oxidation. The resulting nonequilibrium chemistry models will be applied in Sandia's computational fluid dynamics (CFD) and direct simulation Monte Carlo (DSMC) codes to improve their predictive fidelity.

Many advanced engineering technologies that support national security involve nonequilibrium reacting flows. Such flows are generated by reentry vehicles, plasma environments, and detonations. During Earth reentry, gas temperature in the shock region exceeds 10,000 K which leads to air dissociation. The flow in the shock is highly nonequilibrium and chemical kinetics there cannot be characterized by single-temperature Arrhenius rates. Since characterizing such flows in ground or flight experiments is prohibitively expensive, there is currently a lack of high-fidelity nonequilibrium chemistry models that could account for internal energy specific chemical processes. This project will address this challenging R&D gap.

Modeling the Coupled Chemo-Thermo-Mechanical Behavior of Amorphous Polymer Networks

169249
Year 2 of 2
Principal Investigator: J. A. Zimmerman

Project Purpose:

Thermally activated shape-memory polymers (SMPs) have garnered significant attention in recent years for their potential broad range of applications and properties that can be tailored. Several different mechanisms can be employed to achieve the shape-memory effect in polymers, but the two most common ones are the melt transition of semi-crystalline polymers and the glass transition of amorphous polymers. For amorphous polymers, the temporary shape is obtained by deforming the material in its heated rubbery state. Cooling the material below the glass transition temperature (T_g) reduces the molecular mobility of the polymer chains, fixing the deformed shape in a nonequilibrium thermodynamic state. The temporary shape should be fixed indefinitely until the material is heated above the T_g. However, amorphous SMPs can experience a significant loss in shape fixity below T_g when stored for a prolonged period of time in water or in a humid environment. While the absorption of solvents, such as water, can be detrimental to the shape-memory effect of amorphous networks, the phenomena can also be harnessed to athermally activate shape recovery. This alternative to temperature-driven shape recovery can be attractive in applications where the controlled delivery of heat poses an intractable challenge in a surgical environment.

Summary of Accomplishments:

We have developed an effective temperature theory for the coupled thermomechanical behavior of amorphous polymers across the glass transition and applied the model to describe a wide range of shape-memory behavior. In developing the model, we adopted the basic idea that the behavior of the glass can be decomposed into fast kinetic processes at the equilibrium temperature and multiple slowly evolving configurational processes at different effective temperatures. The concept of multiple configurational processes is introduced to accurately represent the broad relaxation spectrum. The kinetic and configuration processes are characterized by different internal energies, configurational entropies, and heat flux, the sum of which gives the properties of the system. The theory decomposes the balance of energy into sub-balances for the kinetic and configurational subsystems, which requires introducing heat conduction between the subsystems. The energy sub-balances are used to develop a reduced entropy inequality that constrains the constitutive relations for heat conduction and internal state variables. We applied theory to describe the thermomechanical behavior of an acrylate shape-memory polymer, where the properties have been previously determined from standard dynamic mechanical analysis and isothermal uniaxial tensile experiments. The results showed that the effective temperature theory was able to reproduce the temperature-dependent stress response through the glass transition, and quantified the effects of physical aging and mechanical rejuvenation on the yield strength of the glass, without introducing additional structural variables. The effective temperature thermodynamics theory provides a unifying framework to model the wide range of nonequilibrium behavior of amorphous polymers across the glass transition.

Significance:

Modeling the nonequilibrium behavior of amorphous polymers is important for improving a wide range of manufacturing processes, design of shape-memory polymer materials and devices, and design for high-rate applications. Predictive models that include temperature- and rate-dependent material behavior are needed to:

1) increase manufacturing process efficiency and precision, 2) tailor processing conditions for targeted material properties, and 3) integrate structural evolution and inelastic deformation to accurately capture responses to impact and blast. The project has the potential to impact a broad range of technologies, including integrated sensors and actuators and manufacturing, by enabling new and integrated functionalities.

Refereed Communications:

R. Xiao and T.D. Nguyen, "Thermomechanics of Amorphous Shape-Memory Polymers," presented at the *IUTAM Symposium on Mechanics of Soft Active Materials*, Technion, Israel, 2014.

R. Xiao and T.D. Nguyen, "Modeling Physical Aging and Mechanical Rejuvenation of Glassy Amorphous Polymers," presented at the *International Conference on the Mechanics of Time Dependent Materials*, Montreal, Canada, 2014.

T.D. Nguyen and R. Xiao, "Thermomechanics of Amorphous Polymers: Applications to Shape-Memory Behavior," presented at the *International Symposium on Plasticity*, Grand Lucayan, The Grand Bahamas, 2014.

Determination of Surface-Mediated Degradation Products in Energetic Materials at Critical Interfaces

170974
Year 2 of 3
Principal Investigator: C. L. Beppler

Project Purpose:

The purpose of this project is to better understand the surface-mediated chemical degradation products that form in energetic materials (EM) through the use of state-of-the-art analysis methods. This project will apply state-of-the-art methods such as electrospray ionization-mass spectrometry (ESI-MS), gas chromatography-thermal conductivity detection (GC-TCD), and other suitable tools to probe the identities and possible formation pathways of surface-mediated EM degradation products.

This study is the first to apply more sensitive tools to better understand how surface-mediated EM degradation occurs at material interfaces. These tools will probe the previously under-examined, non-volatile degradation products in EM, a key deficiency in our knowledge of energetic material degradation. This knowledge will then be fed into the creation of new and more accurate experimental and computational methods to predict critical aging parameters in energetic materials. The knowledge of these key aging parameters can then enable more accurate predictions of how an energetic material will age and provide better criteria for selecting materials that are chemically compatible with EMs.

A current technical challenge in this project is pre-processing and analyzing all the data collected from the analysis of thermally aged EMs by ESI-MS. Software tools are currently being implemented to automate data pre-processing. The new software capabilities also include multivariate statistical data analysis, which is necessary to show statistically significant comparisons of the aged energetic material vs. the pristine, untreated EM samples.

Numerical Methods for Efficient Simulations and Analysis of Circuits with Separated Time Scales

171117
Year 2 of 3
Principal Investigator: M. N. Hsieh

Project Purpose:

The purpose of the project is to develop novel numerical methods for efficient modeling of complex fast/slow circuits (i.e., small circuits with strong, nonlinear oscillations, and separated fast/slow time scales). Circuit-level simulation and analysis can support electrical interface characterization and predict functional performance limits under untestable environments or scenarios. Complex fast/slow circuits can make the computation time of even a single simulation unmanageable. Parallel simulation cannot improve the computation efficiency because these circuits are typically small. Many numerical methods may possibly speed up such simulations by utilizing multiple time variables to efficiently represent circuit signals with widely separated rates of variation (e.g., multirate partial differential equation). However, existing methods become ineffective if the circuits have a small difference between the fast and slow rates of change, have multiple time scales, or have complex quasi-periodic behaviors in the fast time scale. These limitations make the utilization of existing methods inherently risky, and much of the risk lies in identifying a viable solution to overcome each of the limitations. Our circuits of interest may possess complex behaviors that are shown to be the outstanding challenges in this research field. If successful, this project will provide capabilities to simulate and analyze the entire operation cycles of complex fast/slow circuit with high fidelity in manageable time, which is impossible using existing technologies.

High-Fidelity Coupling Methods for Blast Response on Thin Shell Structures

173095
Year 1 of 3
Principal Investigator: M. W. Heinstein

Project Purpose:

The purpose of this project is to conduct a focused investigation of fluid-structure interaction (FSI) coupling algorithms combined with high-resolution shock physics, using level set and unstructured shell modeling to simulate the impact of air blast on thin structures. R&D of new high-resolution methods with compact spatiotemporal discretizations is required for implementation in current codes. Innovative R&D in this project will center on a two-field representation of the coupled FSI. Specifically, rather than inserting the unstructured shell mesh into the Eulerian domain every time step, we will pursue a fundamentally new concept to develop two structure representations with constraints that tie them together with variational consistency. One representation is a Lagrangian shell mesh incorporating modern material and failure modeling. The second is a level set embedded within the structured shock physics grid. Each description of the physics can be implemented with high-fidelity numerical methods applying conservation principles. Much of our focus will be on the formulation and solution of this domain-to-domain coupling problem between these representations producing high-fidelity boundary conditions on each. Finally, the methodology pursued here will be extended with the objective of making advances applicable to current Sandia codes. These methods will have the advantage of being suitable for modern supercomputers.

Modeling Primary Atomization of Liquid Fuels using a Multiphase DNS/LES Approach

173096
Year 1 of 3
Principal Investigator: M. Arienti

Project Purpose:

The purpose of this project is to study the injection dynamics of dense sprays in the context of large eddy simulation (LES) of turbulent combustion through the adoption of an advanced interface-tracking method for multiphase flow. Significant inadequacies in existing models that treat the spray formation (atomization) of liquid fuels are a major barrier to rapid development of advanced, high-efficiency, low-emissions combustion devices. An existing LES framework at Sandia (the code RAPTOR) can treat the full range of scales in turbulent reacting flows in a computationally feasible manner (large energetic scales are resolved and the small sub-grid scales are modeled), but requires the correct initial spray information. The high-fidelity simulation of spray atomization by a second computer code (CLSVOF) is used in this project to develop a model-free database for generating new closure terms for LES.

A semi-Lagrangian framework was selected to extend the current dilute spray model implemented in RAPTOR, using a new kinetic approach devised for strong interactions with the Eulerian flow phase. The kinetic approach is coupled deterministically with the Eulerian fields to avoid statistical noise. An additional advantage of this approach is that it features controlled load balancing by construction. The assessment of the compressible multiphase capability was the major milestone for CLSVOF, whose multiphase Navier-Stokes equations are now completed by a nonlinear equation of state calibrated for sub-critical dodecane. The modeling activity with CLSVOF responds to the need to describe spray atomization at large injection pressures in modern engines. This capability was demonstrated by a baseline simulation of "spray A," one of the engine combustion network suite of industry-relevant diesel injectors that is being experimentally characterized at Sandia and Argonne National Laboratory.

Experiments and Computational Theory for Electrical Breakdown in Critical Components

173097
Year 1 of 3
Principal Investigator: F. J. Zutavern

Project Purpose:

Electrical breakdown is a key issue for many electrical components, either in the need to control it or prevent it from occurring entirely. For example, lightning arresters are designed to protect electrical systems by breaking down when struck by lightning. Alternatively, insulators in high energy density storage, switching, and transmission systems are designed to avoid breakdown using the minimum required volume. Predicting the performance and characteristics of these devices in extreme environments for stockpile and other critical applications is a key issue of national importance. For over a century, component designers have used the breakdown strength of bulk materials as a design guide in many different environments, conditions and configurations. Science-based modeling of this important phenomenon has had limited success in predicting many of the observed characteristics (such as component breakdown strengths, location and size of primary current channels, damage on solid surfaces and in bulk insulating and multi-phase materials, the generation and relative roles of ion and electron distributions in initiating and growing an electrical discharge, and the interaction with solid interfaces near breakdown events) without the help of well-diagnosed discovery experiments.

This project is applying new experimental techniques and diagnostics to the study of electrical breakdown, starting with ultra-short pulse laser-induced terahertz imaging of electron distributions, to provide more information about electrical breakdown than optical imaging. In the past, optical radiation from the recombination of electrons and ions during electrical breakdown has provided a wealth of information about the plasma distribution in regions where both electrons and ions are present. However, this will be the first diagnostic to provide sub-nanosecond images of the highly mobile electron-rich (ion-depleted) regions of the plasma. Other discovery experiments and advanced diagnostics that will also provide new insight into electrical breakdown are being analyzed to understand their scientific issues and potential impact on advance breakdown theory to improve physics-based simulations.

Mechanics of Battery Degradation through Stress-Driven Rearrangement of Percolated Conductive Networks during Discharge and Cycling

173098
Year 1 of 3
Principal Investigator: A. Grillet

Project Purpose:

Mesoscale battery electrode structure and dynamics control electron and ion transport and may determine capacity degradation in rechargeable batteries. We intend to develop an understanding of the process of mechanical degradation on the electrode structure of lithium-ion batteries, focusing specifically on the ionic and electronic percolation pathways. Building on research at the single particle level, we will examine how mechanical changes during cycling cause capacity fade through particle deformations and rearrangements, localized over-potentials, electronic isolation of particles and lithium-ion flux limitations. In particular, we will explore how structural heterogeneity coupled with anisotropic changes at the grain scale causes changes in the electronic conductivity of the percolated network. Understanding capacity fade and reliability of rechargeable batteries will significantly impact our nation's ability to field advanced chemistries for electronics, munitions, and energy storage for renewable sources.

Whereas existing research on battery degradation has focused either at the battery level or on single particle changes, we will take a mesoscale approach, focusing on how microstructural behavior of the percolated electrode network drives macroscale battery performance. By coupling the complex network structure including structural heterogeneities, and correlated particle dynamics due to mechanical changes including anisotropic particle swelling and changes in modulus and porosity/tortuosity, the impact of cycling on battery performance can be understood. To date, this level of sophistication in developing coupled mechanics and performance models of the complex percolated structure of battery electrodes has not been developed, and represents a new way of looking at degradation mechanisms during cycling. This project will develop new experimental techniques to study battery electrodes examining the connectivity of both the particles and porosity as a function of both internal (lithiation) and external (applied) stresses. We will drive new methods of computationally coupling mechanics and electrochemical changes, which will require development of anisotropic constitutive equations and composite network conductivity models to capture the progressive degradation.

Methods for Observing Flow in High-Pressure High-Temperature Flow Experiments

173099
Year 1 of 1
Principal Investigator: M. Nemer

Project Purpose:

In many Sandia applications, there is a need to obtain detailed measurements of interface motion, internal pressures and temperatures. The extreme conditions encountered in abnormal environments challenge conventional methods of direct imaging and measurement. Specific examples include organic material liquefaction and flow in abnormal thermal environments, high-speed confined flows, and shock experiments. Particle image velocimetry (PIV) measurements on high-pressure-temperature flows are difficult because such extreme environments limit the use of optical measurements. Tomographic techniques, such as MRI and CAT-SCANs, while capable of getting 3D structure, require expensive instrumentation and suffer from slow frame rates, making them unsuitable for studying fast dynamic phenomena. Furthermore, MRI scans are not possible on thick-walled metal vessels.

This research utilized a newly developed method for extracting flow information. The needed mathematical formalism is being developed. If successful, the impact of this work would be a novel noninvasive flow-diagnostic technique, capable of providing critical diagnostics for a range of important applications.

Summary of Accomplishments:

We have performed a mathematical analysis demonstrating that we can quantitatively invert to obtain the velocity field for simple flows. An invention disclosure was filed detailing the existence and uniqueness of the inverse solution idea. We have designed a simple experimental setup to test this idea on a real flow.

Significance:

The impact of this work is a novel noninvasive flow-diagnostic technique, capable of providing critical diagnostics for a range of important applications in abnormal environments that are critical to ensuring the safety of the NNSA mission.

A Mesh-Free Method to Predictively Simulate Solid-to-Liquid Phase Transitions in Abnormal Thermal Environments

173194
Year 1 of 3
Principal Investigator: J. A. Templeton

Project Purpose:

Metal melting and encapsulant decomposition significantly impact weapon systems' safety in abnormal thermal environments. Most existing finite element codes are also unable to adequately capture massive geometry changes and liquid relocation. Alternatively, smooth-particle hydrodynamics has been applied to molten aluminum flows, but its formulation precludes phase changes and uncertainty quantification. Other particle formulations, such as the reproducing kernel particle method, are amenable to rigorous error analysis and preserve physical quantities (e.g., viscosity) by retaining the integral form, but have difficulties maintaining high-order numerical quadrature as particles advect. Given the promise of mesh-free methods to accurately model melting and relocation, we are developing a novel mesh-free formulation with error estimation and validation incorporated from inception by resolving the key technological barriers impeding these methods: minimizing integration error as quadrature points move and resolving processes at the solid/liquid and liquid/air interfaces. This computational simulation capability will provide a high-order quadrature mesh-free scheme implemented in a scalable software package. To understand interactions among all relevant processes, models for aluminum melting, oxidation, and flow will be included.

Our work will explore mesh-free strategies for simulating metal melt and relocation that are currently not being investigated at Sandia. While particle methods can model crucial large deformations and surface effects arising in these problems, they are significantly limited because they cannot be rigorously subjected to the verification and validation process for complex topologies. Without quantified uncertainty, the results cannot impact system qualification. Our challenge will be to develop robust integration and interface capturing strategies with precise error estimates and connections to experiments involving melting, surface chemistry, and relocation. If successful, we will enable predictive simulation of phenomena important in abnormal thermal environments.

Fully Coupled Simulation of Lithium-Ion Battery Cell Performance

173655
Year 1 of 3
Principal Investigator: S. A. Roberts

Project Purpose:

Lithium-ion batteries are commonly simulated using a volume-averaged formulation (porous electrode theory), using effective properties and assuming a simplified spherical geometry of the electrode particles. In contrast, a particle-scale simulation applied to real electrode geometries predicts localized phenomena. This research, in collaboration with The University of Texas at Austin, would continue to develop a fully coupled finite volume methodology for the simulation of the electrochemical-thermal equations in a lithium-ion battery cell. Due to the highly complex nature of electrode geometries, these models will operate on any unstructured mesh of arbitrary convex polyhedral cells and, therefore, will be implemented within the MEMOSA software framework of Purdue's PRISM center. Butler-Volmer kinetics at the electrode/electrolyte interface introduce significant nonlinear coupling of all equations. Fully coupling species transport, electrostatics, temperature, and Butler-Volmer kinetics in a stable, efficient, and parallel/scalable computational algorithm for arbitrary geometries is a significant technical challenge. The second part of the project will implement an immersed boundary method to model transport and interface kinetics. This method, which eliminates the need for a conforming mesh as volumes change, would be advantageous when modeling battery electrode volume expansion and stress effects during lithiation. The final part of the project will apply a reduced order version of the particle-scale physics to battery-level simulations without the associated computational cost.

Reducing the Adverse Effects of Boundary-Layer Transition on High-Speed Flight Vehicles

173878
Year 1 of 3
Principal Investigator: K. M. Casper

Project Purpose:

During boundary-layer transition, high-pressure fluctuations are generated on a reentry vehicle that can create significant vibration of internal components. There is an ongoing effort at Sandia to better predict these fluctuations and also understand how they couple to the vibration of the structure. Modern computational capabilities now allow modeling of the fluid-structure interactions in these hypersonic vehicles. These models must be developed from experimental data; however, current structural testing of hypersonic vehicles relies on static tests that do not provide an accurate representation of the fluid-forcing environment in flight. We will make novel measurements of this coupling by introducing controlled pressure disturbances over a flexible panel in hypersonic flow. The flow field and panel response will be characterized using high-frequency pressure and vibration measurements as well as flow-field visualization. High temporal resolution is required to resolve the unsteady flow field at hypersonic speeds, but these diagnostics have only recently attained the frequency response necessary to study this problem.

Significant work is required to develop this coupled experiment. A flexible panel must be created with structural modes that can be excited by the flow. Also, in order to create controlled pressure disturbances, a repeatable flow perturber must be developed, a challenging task in thin hypersonic boundary layers. Finally, the high-speed environment requires instrumentation with good spatial and temporal resolution. We will leverage recent development work focused on high-speed instrumentation to perform these coupled experiments for the first time. This work will provide the first data set on hypersonic fluid-structure coupling and improve current predictive models. However, the potential impact extends well beyond this. A natural extension would be to develop perturber arrays that might be used to reduce the pressure-fluctuation magnitude or drive the frequency content of the fluctuations to ranges at which the structure will not respond. These applications of flow control have never been explored.

Development of a Spatially Resolved Microwave Interferometer (SRMI)

173881
Year 1 of 2
Principal Investigator: P. E. Specht

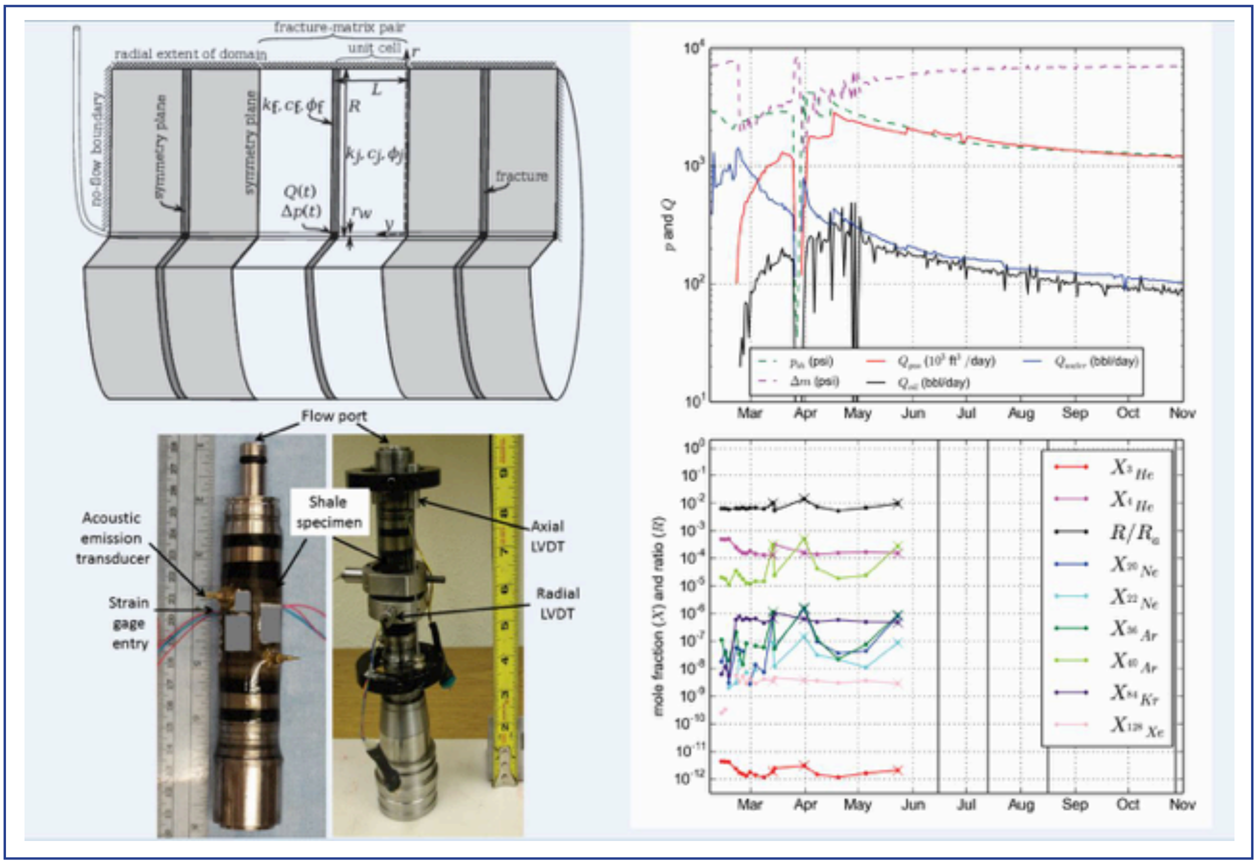
Project Purpose:

A novel, spatially resolved microwave interferometer (SRMI) is being developed to noninvasively image the internal transit of a shock, detonation, or reaction front in energetic media. Current state-of-the-art interferometry techniques, such as VISAR (Velocity Interferometer System for Any Reflector) or ORVIS (Optically Recording Velocity Interferometer System), rely on surface or interface measurements to infer the internal loading condition of the material. Alternate diagnostics embedded in the sample, such as electromagnetic gauges, inherently disrupt the state of the shock or reaction wave being measured. A SRMI will overcome these failings and provide a high-fidelity, spatially resolved diagnostic for internally measuring the real-time transmission of a shock or reaction wave through an energetic material.

Most energetic media is transparent at microwave frequencies. Current microwave interferometers provide a single-point, continuum measurement of the dielectric discontinuity that occurs across a shock or reaction front. A continuum-level response is insufficient to understand the complex wave and material interactions affecting the thermal, mechanical, and chemical response of heterogeneous energetic materials. The SRMI integrates advanced technologies from laser interferometry, microwave interferometry, terahertz spectroscopy, and high-speed imaging to yield a spatially resolved view of the shock or reaction front. The fundamental advancement in the SRMI is the use of an electro-optic crystal to transfer the Doppler shifted microwave information to a laser without loss of fidelity. This eliminates the technical challenges associated with manipulating and recording a microwave beam. Well-established laser interferometry techniques can instead be used to retrieve the information. Spatial resolutions under a micron and temporal resolutions under a picosecond can be theoretically achieved. Such noninvasive, spatially resolved internal measurements of a shock or reaction wave could provide a new and unmatched view of the response of heterogeneous energetic materials, which is necessary for developing advanced, predictive mesoscale models.

GEOSCIENCE

The Geoscience Investment Area seeks to expand the frontiers of knowledge in the following areas: 1) the properties, structure, phenomena and processes associated with the earth's subsurface, surface, and atmosphere and 2) how engineered systems interact with the earth and the earth system. These earth systems and properties impact Sandia national security missions, including energy security, defense, nonproliferation, disaster response, and climate security.



An increased understanding of hydraulic fracturing processes can be realized by a combined approach of modeling, field measurements, and laboratory helium-release-during-deformation experiments. Through these activities, Sandia is developing methods to incorporate temporal measurements of a suite of naturally occurring noble gases at wellheads to reduce uncertainty in fluid production forecasts and improve knowledge of reservoir fracture characteristics and transport processes. (Project 165670)

GEOSCIENCE

Aerosol Aging Processes and their Relevance to Human and Environmental Hazards

161873
Year 3 of 3
Principal Investigator: J. Santarpia

Project Purpose:

To understand the fate of any aerosol in the atmosphere and assess the impacts or hazards they pose, the atmospheric processes that affect the physical, chemical, and biological properties of airborne particulate matter must be characterized. For instance, the viability/toxicity and the fluorescence of chemical and biological warfare (CBW) agents and simulants released into the open atmosphere decay at vastly different rates as compared to those enclosed in conventional laboratory apparatus due to atmospheric chemical interactions and compounds, termed open-air factors (OAF). Because CBW agents cannot be studied outside, there are very few open-air decay rates to inform operational hazard prediction models. Further, there is little understanding about the effects of OAF on the biological detection signatures for agents. Past and current studies indicate that the specifics of how long a biological attack may be detectable by current technologies are presently unknown. Tracers used to simulate the transport of CBW agents, and validate models, often rely on ultraviolet (UV) light induced fluorescence (LIF) for detection. The fluorophores in the tracer material may also be subject to the same degradation processes that affect CBW agents and stimulants. Finally, the radiative and hygroscopic properties of both anthropogenic and naturally occurring super-micron aerosol particles (such as dusts and bacteria) are critically important to understanding Earth's climate processes. Laboratory measurements of these properties after known aging processes are relatively non-existent.

This work proposes to develop new methods to study these complex problems. These problems represent significant gaps in chemical and biological hazard assessment that have had limited study.

Summary of Accomplishments:

We developed a novel system to expose a variety of chemical and biological aerosols to controlled environments. The system is capable of reproducing conditions relevant to urban and remote environments around the world, allowing us to investigate the fate of chemical and biological threat particles in a wide variety of urban environments. We demonstrated the ability of the system to reproduce the solar decay of *Bacillus thurengiensis* var. *kurstaki* from previous ambient tests, as well as the stability of fluorescence of a tracer particle under the same conditions.

Significance:

This work developed new methods to study the complex problems of chemical and biological aerosol fate and provide new information to inform a wide range of problems, including hazard prediction from Weapons of Mass Destruction (WMD) and climate. These results should help enable the predictive capabilities of these fields.

Methane Hydrate Formation on Clay Mineral Surfaces: Thermodynamic Stability and Heterogeneous Nucleation Mechanisms

165668
Year 2 of 3
Principal Investigator: R. T. Cygan

Project Purpose:

We will develop a comprehensive understanding of the heterogeneous nucleation of methane hydrates and their subsequent thermodynamic properties. This will lead to more effective methods to extract subsurface methane (natural gas) from hydrates and better control hydrate formation associated with oil extraction. Methane hydrates, ice-like water cages surrounding methane molecules, have the potential to play a huge role in our nation's energy security. Large untapped hydrate reserves exist in seafloor and Arctic sediments; a recent US geological survey estimates 590 trillion cubic feet of methane hydrate — more than three times the amount of natural gas — is located on the North Slope of Alaska. The ability to utilize and control hydrate reserves is currently hindered by a lack of fundamental understanding of the natural environment's impact on the stability and formation of methane hydrates, which are often found in areas of clay-rich sediments. Most studies on hydrate nucleation and thermodynamic stability have focused on homogeneous systems, whereas heterogeneous systems are found in nature and in technical settings. The addition of nucleating mineral surfaces will impact the outcome of any study performed and will advance this field forward towards an improved knowledge base furthering our ability to utilize its natural fuel sources.

Heterogeneous nucleation and thermodynamic stability of methane hydrates is an understudied phenomenon despite its critical importance. To address this challenge, cutting-edge simulation methods using Sandia's supercomputers will be required. Strategic experiments will both validate and inform the simulations. Even then, the primary scientific risk is that nucleation of a hydrate phase is a rare event. However, the rewards will be substantial and the successful outcome of this project is a comprehensive molecular-level picture of heterogeneous hydrates. Extension to a macroscopic laboratory bench scale enables the rational design of catalysts and inhibitors for hydrate formation and stabilization in energy and fuel applications.

Determination of Aerosol Scattering Characteristics for Atmospheric Measurements

165669
Year 2 of 3
Principal Investigator: M. Arienti

Project Purpose:

The purpose of this project is to assess the radiative properties of realistic, non-ideal aerosols to support Sandia's role in developing optical remote-sensing technology (with reference, for instance, to the Atmospheric Radiation Measurement program in the Arctic). Improved aerosol scattering models are essential in establishing the effect of aerosols on albedo and cloud lifetime, which in turn are important elements of precipitation modeling. Optical remote sensing relies on simplified assumptions (on the dynamics of both individual particles and the airflow) that can impart large uncertainties on the retrieved properties.

Concluding the work from the first year, we have developed and published a four-channel polarization lidar concept for the detection of preferential orientation of atmospheric particulates. There is evidence of preferential orientation of aerosols (for instance, ice crystals) linked to their size and the local turbulence intensity. We have developed an optimum optical configuration for linear and circular polarized incident laser beams based on considerations of data inversion stability and propagation of measurement uncertainties: the theoretical accuracy in the retrieval of backscatter cross sections and depolarization ratios is similar to conventional two-channel configurations while, in addition, the bias due to particulate preferential orientation can be detected and corrected.

The study of the optical properties of ice crystals contaminated by soot (highly absorbing in the visible spectrum) was expanded this year, largely due to the adoption and development of a computer code for modeling composite scatterers of arbitrary shape. We have recovered the previously observed "lens effect," which magnifies the soot absorption cross section even in very small volume percentages, and we are examining the role of inclusion location in relation to the shape of the crystal. To validate these results, we have finalized an experiment for measuring under controlled conditions the optical properties of ice crystals nucleated on soot particles.

Appraisal of Hydraulic Fractures using Natural Tracers

165670
Year 2 of 3
Principal Investigator: J. E. Heath

Project Purpose:

We are developing new methodologies using in situ natural tracers to evaluate local-to-reservoir-scale hydraulic fracturing efficiency, with a focus on application to shale gas. Maximizing fracturing efficiency improves producible reservoir volumes and can mitigate risk to groundwater resources. Current fracture characterization by pressure transient or production analysis and other methods poorly constrains fracture connectivity and hydraulic properties in terms of the integrated impact of fractures on fluid flow. Key reservoir characteristics govern natural tracer release during fracturing, including: 1) the number, connectivity, and geometry of fractures, 2) the distribution of fracture-surface-area to matrix-block-volume, and 3) the nature of multiple fluid phases (e.g., methane dissolved in groundwater or present as a free gas phase). We will estimate fracture characteristics from breakthrough of multiple natural tracers sampled at the wellhead using multirate mass transfer theory (MMT). Favorable attributes include: 1) natural tracer concentrations that start with a well-defined initial condition, 2) a suite of tracers that cover a large range of diffusion coefficients, and 3) diffusive mass transfer out of the matrix into fractures that will cause elemental and isotopic fractionation, providing knowledge on the dominant mass transfer mechanism to the fracture system.

Natural tracers provide useful information in characterizing fracture surface area and transport velocities. However, existing techniques have never been applied in shale gas systems, nor have natural tracer studies considered MMT theory. Previous MMT studies use injected tracers instead of the ubiquitous natural tracers. The existence of multiple phases and the heterogeneity of the matrix in shale gas formations complicate tracer interpretation in these environments, increasing the risk for non-uniqueness of underlying fracture reservoir parameters generated through our improved breakthrough curve interpretation. By considering data from multiple naturally occurring tracers, our project aims to develop techniques for much improved fracture network and fluid flow characterization through data that can be easily collected at wellheads.

Polyfunctional Desorption of Oil from Shales

171069
Year 2 of 3
Principal Investigator: P. V. Brady

Project Purpose:

The purpose of this project is to identify the chemical controls over oil desorption from shales and tight sandstones so that oil recovery can be enhanced. Oil recovery from shales and tight sandstones is very low — 6-8% — compared to 50-80% recovery from traditional oil reservoirs. Part of the oil in shales and tight sandstones is physically occluded and will, therefore, likely never be extracted. But a substantial fraction of the oil is expected to be physically accessible, but chemically bound to the reservoir. By developing theoretical oil wettability maps onto shale and tight sandstone mineral surfaces, we are quantifying the chemical controls over oil adhesion. We are then testing oil-mineral adhesion maps experimentally in the laboratory. Our theoretical models of hydrocarbon adhesion are thus being refined. If successful, this effort should give us a far better understanding of oil-mineral interaction in shales and tight sandstones, and might point to more effective fracking fluids and waterflooding methodologies. This is high risk because chemical adhesion/wettability and waterflooding of shales is in its infancy. Our work has a potentially high R&D return because any improvement in the science of shale oil adhesion that results in improved recovery could have a very large impact over the total amount of shale oil produced in the US.

Detecting Seasonal Changes in Permafrost using in situ Seismic Velocities, Near-Field Soil Moisture Monitoring, and Remote Sensing

171381
Year 2 of 3
Principal Investigator: R. Abbott

Project Purpose:

The Arctic is important to Earth's climate system. In 2012, Arctic sea ice retreated the furthest in recorded history, opening the Arctic to commerce, resource exploration, and national security threats. The melting of Arctic ice also increases sea surface temperatures, which then leads to increased storm severity around the globe. The melting of permafrost releases methane, which has been locked in the frozen layers, potentially causing further increases in Earth's temperature.

Current climate models do not have sufficient data to accurately predict the impact these factors will have on climate. The Arctic is not a homogeneous area in terms of precipitation, depth to permafrost, distance from the sea, etc. Therefore, data need to be collected from a variety of areas (coastal, inland, high and low precipitation, etc.). To effectively capture these data, remote sensing methods that can collect accurate data over multiple scales are needed. These methods do not currently exist. Similarly, precipitation in the Arctic is difficult to measure. Differentiating between snow that is falling vs. snow that is being moved by the wind is essential for accurate water balances but difficult to achieve in practice.

This project will apply recent advances in seismic research and soil moisture monitoring to the Arctic for the first time. The data from those efforts will be coupled with remote sensing data originally collected for national security purposes to determine if remote methods can be used to accurately collect data for use in climate models. Although Sandia has performed research in each of these areas in the past, this will be the first time that we will apply them to the climate arena. Since none of these techniques have been deployed in the Arctic, there is a high level of risk for the project. Results from this effort will contribute to a DOE Office of Science goal of improved understanding of Arctic water budgets.

Monitoring, Understanding, and Predicting the Growth of Methane Emissions in the Arctic

173100
Year 1 of 3
Principal Investigator: H. A. Michelsen

Project Purpose:

Concern over Arctic methane (CH_4) emissions has increased following recent discoveries of poorly understood sources and predictions that methane emissions from known sources will grow as Arctic temperatures increase. Methane has a 25-fold higher global warming potential than CO_2 and is believed to cause ~50% of the net radiative forcing of CO_2. The calculated capacity of the warming Arctic to produce methane is enormous, and the warming effect of CH_4 could surpass that of CO_2. Methane sources predicted to increase include: thawing terrestrial permafrost, shallow oceanic methane hydrates, and submerged permafrost. Recent studies revealed an unexplained methane source associated with cracks in sea ice and a potentially important open ocean source. A few incomplete datasets are available to study Arctic methane emissions, and new efforts are required to detect increases and explain sources without being confounded by the multiple sources. Methods for distinguishing different sources are critical. We plan to conduct measurements of atmospheric methane and source tracers and couple these measurements with global atmospheric modeling and back-trajectory analysis to identify, characterize, and assess the climate impact of Arctic methane sources. The unique data and analysis will address a timely and high-profile scientific question. Understanding Arctic methane sources will help inform decisions related to human activity (such as oil and gas exploration) at high latitudes.

We will address uncertainties in Arctic methane sources and their potential impact on climate. We will characterize methane sources using high-resolution atmospheric chemical transport models and tracer measurements and will model the Arctic climate using the state-of-the-art high-resolution Spectral Element Community Atmosphere Model (CAM-SE) developed at Sandia. We propose leveraging the Sandia-managed atmospheric research station in Barrow, Alaska to deploy newly developed trace gas analyzers. This project incorporates inherent risk associated with the uncertainties in the novel use of tracers and the complexity of inversions on multiple tracers in the Arctic.

Technology for Subsurface Imaging with Backscattered Muons

173101
Year 1 of 2
Principal Investigator: N. Bonal

Project Purpose:

The purpose of this project is to develop subsurface imaging using upgoing muons. Subsurface imaging of underground structures, such as tunnels and caverns, is important to Sandia's missions of energy surety, nonproliferation, and border and infrastructure security. Muons are subatomic particles produced in the upper atmosphere, which penetrate Earth's crust up to a few kilometers. Their absorption rate depends on the density of the materials including fluids through which they pass. Measurements of muon flux rate at differing directions provide density variations of the materials between the sky and detector from those directions, much like a CAT scan. Traditional muon imaging focuses on more prevalent downgoing muons, but requires below-target detectors — a major obstacle to widespread use. Exploratory work in FY 2014 demonstrated that upgoing muon fluxes appear sufficient to achieve target detection. In FY 2015 and FY 2016, we plan to eliminate noise from downgoing muons by adding scintillator to the drift tube detector to determine muon directionality. Currently, muon tomography can resolve features to the sub-meter scale. However, their practical use is uncertain due to dependencies among resolution, duration of acquisition, density contrast, size of the target, and distance between target and detector remain undefined. To widen the performance envelope of the approach, 3D earth structural variations, integration time, size of target, distance from target, and density contrast of targets with surrounding material will be constrained through a combination of modeling and experimental verification.

Fundamental Study of Disposition and Release of Methane in a Shale Gas Reservoir

173102
Year 1 of 3
Principal Investigator: Y. Wang

Project Purpose:

The boom in shale gas production through hydrofracturing may reshape the energy production landscape in the US. However, one troubling issue related to shale gas extraction is the decline in wellbore production by up to 95% over the first three years with a recovery rate less than 10%. Maximizing wellbore production and extending the production life cycle are crucial to realize the energy security benefits of shale gas. This effort has been hindered by a lack of mechanistic understanding of gas disposition and release in shale gas reservoirs. Existing knowledge drawn from conventional gas-oil reservoirs is not applicable to shale formations characterized by nanometer-scale pore sizes and extremely low permeability. Gas in shale (mainly methane) exists as a compressed gaseous phase or an adsorbed phase in nanopores, with the latter accounting for up to 85% of total gas in place (GIP). We will perform an integrated experimental and modeling study to fundamentally understand two important processes that directly control GIP in a reservoir and wellbore production: methane partitioning in the nanopores of mudstone matrices and methane transport from low-permeability matrices to fractures. We will first carefully characterize pore geometry and pore-size distributions of representative shale samples. We will then measure methane sorption isotherms, desorption kinetics, and transport properties on selected shale samples, either crushed or intact, under simulated reservoir conditions, using our newly developed high temperature/high pressure (HTHP) systems and microanalysis techniques. The data will be synthesized, using novel nanogeochemistry and nanofluidics concepts and molecular dynamic simulations to establish needed constitutive relationships for predicting and optimizing shale gas wellbore production. The project will leverage Sandia's unique expertise in material science, nanogeochemistry, HTHP geochemistry, and high-performance computation capability. If successful, this work will position Sandia at the forefront of shale gas study and greatly expand Sandia's research footprint in nanogeoscience as well as prediction of material behaviors in extreme environments.

Predicting the Occurrence of Mixed Mode Failure Associated with Hydraulic Fracturing

173662
Year 1 of 3
Principal Investigator: S. J. Bauer

Project Purpose:

The objective of this study is to understand the nature of the extension to shear fracture transition in fine-grained unconventional reservoir rocks and develop a universal failure criterion that is scalable by easily measured rock properties such as tensile strength, uniaxial compressive strength, porosity, grain size, and composition. Using these properties and the in situ reservoir stress state, the failure criterion can be combined with fracture mechanics to predict the mode of off-crack failure, fracture orientation, and small-scale damage likely to occur during hydraulic fracturing.

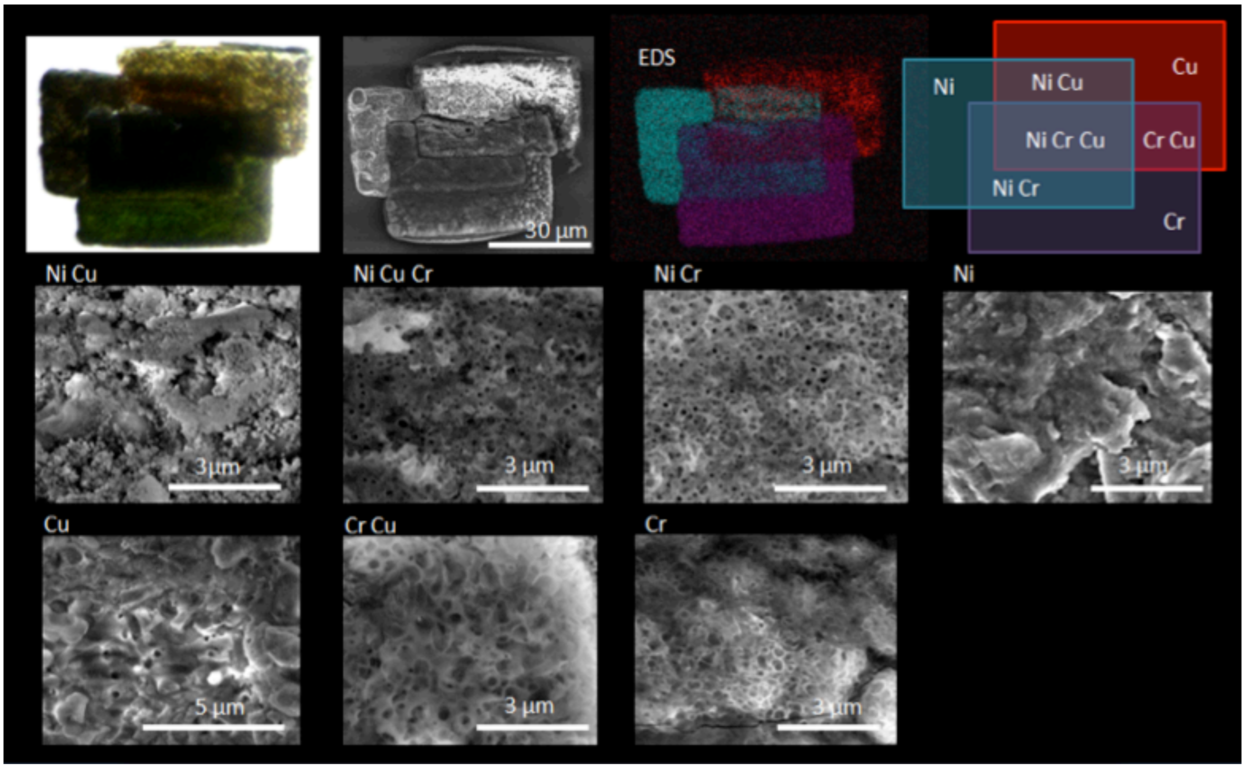
Development of multi-physics models validated by sophisticated experiments and observations presents a significant technical challenge; the complexity and integration of this approach to develop a universal failure criteria provides the framework for this effort and will be used to develop a physics-based understanding/ assessment of the rock failure process.

Sandia's unique high-pressure geomechanics laboratory capabilities will be used to explore fundamental physical processes encountered during the fracture process. The integrated experiment/observation/analysis approach will lay the foundation for improved understandings of the flow and transport in rock in response to stimulation, leading to increase production and recovery from these resources. This work is in collaboration with Texas A&M University.

The work completed, thus far, includes successful completion of 24 triaxial extension experiments on three lithologies of sedimentary rock. The lithologies represent a range of material ductility. The results of these tests will be used to develop a new failure criteria at the low mean stress conditions studied. The failure criteria will be applied to evaluate fracture propagation during hydrofracture.

MATERIALS SCIENCE

R&D sponsored by the Materials Science Investment Area strives to *discover* new phenomena, to *create* new classes of materials with novel synthesis techniques and processing approaches, and to *understand and control* materials' structures and properties. The goal is to foster a bold, vibrant, ground breaking, materials science base of world-renown, which serves as the foundation for developing the critical and differentiating technical capabilities that will be needed in the future to support our national security missions.



Optical (top left), scanning electron microscopy, and energy-dispersive x-ray spectroscopy (top right) images of a fully iterated and spatially patterned, three element alloy system. The development of nanoscale alloys with arbitrary form and controlled composition requires novel material syntheses and manufacturing procedures. New chemical strategies will enable engineering materials with greater compatibility for high resolution, laser-driven 3D manufacturing. (Project 164677)

MATERIALS SCIENCE

In Situ Study of Dynamic Phenomena at Metal Nanosolder Interfaces using Aberration-Corrected Scanning Transmission Electron Microscopy

158822
Year 3 of 3
Principal Investigator: P. Lu

Project Purpose:

Controlling metallic nanoparticle (NP) interactions plays a vital role in the development of new joining techniques (nanosolder) that bond at lower processing temperatures but remain viable at higher temperatures. The primary objective of this project is to develop a fundamental understanding of the actual reaction processes, associated atomic mechanisms, and the resulting microstructure that occur during thermally driven bond formation concerning metal-metal nanoscale (<50 nm) interfaces.

In this project, we have studied metallic NPs interaction at the elevated temperatures by combining in situ transmission electron microscopy (TEM) using an aberration-corrected scanning transmission electron microscope (AC-STEM) and atomic scale modeling such as molecular dynamic (MD) simulations. Various metallic NPs such as silver, copper, and gold (Ag, Cu, and Au, respectively) are synthesized by chemical routines. Numerous in situ experiments were carried out with focus of the research on study of the Ag-Cu system. For the first time — using in situ STEM heating experiments — we directly observed the formation of a 3D epitaxial Cu-Ag core-shell nanoparticle during the thermal interaction of Cu and Ag NPs at elevated temperatures (150 - 300 °C). The reaction takes place at temperatures as low as 150 °C and was only observed when care was taken to circumvent the effects of electron beam irradiation during STEM imaging. Atomic scale modeling verified that the Cu-Ag core-shell structure is energetically favored, and indicated that this phenomenon is a nanoscale effect related to the large surface-to-volume ratio of the NPs. The observation potentially can be used for developing new nanosolder technology that uses Ag shell as the “glue” that sticks the particles of Cu together.

Summary of Accomplishments:

We have successfully synthesized various metallic NPs such as Ag, Cu, and Au using chemical routes, and carried out numerous in situ experiments. In particular, experimental efforts on Ag-Cu systems have led to discovery of formation of the core-shell Ag/Cu structure at reaction temperatures as low as 150 °C. Molecular dynamics (MD) and Monte Carlo (MC) models indicated that the core-shell structure is thermodynamically preferred and is a nanoscale effect related to the large surface-to-volume ratio of the NPs. These observations potentially can be used for developing new nanosolder technology that uses Ag shell as the “glue” that sticks the particles of Cu together.

Significance:

The technical outcomes of this project have led to several new projects, impacting our national security mission. The modeling work throughout the project has led to further development of the modeling tool, a phase-field model that can used to simulate the reaction of the nanoscale alloys at high temperatures. In addition, we have developed new TEM characterization techniques and a phase-field modeling tool that can be used for future materials research at Sandia.

Establishing a fundamental understanding of specific interfacial mechanisms in new metal/metal NP bonding processes is critical to basic science and will enable development of next-generation solders critical to many mission-relevant technologies. The realization of low-melting temperature metallic nanosolders could eliminate concerns with product processing, product reliability, and manufacturing changes introduced with conventional solders. Success in achieving these goals will further strengthen Sandia's leadership position in the research, development, and applications of advanced materials.

Refereed Communications:

M. Chandross, "Bonding of Metallic Nanoparticles," presented at the *TMS 2014: Annual Meeting and Exhibition*, San Diego, CA, 2014.

M. Chandross, "Bonding of Metallic Nanoparticles," presented (keynote) at the *Second International Conference on Metallic Materials and Processing*, Las Vegas, NV, 2014.

P. Lu, M. Chandross, T.J. Boyle, B.G. Clark, and P. Vianco, "Equilibrium Cu-Ag Nanoalloy Structure Formation Revealed by In Situ Scanning Transmission Electron Microscopy Heating Experiments," *APL Materials*, vol. 2, p. 22107, 2014.

P. Lu, T.J. Boyle, B.G. Clark, and M. Chandross, "In Situ TEM Study of Cu and Ag Nanoparticle Interaction," *Microscopy and Microanalysis*, vol. 19, pp. 448-449, August 2013.

P. Lu, et al., "In Situ TEM Study of Cu-Ag Nanoparticle Thermal Interaction," presented at the *25th Rio Grande Symposium on Advanced Materials*, Albuquerque, NM, 2013.

P. Lu, J. Xiong, M. Van Benthem, and Q. Jia, "Atomic-Scale Chemical Quantification of Oxide Interfaces using AC-STEM EDS," presented (invited) at the *Materials Science and Technology,* Montreal, Quebec, Canada, 2013.

P. Lu, E. Romero, S. Lee, J. L. MacManus-Driscoll, and Q. Jia, "Chemical Quantification of Atomic-Scale EDS Maps under Thin Specimen Conditions," to be published in *Microscopy and Microanalysis*.

M. Chandross, "Energetics of the Formation of Cu-Ag Core-Shell Nanoparticles," to be published in *Modeling and Simulation in Materials Science and Engineering*.

P. Lu, L. Zhou, M.J. Kramer, and D.J. Smith, "Atomic-Scale Chemical Imaging and Quantification of Metallic Alloy Structures by Energy-Dispersive X-Ray Spectroscopy," *Scientific Reports*, vol. 4, p. 3945, February 2014.

P. Lu, J. Xiong, M. Van Benthem, and Q. Jia, "Chemical Quantification of Atomic- Scale EDS Maps under Thin Specimen Conditions," *Microscopy and Microanalysis*, vol. 19, pp. 1298-1299, August 2013.

Deciphering Adsorption Structure on Insulators at the Atomic Scale

158823
Year 3 of 3
Principal Investigator: K. Thüermer

Project Purpose:

Whether to understand ice nucleation in clouds, lubricant degradation in micromachines, or aqueous electrochemical kinetics, one wants a molecular-level knowledge of water-solid interactions. Water behavior at interfaces has, therefore, been the subject of hundreds of studies. Still, even the simplest issue, the structure of the first water layer on a solid surface, has been hard to resolve. For three decades, low temperature, 2D wetting layers on close-packed precious metal surfaces were thought to be "ice like" arrangements of water molecules, strained into registry. In the past year, via scanning tunneling microscopy (STM) and density functional theory (DFT)-supported interpretation, we overturned that idea, discovering the remarkably non-ice-like molecular arrangement adopted by water on a platinum surface, Pt(111). That success offers the prospect of understanding how water binds to the more stable materials: oxides, sulfides, and salts, of which the world is largely comprised. The obstacle is that these materials are generally insulators, for which high-resolution microscopic techniques have been unavailable. Molecular-scale images were indispensable to solving the Pt(111) wetting-layer structure. We can expect that high-resolution imaging will be equally important to understanding water on the more common materials.

By exploiting an atomic force microscopy (AFM) breakthrough, we aim to be the first to perform atomic-resolution studies of adsorbates on insulating surfaces relevant to environmental and technological processes bearing on national needs. Unprecedented resolution has been achieved with a novel tuning fork type sensor known as "Q-plus." Proof-of-principle of the Q-plus technique, atomic-resolution AFM of an adsorbed pentacene molecule, suggests breakthrough possibilities for molecules on oxides, assuming the technique proves robust enough; the risk, to provide similarly high resolution images of delicately bonded, adsorbed water. Our first goals are the wetting of muscovite and kaolinite, oxides ubiquitous in nature, implicated as cloud-seed materials, and subjects of many experimental and theoretical studies with no definitive conclusions. We will attempt to decipher adsorbed water-molecule arrangements by combining atomic-level imaging with DFT-based interpretation.

Summary of Accomplishments:

To allow experiments on insulators, we added a previously purchased Q-plus AFM module to our existing STM. Since our microscope was the first retrofitted system, there were various hardware and software problems initially preventing operation. Through extensive testing and debugging, we eliminated all these problems. Establishing AFM's capability to routinely resolve molecular steps on ice surfaces (nobody had done this before), positioned us to examine growth morphology of thick ice films beyond the reach of STM.

Our AFM experiments revealed that thicker films grow via double spirals around screw dislocations with a double burgers vector, a mechanism that explains the nucleation-free formation of hexagonal ice at low temperature. These AFM experiments combined with earlier STM experiments yield a comprehensive picture of the thickness-dependent growth of ice films at low temperature. We learned that the crystal structure of ice deposited at low temperatures onto Pt switches twice as films grow thicker. Isolated 3D clusters grow via layer nucleation as hexagonal ice. Following coalescence, cubic ice is produced in growth spirals created by screw dislocations above substrate steps. Eventually, at larger thickness, double spirals become dominant, causing the preferential formation of hexagonal ice.

The DFT effort focused on finding the lowest-energy configuration of the one-molecule thick wetting layer of water on muscovite (mica). We discovered that wetting is controlled by how exactly a water layer wraps around the K^+ ions protruding from the mica surface. Tightly bound structures have lower water coverage, allowing K atoms to be embedded and hydrated. We learned the importance of optimizing H-bonds also between water and substrate O atoms.

DFT also sheds light on the experimentally observed sensitivity of the mica surface to preparation conditions: K atoms can easily be rinsed off by water flowing past the mica surface, consistent with our AFM experiments on ice/mica.

Significance:

Availability of adequate pure water is a vital homeland security interest; thus, we need to understand, at the molecular scale, ice nucleation on cloud-seed materials, and interactions between flowing water and minerals. In this project we improved on the "state of the art" of examining the formation of the two ice phases that occur at atmospheric pressure by introducing Q-plus AFM into ice research. Our DFT work improved on the previous state of our understanding of wetting of the "classic geoscience system," muscovite mica. Sandia is now much better positioned to examine delicate insulator surfaces at a molecular-layer level.

Refereed Communications:

K. Thürmer, "Nucleation and Growth of Ice Films on Metal Surfaces," presented at the *ACS National Meeting and Exposition*, San Francisco, CA, 2014.

P.J. Feibelman, "K^+ Hydration in a Low-Energy, Two-Dimensional Wetting Layer on the Basal Surface of Muscovite," *The Journal of Chemical Physics*, vol. 139, p. 075705, 2013.

K. Thürmer and S. Nie, "Formation of Hexagonal and Cubic Ice during Low-Temperature Growth," in *Proceedings of the National Academy of Sciences*, pp. 11757-11762, 2013.

K. Thürmer, "Nucleation and Growth of Ice Films on Metal Surfaces," presented at the *CECAM Workshop*, Zurich, Switzerland, 2014.

Crystalline Nanoporous Frameworks: a Nanolaboratory for Probing Excitonic Device Concepts

158825
Year 3 of 3
Principal Investigator: M. D. Allendorf

Project Purpose:

Electro-optical organic materials hold great promise for the development of high-efficiency devices based on exciton formation and dissociation, such as organic photovoltaics (OPV) and organic light-emitting devices (OLEDs). However, the external quantum efficiency (EQE) of both OPV and OLEDs must be improved to make these technologies economical. Efficiency rolloff in OLEDs and inability to control morphology at key OPV interfaces both reduce EQE. Only by creating materials that allow manipulation and control of the intimate assembly and communication between various nanoscale excitonic components can we hope to first understand and then engineer the system to allow these materials to reach their potential. The aims of this project are to: 1) develop a paradigm-changing platform for probing excitonic processes composed of crystalline nanoporous frameworks (CNFs) infiltrated with secondary materials (such as a complementary semiconductor), 2) use them to probe fundamental aspects of excitonic processes, and 3) synthesize prototype OPVs and OLEDs using infiltrated CNF as active device components. These functional platforms will allow detailed control of key interactions at the nanoscale, overcoming the disorder and limited synthetic control inherent in conventional organic materials. CNFs are revolutionary inorganic-organic hybrid materials boasting unmatched synthetic flexibility that allow tuning of chemical, geometric, electrical, and light absorption/generation properties. For example, bandgap engineering is feasible and polyaromatic linkers provide tunable photon antennae; rigid 1-5 nm pores provide an oriented, intimate host for triplet emitters (to improve light emission in OLEDs) or secondary semiconducting polymers (creating a charge-separation interface in OPV). These atomically engineered, ordered structures would enable critical fundamental questions to be answered concerning charge transport, nanoscale interfaces, and exciton behavior that are inaccessible in disordered systems. Implementing this concept also creates entirely new dimensions for device fabrication that could improve performance, increase durability, and reduce costs with unprecedented control of over properties.

Summary of Accomplishments:

Our multidisciplinary team has combined theory, synthetic chemistry, and advanced diagnostics to understand critical energy transfer processes in highly organized supramolecular CNFs. Novel CNFs and CNF composite materials were developed and synthesized, enabling the investigation of light harvesting and energy transfer in a metal-organic framework (MOF) infiltrated with donor and acceptor molecules of the type typically used in organic photovoltaic devices (thiophenes and fullerenes, respectively). Synthetic efforts included not only traditional solvothermal approaches, but also innovation of custom “layer-by-layer” CNF syntheses that afford exceptional control over CNF structure and chemistry during surface-based CNF growth. The results show that CNFs can provide multiple functions: as a light harvester, as a stabilizer and organizer or the infiltrated molecules, and as a facilitator of energy transfer. The infiltration concept was used to study optoelectronic phenomena for excitonic materials, but also led to the discovery of an electrically conducting composite framework. The tailorability and high conductivity of this material are unprecedented and spawning several provisional technical advances. Computational design of CNF linker groups informed the development of new linker molecules capable of both visible light harvesting and charge separation and transport. The predictions were validated by ultraviolet-visible absorption spectroscopy, demonstrating that rational design of CNFs for light-harvesting purposes is feasible. Finally, we incorporated tailored CNFs into a variety of photovoltaic device configurations, most notably dye-sensitized solar cells (DSSCs). Results suggest that CNF thin films can be used as the active absorbing element in a sensitizer in a DSSC, supporting the idea that CNFs can serve as active layers in excitonic devices. Overall, this project provides several crucial proofs-of-concept demonstrations of the potential applicability of CNFs in optoelectronic devices.

Significance:

This research focused on the development of technologies associated with energy transfer, with most significant potential impact to renewable energy production (photovoltaics) and low cost lighting (light-emitting diodes), which are both nationally and globally vital technical priorities. Research performed has contributed to the understanding of new molecular and nanoscale processes associated with energy transfer, central to these technologies.

Refereed Communications:

K. Leong, M.E. Foster, B.M. Wong, E.D. Spoerke, D.V. Gough, J.C. Deaton, and M.D. Allendorf, "Energy and Charge Transfer by Donor-Acceptors Pairs Confined in a Metal-Organic Framework: A Spectroscopic and Computational Investigation," *Journal of Materials Chemistry A*, vol. 2, pp. 3389-3398, January 2014.

D.V. Gough, T.N. Lambert, D.R. Wheeler, M.A. Rodriguez, M.T. Brumbach, M.D. Allendorf, and E.D. Spoerke, "Controlled Nucleation and Growth of Pillared Paddlewheel Framework Nanostacks onto Chemically Modified Surfaces," *ACS Applied Materials and Interfaces*, vol. 6, pp.1509-1514, February 2014.

K. Leong, M.E. Foster, B.M. Wong, E.D. Spoerke, D.V. Gough, J.C. Deaton, and M.D. Allendorf, "Nano-Ordering of Donor-Acceptor Interactions using Metal-Organic Frameworks as Scaffolds," *Photovoltaics for the 21st Century 9, ECS Transactions*, vol. 58, pp. 21-28, 2013.

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V. Stavila, A.A. Talin, and M.D. Allendorf, "MOF-Based Electronic and Opto-Electronic Devices," *Chemical Society Reviews*, vol. 43, pp. 5994-6010, May 2014.

M.D. Allendorf, "Emergent Properties using the Guest@MOF Concept," presented (invited) at the *Metal-Organic Frameworks: Experiments and Simulations*, Telluride, CO, July 2014.

A.A. Talin, M.E. Foster, V. Stavila, A. Ford, F. El Gabaly, F. Léonard, and M.D. Allendorf, "Molecule@MOF: A New Class of Electronic Materials," presented (invited) at the *Fall Electrochemical Society Meeting*, Cancun, Mexico, 2014.

A.A. Talin, A. Centrone, P. Haney, V. Stavila, A.C. Ford, M.E. Foster, R A. Kinney, V. Szalai, H.P. Yoon, F. Léonard, and M.D. Allendorf, "Tunable Electrical Conductivity in Metal-Organic Framework Thin Film Devices," *Science*, vol. 343, pp. 66-69, January 2014.

M.D. Allendorf, A.A. Talin, J.A. Greathouse, T.N. Lambert, E.D. Spoerke, V. Stavila, and B.M. Wong, "The Power of Empty Space: Metal-Organic Frameworks as Electronic Materials," keynote lecture at *EuroMat*, Seville, Spain, 2013.

M.D. Allendorf, “Pleasures and Pitfalls of Guest Molecules in MOFs,” presented (invited) at the *Characterization of Nanoporous Materials Workshop*, Stanford, CA, 2014.

M.D. Allendorf, “Nanoporosity and the Welcome Guest: Metal-Organic Frameworks as Active Components of Electronic Devices,” presented (invited) at the *ACS Fall 2014 Meeting*, San Francisco, CA, 2014.

M.D. Allendorf, A.A. Talin, M.E. Foster, V. Stavila, and F. Léonard, “Molecule Meets MOF: Bridging the Gap between Organic and Inorganic Electronic Materials,” presented (invited) at the *SPIE Optics + Photonics Conference*, San Diego, CA, 2014.

E.D. Spoerke, J.S. Wheeler, S. Wolf, D.V. Gough, M.E. Foster, K. Leong-Hau, V. Stavila, T.N. Lambert, and M.D. Allendorf, “Optoelectronic ‘Tinker Toys’: Supramolecular Nanocomposite Frameworks for Next Generation Photovoltaics,” presented at *Composites at Lake Louise-2013*, Lake Louise, Alberta, Canada, 2013.

Understanding Tantalum Oxide Memristors: An Atoms-Up Approach

158828
Year 3 of 3
Principal Investigator: M. Marinella

Project Purpose:

Dynamic random access memory (DRAM) and flash memory technologies are nearing physical scaling limits and are starting to require significant switching energy compared to other components of modern computing systems. An International Technology Roadmap for Semiconductors (ITRS) report has determined that memristive (also referred to as redox) memory is one of the two most promising new memory technologies due to its unprecedented scalability, speed, pJ/bit switching energy, endurance, and retention and has recommended that it receive increased research focus. Government customers have already invested in memristor technology for neuromorphic computing and as a rad-hard memory. However, current state-of-the-art memristors continue to exhibit serious uniformity and reliability problems; for example, resistances can vary by several orders of magnitude for devices within the same array. Industry is using Edisonian approaches to these problems, resulting in slow, incremental progress. The physical mechanisms enabling switching between high and low resistance states is thought to involve the motion of oxygen vacancies in a region that is only tens of nanometers thick. However, we still cannot definitively answer the question – What is moving where, and how? Thus, the central scientific problem is to identify the physical and chemical changes responsible for resistive switching. This will enable us to engineer reliable devices with predictable electrical behavior. Memristors present Sandia with a time-sensitive opportunity to achieve this understanding and significantly advance the field of microelectronics as a whole, while enabling important government applications.

Industry has favored trial and error experimental approaches that often result in minor, incremental improvements. We will implement a scientific approach using novel lateral structures to perform a set of linked experiments that results in a physical model of memristor switching. A comprehensive scientific model of this phenomenon will result in a groundbreaking advancement of this technology, relevant to both commercial and government applications.

Summary of Accomplishments:

We made notable progress in our ability to fabricate and characterize tantalum oxide switching films and device structures, and gained an understanding of the electrical and thermal behavior as expressed through new models. The most significant accomplishments are summarized in the following:

1) We developed a technique to fabricate films of a specific tantalum oxide stoichiometry required for optimal switching, despite the tendency of the tantalum oxide system to favor Ta_2O_5 (TaO_2 is favored for switching).
2) We created a novel, ultra-thin film stoichiometry characterization technique known as Rutherford forward scattering and elastic recoil detection.
3) We developed an x-ray photoelectron spectroscopy (XPS) characterization method to separate the states of Ta^{1+} through Ta^{5+} in a TaO_x switching film. This led to the discovery that films with identical stoichiometries may be made up of different configurations of Ta oxidation states, and that Ta^{4+} gave exceptional switching behavior.
4) An analytical model of both SET and RESET switching was derived by solving the Fourier equation for the cylindrical filament, which very closely fit the observed electrical results. This led to the discovery that TaO_x memristors have two state variables, conductivity and switching filament radius, responsible for switching, and multiple configurations can give a particular resistance.

5) The first major study of the effect of displacement damage due to heavy ions, and total ionizing dose due to x-ray and protons was produced. This has spurred significant work in the worldwide research community and significant interest in TaO_x memristors as a radiation hardened memory.
6) Nanoscale TaO_x memristors were switched in situ, in Sandia's aberration-corrected scanning transmission electronic microscope (AC-STEM), and high resolution spatial maps of electron electron energy loss spectroscopy (EELS) spectra were taken the device states. These recent results are suggesting that the standard model of resistive switching in TaO_x may not apply in key resistance ranges.

Significance:

This project has put Sandia at the forefront in bipolar metal oxide memristor research and allowed us to advance the scientific frontier of this topic — a field, which has gained significant attention since this project started. Fabrication and characterization of subtle aspects of memristors films, and our understanding of the multi-state electrical behavior will allow us to make devices that are ideal for brain inspired computing. The pioneering work on radiation effects on TaO_x devices, done in this project, helped inform and spawn a subsequent project to create a radiation hardened memristor memory.

Refereed Communications:

M.J. Marinella, P.R. Mickel, A.J. Lohn, D.R. Hughart, R. Bondi, D. Mamaluy, H.P. Hjalmarson, J.E. Stevens, S. Decker, R.T. Apodaca, B. Evans, J.B. Aimone, F. Rothganger, C.D. James, and E.P. DeBenedictis, "Development, Characterization, and Modeling of a TaO_x ReRAM for a Neuromorphic Accelerator," to be published in *Trans ECS 2014*.

M. Brumbach, P.R. Mickel, A.J. Lohn, A.J. Mirabal, M.A. Kalan, J.E. Stevens, and M.J. Marinella, "Evaluating Tantalum Oxide Stoichiometry and Oxidation States for Optimal Memristor Performance," *Journal of Vacuum Science and Technology A*, vol. 32, p. 051403, 2014.

P.R. Mickel, A.J. Lohn, C.D. James, and M.J. Marinella, "Isothermal Switching and Detailed Filament Evolution in Memristive Systems," *Advanced Materials*, vol. 26, pp. 4486-4490, 2014.

M.J. Marinella, "Emerging Resistive Switching Memory Technologies: Overview and Current Status," in *Proceedings of the IEEE International Symposium, Circuits and Systems*, pp. 830-833, 2014.

P.R. Mickel, A.J. Lohn, and M.J. Marinella, "Memristive Switching: Physical Mechanisms and Applications," *Modern Physics Letters B*, vol. 28, p. 1430003, 2014.

D.R. Hughart, A.J. Lohn, P.R. Mickel, S.M. Dalton, P.E. Dodd, M.R. Shaneyfelt, A.I. Silva, E. Bielejec, G. Vizkelethy, M.T. Marshall, M.L. McLain, and M.J. Marinella, "A Comparison of the Radiation Response of TaO_x and TiO_2 Memristors," *IEEE Transactions on Nuclear Science*, vol. 60, pp. 4512-4519, December 2013.

J.E. Stevens, A.J. Lohn, S.A. Decker, B.L. Doyle, P.R. Mickel, and M.J. Marinella, "Reactive Sputtering of Substoichiometric $Ta2O_x$ for Resistive Memory Applications," *Journal of Vacuum Science and Technology A*, vol. 32, p. 021501, 2014.

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A.J. Lohn, P.R. Mickel, and M.J. Marinella, "Analytical Estimations for Thermal Crosstalk, Retention, and Scaling Limits in Filamentary Resistive Memory," *Journal of Applied Physics*, vol. 115, p. 234507, 2014.

Understanding and Exploiting Bilayer Graphene for Electronics and Optoelectronics

158829
Year 3 of 3
Principal Investigator: S. W. Howell

Project Purpose:

Bilayer graphene (BLG) offers advantages that its more common form, monolayer, does not. Most prominently, a dynamic, "tunable" bandgap can be readily induced in BLG using electrical fields. Understanding this tunability presents a significant scientific challenge that could enable new, potentially disruptive, graphene devices, as is envisioned by the latest International Roadmap for Semiconductors. A lack of fundamental understanding, however, has limited the realization of advanced BLG devices. For example, graphene's electronic properties are exceptionally sensitive to the materials surrounding it in a device. Additionally, there is limited understanding of the factors determining the magnitude and uniformity of the induced bandgap. In response, this project leverages our capabilities in BLG synthesis, characterization, device fabrication, and modeling in order to fundamentally understand BLG properties, thereby providing a scientific foundation for future graphene electronics and optoelectronics.

This project aims to: 1) understand the interaction between BLG's 2D charge carriers and the metals/dielectrics intrinsic to device integration, 2) understand the many-body electronic and optical properties of the system, and 3) demonstrate a gated BLG device having the potential for disruptive capabilities in electronics and as an infrared detector. The project operates with the belief that BLG is the best platform to study these phenomena and has the greatest promise to fully leverage graphene's inherent advantages. Most importantly, BLG exhibits a tunable bandgap when exposed to a transverse electric field. There has been no definitive realization of scalable BLG devices, however, due to the limited availability of the material itself and an incomplete understanding of how integration processes alter graphene's properties. Utilizing our differentiating competency to produce large area, high-quality, BLG combined with our ability to fabricate, characterize, and model these structures, we are uniquely positioned to address these problems and establish Sandia as the "go to" national resource for graphene nanoelectronics.

Summary of Accomplishments:

1) We continued the development of a scalable fabrication process to fabricate dual-gated bilayer graphene field effect transistors (BLG-FETs). We combined large-area BLG synthesis, on semi-insulating silicon carbide (SiC), with advanced ion implantation to create a scalable approach for forming a bottom gate within the SiC. Similar to that employed in silicon processing, ion implantation can be utilized to create a conductive channel within the SiC. The conductive channel may then serve as the contact for the bottom gate of an epitaxial graphene device.
2) We demonstrated dual-gated BLG-FET operation, the first demonstrations using this scalable fabrication approach. Our group was the first to create dual-gated graphene devices using such an approach showing: 1) the approach's feasibility and 2) that incomplete activation of the ion-implanted dopants can reduce the capability of the back gate by over 2 times.
3) We observed an increase in domain size and quality when O2 is used during graphene chemical vapor deposition (CVD) growth, an important step towards large-scale economic production of electronic-grade graphene.

Significance:

The development of a critical scientific understanding of the interaction between graphene layers enables the production of "designer" 2D crystal systems with novel device properties. The development of a dual-gated device architecture, that can tune the electronic properties of BLG in real time and is scalable for mass production, enables new reconfigurable electronic and optoelectronic device concepts. The scientific understanding of large-area CVD graphene growth enables routes to economic production of electronic-grade graphene for potential commercial and national security applications.

Refereed Communications:

S.W. Howell, et al., "Continued Development of Dual-Gated Bilayer Graphene Device Structures," presented at the *SPIE NanoScience and Engineering*, San Diego, CA, 2014.

T. Ohta, "Electronic Dispersion in Two Overlapping Graphene Sheets: Impacts of Long-Range Atomic Ordering and Periodic Potentials," presented at the *9th International Symposium on Atomic Level Characterizations for New Materials and Devices*, Kona, HI, 2013.

T.E. Beechem, T. Ohta, B. Diaconescu, and J.T. Robinson, "Rotational Disorder in Twisted Bilayer Graphene," *ACS Nano*, vol. 8, pp. 1655-1663, January 2014.

T. Ohta, "Electronic Dispersion from Long-Range Atomic Ordering and Periodic Potentials in Two Overlapping Graphene Sheets," presented at the *60th Annual AVS International Symposium and Exhibition*, Long Beach, CA, 2013.

Y. Hao, et al., "The Role of Surface Oxygen in the Growth of Large Single-Crystal Graphene on Copper," *Science 8*, vol. 342, pp. 720-723, November 2013.

Alloys and Composites for Strong and Tough Freeform Nanomaterials

164677
Year 3 of 3
Principal Investigator: B. J. Kaehr

Project Purpose:

The pursuit of nanotechnologies has largely focused on the physics and chemistry of low dimensional materials and their potential impact on areas such as electronics, catalysis, and medicine. However, a crucial class of materials remains largely unexplored at the smallest scales, namely alloys and composites that dominate modern manufacturing for mechanically robust (macroscopic) structures and devices. Of critical importance is the ability to manufacture 'freeform' 3D designs and shapes using techniques such as casting.

The question arises: can engineered materials with freeform shapes be fabricated at nanoscales? Despite advances for developing nanomaterials with controlled composition, current synthetic practices generally limit forms to particles and wires. The development of nanoscale alloys with arbitrary form and controlled composition will require new material syntheses and manufacturing procedures.

We will address this wholly unexplored area of materials science by adapting recent breakthroughs in 3D nanofabrication toward the synthesis of mechanically robust freeform alloys and composites. Specifically, we will focus on 3D direct write methodologies for nanoscale materials comprised of alloys of iron (steels) and determine generalized strategies applicable to other alloy systems (e.g., Ti, Ni, Cu, Al). The challenges that arise for maintaining strength and toughness as features sizes approach minimum grain size, crack length, etc., will be mitigated via concurrent development of hierarchical freeform composites.

Recent advances in 3D printing have begun to usher in a new era for rapid prototyping. Considering available methodologies such as robocasting, stereolithography, and laser sintering only multiphoton lithography (MPL) has the capability to fabricate feature sizes <100 nm. However, the range of materials compatible with this technique is currently very limited. The planned work will aim to substantially broaden this material space by building upon recent breakthroughs for MPL of metals and composites. Beyond advancing fundamental nanoscience, realizing nanoscale freeform alloys will facilitate design and fabrication of next-generation 3D device architectures.

Summary of Accomplishments:

This project has developed a new methodology for optically driven additive manufacturing that is applicable across a broad range of metals, metal oxides, and alloys at ~1 micron level scale. Unlike laser sintering of powder, gaseous precursors, or nanoparticle ink printing, we have shown that material systems can be directly patterned via localized hydrothermal reaction volumes (HT-voxels) in aqueous solutions. Laser energy is focused onto an optical absorber (such as a metal) in contact with a solution containing one or more dissolved metal precursors (e.g., metal salts). Structures can be continually drawn out from this 'hot edge.' The generalizability of this approach is due to the hydrothermal chemistry underpinning material deposition, and we have investigated physical aspects of the localized temperature and pressure (using a picosecond acoustic thermometry technique) to better understand and tailor the reaction conditions. Admittedly, many of the initial structures produced using these procedures require subsequent processing to arrive at desired properties. Thus, we have shown in situ (laser) annealing of materials such as copper, copper/nickel, and copper/zinc can be achieved under vacuum-less conditions. We have formulated and begun tests on resist systems based on hydrated gels to extend this technique toward 3D printing at the smallest scales. Overall the development of this technique has the potential to simplify mixed material manufacturing (sequential deposition followed by simple rinsing), cost (inexpensive, widely available precursors), and provide a route toward 3D printing of a majority of the periodic table at micro- to sub-micro resolution.

Significance:

Direct patterning of conductive, catalytic, and other functional components with precise compositions and potentially free-form shapes is of critical importance for future additive manufacturing approaches that will enable next-generation electronic, photonic, and mechanical devices. Here, we have developed a foundational and generalizable approach that is analogous to bulk chemical synthesis of many nanomaterials but confined to the tight focus of a laser beam. By extending optical direct write methods to these new material systems, all device components — from electrical elements to packaging — can potentially be processed via 3D printing.

Refereed Communications:

B.M. Foley, C.S. Gorham, J.C. Duda, R. Cheaito, C.J. Szwejkowski, C. Constantin, B.J. Kaehr, and P.E. Hopkins, "Protein Thermal Conductivity Measured in the Solid State Reveals Anharmonic Interactions of Vibrations in a Fractal Structure," *The Journal of Physical Chemistry Letters*, vol. 5, pp. 1077-1082, March 2014.

LEEM-PEEM Studies of Localization Mechanisms in InGaN-Based Heterostructures

165692
Year 2 of 3
Principal Investigator: T. Ohta

Project Purpose:

Scientific insight is crucial for improving the efficiency of optoelectronic devices that target energy mission needs. An example is indium gallium nitride (InGaN) light-emitting diodes (LEDs) for energy efficient solid state lighting (SSL). A key fundamental question is: Why do blue-emitting InGaN alloys have high radiative efficiency despite having threading-dislocation (TD) densities that quench light emission in traditional semiconductors? It is hypothesized that structural and compositional inhomogeneities localize carriers away from crystalline defects, but the nature and degree of localization, its correlation with defects, and its dependence on composition are controversial. The nanoscale properties that influence carrier localization may also contribute to long-standing (~15 year) roadblocks to high efficiency SSL, including the "green-yellow gap" in LED efficiency (where the efficiency of InGaN degrades at longer wavelengths) and the "efficiency droop" observed for InGaN LEDs operated at high currents. To circumvent these roadblocks, we envision the implementation of spectroscopic low energy electron microscopy-photoemission electron microscopy (LEEM-PEEM) on test device structures as a new approach to revealing key structure-property relationships vital for understanding the carrier localization mechanisms impacting efficiencies.

We will use spectroscopic LEEM-PEEM to probe the surface potential, occupied electron density-of-states (DOS), and alloy composition of InGaN alloys with micro- to nanometer spatial resolution. Combined with controlled growth studies, time-resolved optical spectroscopy, and detailed modeling of as-grown surface morphology/composition, these studies will enable unprecedented insight into the connection between microscopic/nanoscale materials properties and efficiency limitations of InGaN LEDs. The planned work leverages two world-class capabilities exclusively co-located at Sandia: our new spectroscopic LEEM-PEEM and state-of-the-art InGaN materials growth and characterization. The major thrust will be to explore the nanoscale materials properties that lead to carrier localization in InGaN, their correlation with materials defects, and the overall impact of these phenomena on InGaN LED efficiency.

Ion-Conduction Mechanisms in NaSICON-Type Membranes for Energy Storage and Utilization

165694
Year 2 of 3
Principal Investigator: A. H. McDaniel

Project Purpose:

Next-generation metal-ion conducting membranes are key to developing technologies like metal-air batteries or flow batteries that will enable grid-scale electrical energy storage, and thus, facilitate the integration of intermittent renewable sources into the US energy infrastructure. NaSICON-type materials, where the acronym stands for sodium super ionic conductor, are a broad class of compounds with $AM_1M_2 (PO_4)^3$ stoichiometry and the choice of either "A" or "M" cation is widely variable. Phosphorus can also be substituted by silicon, Si. Other than stoichiometry, the defining feature of this material class is the formation of a 3D crystallographic framework that contains interconnected channels within which the mobile conducting ions are encapsulated by the "A" site(s). With these materials, it is possible to make batteries, fuel cells, gas sensors, catalyst supports, and even develop technologies for remediating radioactive waste. The challenge is to design NaSICON with optimal ion mobility and chemical stability. Current research involves a heuristic approach to probing the enormous array of possible material compositions that manifest ion conductivity in NaSICON. A comprehensive molecular-level picture of the factors that influence ion conduction is missing.

The objective of this project is to analyze transport chemistry using a combination of in situ studies of structure, composition, and bonding, combined with first principles theory and modeling, to develop an atomistic understanding of mechanisms that give rise to ion conductivity. We will use synchrotron-based x-ray diagnostics to probe the electronic structure of well-controlled, model NaSICON systems while in operation (i.e., conducting Na ions at relevant conditions under an applied field). A unique research platform developed by Sandia will be used to measure x-ray absorption spectra. First principles theory and modeling will be used to interpret the experimental observations and enhance understanding of atomistic processes. This combination of novel experimental methodology and theory is truly innovative and represents a holistic approach to understanding ion conduction in NaSICON.

Programmable Nanocomposite Membranes for Ion-Based Electrical Energy Storage

165696
Year 2 of 3
Principal Investigator: E. D. Spoerke

Project Purpose:

Capabilities and limitations of modern electrical energy storage (EES) are dominated by ion transport and storage. High volume, rate-limited ion intercalation in batteries yields high energy density but limited power; conversely, fast ion transport restricted to electrode surfaces facilitates high power densities with reduced capacity in ultracapacitors. Mating high energy density and high power density will require innovative new strategies for ion transport and storage. We present a new approach to ion-based EES, inspired by biological systems in which currents and voltages are generated through the manipulation of ion concentration gradients. Utilizing energy-dissipative ion pumps and gated ion-selective channels, electric eels, for example, manipulate large ion gradients across membranes, generating and discharging 1A of current at over 600 volts. We intend to translate these concepts to a synthetic system, focusing on scientific phenomena that would allow ion pumps and programmable ion channels in engineered materials to control the transport, accumulation, and dissipation of ions for EES. Combining our expertise in nanomaterials chemistry, biointegration, and electrochemistry, with advanced characterization and computation, we aim to create and understand new materials capable of systematically regulating ion concentration gradients. Our studies will focus on the cooperation of a “pump membrane,” comprising light-powered ion pumps (bacteriorhodopsin), with a nanoporous “gate membrane,” functionalized with novel programmable ion gating chemistries, to explore controlled ion transport in this bio-inspired synthetic system. Knowledge and capabilities established will facilitate critical improvements in existing technologies (e.g., battery separators, water treatment technologies) and will provide a platform to develop a technology utilizing volumetric storage of unbound ionic charge to facilitate high rate, high capacity EES. Developing a fundamental scientific understanding of this promising capability will position Sandia as a leader in an evolving field of bio-inspired energy storage.

Science-Based Design of Stable Quantum Dots for Energy-Efficient Lighting

165697
Year 2 of 3
Principal Investigator: J. E. Martin

Project Purpose:

Fluorescent and solid state lighting rely on rare earth elements (Y, Eu, Tb, and Ce) for which shortages are expected. We will pursue the replacement of these rare earth elements with photoluminescent quantum dots (QDs). To meet the extreme demands of lighting requires that QDs have greatly improved photo and thermal stability. Increased stability can be achieved by coating the QDs with suitable shell materials, but these lead to stresses that generate defects both at the heterojunction and within the lattice. Such defects serve as nonradiative recombination centers that greatly reduce the quantum yield. To design QDs that have both high stability and quantum yield, we will use alloying of both the cores and the shells. Continuum calculations show that alloying will greatly reduce the strains that lead to defect formation. We will use atomistic modeling to predict those graded compositions that have the highest stability to defect formation. Defect formation will be identified through photophysical characterization and with Sandia's unique Z-contrast aberration-corrected scanning electron transmission microscope (AC-STEM).

We will synthesize CdSe or CdTe quantum dot cores using a high temperature process. Shells will be synthesized using heterogeneous nucleation to create Type II heterostructures. These shells, and successive stabilizing shells, will be composition graded to reduce lattice mismatch strains, with the final layers being graded to either ZnS or ZnSe. These heterostructures will be analyzed with Z-contrast AC-STEM before and after thermal cycling and high fluence photoexcitation to determine if defect generation is correlated to the change in photoluminescence. Atomistic modeling will be used to compute the strains throughout the QD and to determine if these can nucleate defects, both at the critical core/shell heterojunction, as well as within the core and first shell. At this time, there has been no effort to combine atomistic modeling and experiment to optimize these nanomaterials, and the planned research will comprise a significant innovation in this field.

Predicting Growth of Graphene Nanostructures using High-Fidelity Atomistic Simulations

165698
Year 2 of 3
Principal Investigator: N. C. Bartelt

Project Purpose:

Graphene continues to attract widespread attention due to its outstanding electronic and optical properties for next-generation electronics. In future applications, device functionality critically depends on producing graphene nanomaterials with high quality and uniformity (with few or no defects). Inserting these novel electronic materials into real world devices requires discovering improved understanding to better control growth. Among the numerous methods for graphene synthesis, chemical vapor deposition (CVD) growth on transition metal substrates stands out for producing large-area films amenable to commercial applications. In particular, large-area graphene growth on copper (Cu) foils (the most commonly used substrate) shows the greatest promise because low solubility of carbon in Cu inherently favors single-layer graphene growth. However, despite its potential, the detailed mechanisms or conditions for controlled graphene growth are unknown or very poorly characterized, often leading to a wide variety of nanostructures. Specifically, how graphene grows on different Cu facets, what controls its in-plane orientation, and how intrinsic Cu defects affect nucleation and defect formation remain inadequately understood. Indeed, even how graphene is aligned, in terms of its crystallography, with Cu itself remains an open question. Consequently, it is extremely difficult to design experimental procedures that will lead to reproducible, controlled growth of optimal nanostructures. A theoretical understanding of the detailed mechanisms of graphene growth is needed to help tailor the experimental conditions to generate high-quality graphene nanostructures. The aims of this project are to: 1) develop a paradigm-changing computational capability for predicting the growth of graphene nanostructures on a metallic substrate, 2) validate the capability through comparison to experimental observations of graphene growth on Cu, 3) use this predictive tool to understand the fundamental mechanistic processes and conditions (temperature, pressure, deposition rate, and substrate orientation) that govern high-quality growth, and 4) perform a proof-of-concept demonstration to down-select a subset of candidate growth experiments for graphene nanostructures to be carried out under specific conditions.

Tunable Quantum Dot Solids: Impact of Interparticle Interactions on Bulk Properties

165700
Year 2 of 3
Principal Investigator: M. B. Sinclair

Project Purpose:

The project will develop a fundamental understanding of the relationship between nanoparticle interactions and the different regimes of charge and energy transport in semiconductor quantum dot (QD) solids. QD solids comprising self-assembled semiconductor nanocrystals such as lead selenide (PbSe) are currently under investigation for use in a wide array of applications including light emitting diodes, solar cells, field effect transistors, photodetectors, biosensors, lasers, and thermoelectrics. These unique materials exist at the crossover between isolated particles and bulk materials. They retain many of the attractive features of the isolated particles such as size-tunable bandgaps, but interparticle interactions modify their behavior and cause charge and energy delocalization. At present, the relative contributions of charge and energy transport to device performance are not well understood. For example a QD solid solar cell with an efficiency of ~5% was recently demonstrated but conflicting explanations of the underlying mechanism have been proposed: exciton migration and dissociation at the electrodes, and direct photogeneration of electron-hole pairs. Device optimization requires a quantitative fundamental understanding of the means by which interparticle interactions lead to collective bulk behavior. The current state of the art in the study of interparticle effects relies on the utilization of different capping ligands to control the interparticle separation. However, the large number of other variables that change as the ligand is varied clouds the interpretation of experimental results. We will use a Sandia-developed mechanical compression method, in conjunction with nanoparticle self-assembly, to fabricate QD solids with precisely controllable interparticle spacing. State-of-the-art optical probes, including ultrafast spectroscopy and non-contact photoconductivity, will be used to characterize QD solid behavior spanning the range from widely separated nanoparticles to sintered nanoparticle superlattices — all within a single, highly ordered QD solid sample. This approach allows for an unambiguous unraveling of the behavior of this unique class of solids and will enable new directions in materials science for a variety of national security missions.

Crossing the Membrane Barrier: Implications for Developing Medical Therapeutics

165824
Year 2 of 3
Principal Investigator: C. Ting

Project Purpose:

The interaction of nanoparticles with lipid membranes is a common motif underlying a number of important phenomena in biology, ranging from cytotoxicity to viral cell entry to transmembrane protein insertion. Inspired by nature, membrane-nanoparticle composites are a new class of functional materials comprised of nanoparticles and diblock copolymers. The versatility of polymer chemistries offers controllable design of diverse vesicle properties and morphologies beyond the range achievable through lipids. The nanoparticles, in turn, impart novel functionalities (for example, magnetic, optical, or fluorescence) to these materials.

Thermal fluctuations are important in these systems and many interesting processes involve thermally activated (rare) events. We will address the difficult problem of activation in soft matter, with a particular focus on polymeric membranes. Besides the long time scales associated with these rare events, a significant challenge arises because of the high dimensional free energy surface due to the complex molecules comprising the membranes. Hence, with any sizable nucleation barrier, direct computer simulation is unfeasible. The potential of mean constraint force method attempts to overcome this challenge by artificially choosing a reaction coordinate, which (in general) does not coincide with the true transition pathway. The transition path sampling method, while in principle applicable to any activated process, is impractical for systems involving large assemblies of complex molecules. Our method combines the hybrid particle field, external potential dynamics, and the string method to overcome these challenges.

While method development is ongoing, we will continue to explore a wide range of previously intractable rare event problems in biological and synthetic soft matter systems. This work paves the way for a molecular-based understanding of membrane-nanoparticle interactions, which can benefit a variety of applications, including the design of functional materials and novel medical therapeutics. In the latter case, the nanoparticle may be a pathogen or therapeutic agent (e.g., gene/drug) that must be blocked from or allowed entry into a cell.

The PI is a Sandia Truman Fellow.

The Role of Grain Boundary Energy on Grain Boundary Complexion Transitions

165825
Year 2 of 2
Principal Investigator: S. M. Foiles

Project Purpose:

The thermodynamics of grain boundaries strongly influence the evolution of microstructure, which has a major influence on materials properties. Grain boundary complexions, a relatively new concept in materials science, are interfacial phases with distinct structures and compositions. Transformations between complexions can occur as a function of temperature, interfacial chemistry, stress, and grain boundary misorientations. Initial results indicate that complexion transitions change the relative interfacial energy of the grain boundaries and lead to a significant increase in the anisotropy of the grain boundary character distribution. These combined results suggest that the transitions may favor specific high-energy grain boundary planes. The goal of this work is to test this hypothesis.

If we can understand and control complexions, it will be possible to control microstructure development and predictably develop new materials. However, there is little basic knowledge about the thermodynamics and kinetics of the transformations between different complexions. In particular, it is not understood what controls the nucleation of complexion transitions. The current project addresses this gap.

It is hypothesized that grain boundary energy is influential in determining when or if a complexion transition will occur. Comparison of relative grain boundary energies and the population of abnormal grains at the interface of single crystal and doped-polycrystalline alumina link the nucleation of grain boundary complexion transitions to the reduction of grain boundary energy.

Doped alumina samples will be prepared, polished, and thermally etched. Contact mode atomic force microscopy will measure the topographic images of the grain boundaries. Mullins' analysis allows the relative grain boundary energy to be calculated from the measurements. Measuring a large number of thermal grooves effectively samples over the anisotropy of the material and allows for the characterization of the distribution of interfacial energies of a given sample. The observed boundary energies will then be correlated with the observation of complexion transitions.

This work is in collaboration with Carnegie Mellon University.

Summary of Accomplishments:

A grain boundary complexion is a distinct equilibrium structure and composition of a grain boundary. A complexion transformation is then a transition from a metastable to an equilibrium complexion at a specific temperature, pressure, chemical potential, and grain boundary character. Previous work indicates that, in the case of doped alumina, a complexion transition that increased the mobility of transformed boundaries and resulted in abnormal grain growth also caused a decrease in the mean relative grain boundary energy as well as an increase in the anisotropy of the grain boundary character distribution (GBCD). This project investigated the hypothesis that the rates of complexion transitions that result in abnormal grain growth (AGG) depend on grain boundary character and energy. Furthermore, the current work expanded upon this understanding and tested the hypothesis that it is possible to control when and where a complexion transition occurs by controlling the local grain boundary energy distribution.

These investigations show that the grain boundary energy anisotropy and temperature are the important parameters influencing the nucleation of the grain boundary complexion transition in Y-doped alumina. With this knowledge, it is possible to control and predict when and where a transition will occur. It is expected that similar trends can be observed in other ceramic and metallic systems. Specifically, it would be interesting to compare these results to a material that displays highly faceted abnormal grain morphology and complexion transitions involving intergranular films, such as the calcium-doped alumina system.

Significance:

Complexion transitions in ceramics are an important aspect of the processing design of ceramic materials. The improved fundamental understanding of these transitions may lead to novel materials for applications such as high-temperature structural materials or thermal barrier coatings.

Refereed Communications:

S.A. Bojarski, M.P. Harmer, and G.S. Rohrer, “Influence of Grain Boundary Energy on the Nucleation of Complexion Transitions,” *Scripta Materialia*, vol. 88, pp. 1-4, 2014.

S.A. Bojarski, M. Stuer, Z. Zhao, P. Bowen, and G.S. Rohrer, “Influence of Y and La Additions on Grain Growth and the Grain Boundary Character Distribution of Alumina,” *Journal of the American Ceramic Society*, vol. 97 pp. 622-630, 2014.

Multiscale Modeling of Hybrid SMA Composites

166636
Year 2 of 3
Principal Investigator: T. E. Buchheit

Project Purpose:

To pursue research of mutual interest to both Texas A&M and Sandia, we will focus on two areas for investigation — constitutive modeling of nano- and microscale phenomena and multiscale modeling of hybrid composites for computationally enabled design and modeling. A hybrid shape memory alloy (SMA) - MAX phase ceramic (Ti_2AlC) composite currently being developed at Texas A&M will be used as an example material system. The focus of this research effort, however, will be on developing a framework applicable to a broader range of high-performance material systems whose deformation behavior is governed by complex inelastic micromechanical mechanisms. Such a tool is needed to address both current and future engineering problems facing both institutions.

Importantly, the new framework will explicitly account for microstructure and have the ability to simulate multiphase materials, thus enabling the analysis and design of advanced material systems.

Creating a Novel Silicon Substrate for the MOCVD Growth of Low Defect GaN

168763
Year 2 of 3
Principal Investigator: A. A. Allerman

Project Purpose:

Current green light-emitting diodes (LEDs) on gallium nitride (GaN) suffer from a host of problems including wavelength shift, power droop, high defect concentrations, and high manufacturing costs. GaN is traditionally grown on small (2-inch), expensive sapphire wafers. It is the lattice and thermal mismatch between the substrate and GaN itself that causes dislocations to form. GaN has been grown on silicon (Si), traditionally in the uncommon orientation, to alleviate the mismatch problem, but the quality is still not as good as GaN on sapphire. We intend to engineer a process to grow device quality GaN on traditional (100) Si substrates.

Growth of GaN on Si would open up the market for GaN LED production. Processing time and costs would drop dramatically because the semiconductor industry already has the tools and raw materials. However, growth of GaN on Si presents challenges. We have recently shown that GaN can be grown on the sidewalls of nano-grooved Si, as well as that nanopatterning sapphire substrates can alleviate defect density. Combining these ideas, a nanopatterned but conventional electronic grade oriented Si wafer could prove a cheap, scalable substrate for GaN growth. Our process would use standard Si instead of the uncommon type and a fast lithography and etching technique to form a nanopatterned substrate for epitaxial growth. Initial results suggest the achievement of very low dislocation density material. This shall form the basis for the goal of fully coalesced GaN templates and devices on standard Si substrates.

Multi-Resolution Characterization and Prediction of Environmentally Assisted Intergranular Fracture

173116
Year 1 of 3
Principal Investigator: R. A. Karnesky

Project Purpose:

Material fracture in the US costs over $119 billion annually. Environmental influences such as hydrogen, irradiation, and high temperatures render ductile alloys susceptible to brittle fracture. Unexpected component failures lead to unacceptable consequences such as the release of flammable or radioactive chemicals. These failures impact gas transfer systems, hydrogen for transportation, and nuclear power generation and waste storage.

There is a critical need for predictive materials understanding to successfully and safely engineer high-consequence systems. At present, however, most procedures for managing materials in such environments rely on extensive experimental databases in the form of empirical crack growth equations, and are implemented into structural analysis codes. These procedures cannot be reliable without thorough experimental data because of complex interactions of environmental influences with deformation mechanisms and microstructure. In response, we will develop a validated science-based computational capability to move beyond the empiricism of current analytical methods.

Our multiphysics, multiresolution framework couples simulations and unique validating experimental techniques at multiple length scales. By coupling cutting-edge modeling and characterization with a thoroughly understood material, the resulting model can predict transient fracture resistance. Deliverables open new core capabilities needed by Sandia and the DOE for interpreting effects of environmental variables and their interactions with microstructure. Rather than having models that simply "support" experimental work, the predictive framework can be exploited for materials engineering.

Our grain-level model, validated by mechanical tests, is based on the Material Point Method and integrates features from kinetic Monte Carlo and phase-field coupled with crystal plasticity. It is informed by atomistic models and experiments. Grain boundary chemistry and cohesion will be modeled with density functional theory and validated by transmission electron microscopy (TEM) and atom-probe tomography. Active mechanisms observed during in situ TEM will be compared to molecular dynamics. This coupled approach is needed for true predictive capabilities.

Phonon Scattering at Mobile Ferroelastic Domain Walls: Toward Voltage Tunable Thermal Conductivity

173117
Year 1 of 3
Principal Investigator: J. Ihlefeld

Project Purpose:

The technical challenge to be addressed in this project is an ability to actively modify thermal conductivity in a solid-state material over a broad temperature range using nonmechanical stimuli. If successful, this will enable active and low-power thermal emission and heat control. To date, altering thermal conductivity in a material at noncryogenic temperatures has only been achieved by applying a mechanical strain, by traversing a narrow phase transition, or by changing the physical dimensions of material itself. This project will develop a means to achieve voltage tuning of thermal conductivity by harnessing mobile coherent interfaces (domain walls) in ferroelectric materials to scatter heat-carrying phonons. By adjusting domain wall spacing to be smaller than the phonon mean free path, phonon domain wall scattering will become the dominant mechanism leading to manipulation of thermal conductivity. Electric fields can sweep these interfaces out of the material and will result in increased thermal conductivity. This has not been demonstrated previously at noncryogenic temperatures and is only recently possible to measure owing to advanced film preparation and thermal characterization instruments.

An ability to actively control thermal transport in a solid-state material over a broad temperature range is an elusive technological goal. This project seeks to develop the underlying science and technology utilizing ferroelectric materials, which contain mobile interfaces, and electric fields. The fundamental variables controlling phonon scattering at these interfaces are poorly understood, and the phenomenon has not been well studied in thin films. Utilizing empirical results and phase field modeling, the necessary understanding to harness this effect will enable the first ever demonstration of field-tunable thermal conductivity at non-cryogenic temperatures. Combined, this improved understanding could be used to inform further technology development and application-specific proposals following this project.

In Situ Study of Surface-Mediated Explosive Degradation using Surface Enhanced IR-Vis Sum Frequency Generation

173118
Year 1 of 3
Principal Investigator: D. Farrow

Project Purpose:

Degradation of explosives at the bridgewire/explosive interface, where the bridgewire initiates detonation by plasma induced shock, is known to change component performance. It has been observed that losses of <1% of total material in a bridgewire detonator can change function time and substantially reduce component lifetime. Two proposed mechanisms are: 1) low levels of ionizing radiation generate free electrons in the bridgewire that cleave a N-O bond in the explosive at the bridgewire interface and 2) chemical reactions at the metal interface (e.g., corrosion) bringing reactive species in contact with the explosive. Furthermore, products of explosive degradation may also corrode the bridgewire. No tool currently exists for in situ identification of short-lived intermediates at a buried interface. Current methods are only sensitive to bulk material (Raman spectroscopy), cannot access the organic/metal interface (mass spectroscopy) or cannot detect species in low concentration infrared-visible sub-frequency generation (IR-Vis Sum Frequency Generation, SFG).

We will build a novel platform to directly observe low concentrations of reactive species at buried organic/metal interface for the first time. We will improve on the state of the art by: 1) combining heterodyne SFG and surface enhancement of SFG signal by vapor depositing thin films of explosive over nanopatterned metal surfaces (e.g., gold and copper) and 2) use the nanostructure/film interface as a model for the explosive/bridgewire interface — exposing it to reactive stimuli and then probing surface mediated reactions in situ. If successful, we will make the first direct observation of reactive intermediates driving ionization and corrosion-mediated aging at the explosive/bridgewire interface. This approach could provide mechanistic information about surface mediated explosive degradation critical to explosive component surveillance and design efforts at Sandia. It is also a novel approach for detecting chemical and material change at any buried film/metal interface with increased sensitivity applicable to a wide variety of energetic and nonenergetic components (batteries, organic electronics, etc.) with possible remote sensing applications.

Scanning Ultrafast Electron Microscopy for Charge Carrier Lifetime Imaging with High Spatial Resolution

173119
Year 1 of 3
Principal Investigator: J. R. Michael

Project Purpose:

In this work, we will develop, build, and use an innovative new scanning ultrafast electron microscope (SUEM) dedicated to the probing of semiconductor structures and devices in order to understand carrier dynamics and carrier lifetimes. SUEM will allow ultra-short time resolved imaging through the use of an electron beam that is pulsed in synchronicity with a laser beam used to excite the sample. Thus, dynamic processes on short time scales can be imaged with high spatial resolution and high temporal resolution. This SUEM will be used to answer important questions about impurities and charge carriers in semiconductor devices and structures providing semiconductor performance information that was previously impossible to obtain.

High Fidelity Modeling of Ionic Conduction in Solids

173121
Year 1 of 3
Principal Investigator: F. P. Doty

Project Purpose:

A critical gap exists in our understanding of mechanisms and kinetics of ionic conduction in solids. For example, thallium bromide, TlBr, is the only room-temperature semiconductor with properties and performance rivaling cadmium zinc telluride (CdZnTe) for gamma ray spectrometers, however, ionic conduction related to structural disorder causes failure after weeks of operation. Changes in microstructure of TlBr and other ionic conductors are greatly accelerated by ion transport. Therefore, to design materials for optimum performance and low life-cycle cost, we must understand structure evolution and ionic transport under realistic service conditions. Prior work focused on atomic-scale calculations of defect formation and migration energies, and addressed neither kinetics nor large-scale disorder, which can dominate ion transport and induced microstructure evolution. Traditional molecular dynamics methods can capture kinetics and structural disorder on appropriate length and time scales, but do not explicitly address electrostatic forces, which drive ionic motion through bulk materials. Therefore, a new approach is required to bring realistic understanding to ionic transport in disordered solids.

We intend to develop a hybrid transport model based on high fidelity interatomic potentials and electrostatic forces. In particular, ion transport and structure evolution will be directly studied with molecular dynamics (MD) simulations using a high-fidelity interatomic potential and a novel variable charge model that captures the electric field induced forces on atoms as obtained from density functional theory (DFT). Innovative, enabling concepts include: 1) dedicated models to independently treat interatomic potential and variable charge effects both simplifies the method and improves accuracy, 2) use of electrostatic forces, rather than charges, solves the problem in previous models that atomic charges are ill defined in DFT due to distributed electron density, and 3) our novel analytical variable charge model significantly improves calculation efficiency over literature numerical variable charge models.

Understanding and Overcoming Materials Challenges for AlN: A Scientific Foundation for Next-Generation Power Electronics

173122
Year 1 of 3
Principal Investigator: A. Armstrong

Project Purpose:

This research will lay the foundation for ultra-wide bandgap (UWBG) semiconductor material science by transmuting aluminum nitride, AlN, with bandgap energy (Eg) of 6.2 eV from an electrical insulator to an electrically conductive material with fully tunable conductivity type. This will enable a revolution in power electronics because the breakdown voltage (Vbr) grows rapidly with Eg. UWBG-based power switches with Vbr upwards of 100 kV becomes plausible for enabling energy technology revolutions such as DC electrical grids with greatly improved efficiency. AlN is attractive due to its large Eg and compatibility with existing semiconductor technology. However, AlN is electrically insulating and must be made conductive to function as an electronic material. Typical methods of controlling electrical conductivity for semiconductors (e.g., impurity doping and minimizing crystal defects) fail for AlN because thermodynamics drives spontaneous defect formation that completely compensates dopants. New methods must be discovered to control the electrical conductivity of AlN.

This project seeks to demonstrate controllable electrical conductivity for AlN for the first time using the strong piezoelectricity and non-centrosymmetric lattice to produce electrical conductivity without dopants. We will employ advanced defect spectroscopy to understand the physical origin and properties of defects in AlN and mitigate their impact on electrical properties. Quantum kinetic theory will be developed to assess electrical transport phenomena in AlN by treating the largely unexplored physics of carrier scattering in AlN including strong electron-phonon coupling and quantum memory effects.

This project looks beyond current national security mission needs and anticipates future needs by addressing scientific problems that will arise when AlN inevitably becomes the technological focus for next-generation power electronics and deep ultraviolet optoelectronics. We approach what are regarded as simple tasks for conventional semiconductors (e.g., doping) and re-examine them to surmount new challenges attendant with semiconductors very large Eg.

Harnessing Multiscale Periodicity of 2D-Crystals for Flexible Adaptable Broadband Optics

173124
Year 1 of 3
Principal Investigator: T. E. Beechem, III

Project Purpose:

The library of isolated 2D crystals grows daily. Beyond graphene, atomically thin nitrides, oxides, and transition metal dichalcogenides (e.g., MoS_2) along with many others are now available and routinely stacked to create hybrid 2D solids. Importantly, when 2D crystals are combined, properties change. The mobility of graphene, for instance, is greatly improved when overlaid on hexagonal boron nitride (hBN). Similarly, arbitrarily stacked graphene transforms from a broadband to bandpass optical absorber. Such changes occur because of interactions between atomic layers. These interactions take place over a new, larger scale (100's of Å), periodicity manifested by the moiré superlattice that evolves between the layers. Combined with the intrinsic atomic periodicity (~1Å), a moiré potential hybridizes the electronic bandstructure of the entire system. Leveraging the interlayer interactions and the resulting multiscale periodicity provides, therefore, a means to create new 2D solids having tailored and engineered properties. Realizing this possibility, however, rests on fundamental understanding linking interlayer interactions, the interplay of differing length scales of periodicity, and the original properties of each 2D crystal. We pursue this fundamental understanding to develop new optical materials impacting a broad spectral range that exhibit operational adaptability and mechanical flexibility.

While understood theoretically and demonstrated experimentally, the interplay of 2D solids, interlayer interactions, and multiscale periodicity, has neither been examined systematically nor leveraged purposely. This is our objective. We will combine our differentiating capabilities to fabricate several different 2D solids, predict their bandstructure, and characterize their responses in order to:

1) Quantify, evaluate, and understand the strength of interlayer interaction in 2D solids to assess how these interactions change the solid's electron dispersion via the superposition of differing length scales of periodicity
2) Manipulate these interactions via externally applied perturbations (e.g., strain, doping, and temperature, etc.) to demonstrate the adaptability/robustness of these phenomena
3) Leverage our understanding for function via the creation of hybrid solids with enhanced or adaptable optical responses

Utilization of Reactive Metal Films for Self-Healing Metal Matrix Composites

173653
Year 1 of 3
Principal Investigator: D. P. Adams

Project Purpose:

Failures involving fatigue, creep, and fracture can readily occur in service if materials are designed and used inappropriately. The traditional approach to mitigate failure is to increase strength, which delays the inevitable without solving the problem. Thus, the focus of this research is to develop a technique to heal and repair damage through the combination of reactive multilayer thin films and self-healing metal matrix composite technology. To date, liquid-assisted self-healing advanced composites which consist of a metal alloy reinforced with shape memory alloy (SMA) wires have been developed that show a 90% recovery of strength. Self-healing in these advanced alloys is achieved by the application heat, which creates a clamping force generated by the SMA combined with the liquation of the matrix. We will utilize reactive metal foils combined with the advanced alloy to provide both heating and sealing of surface cracks. This approach has not been previously investigated and provides the opportunity to: 1) understand and characterize the fundamental relationships between matrix liquation and heat flow produced by the reactive films, 2) to optimize matrix melting behavior, composite properties, and exothermicity of the reactive film, and 3) to develop fabrication techniques that meld the properties of self-healing and reactive films. This technology has the potential to significantly reduce costs by allowing the on-site repair of surface cracks with the value-added characteristic of self-healing for increased reliability.

This research merges two technologies to meet the need for field repair of self-healing materials. Using a systems-based design approach, composite structures will be developed to confirm the viability of this pairing. Simultaneously, this research will create a methodology for selecting multilayer-metal matrix composite (MMC)/reactive foil combinations for tailored and enhanced repair methodology. The work is in collaboration with the University of Florida.

Engineering Bioelectronic Signal Transduction using the Bacterial Type III Secretion Apparatus

173670
Year 1 of 3
Principal Investigator: D. Y. Sasaki

Project Purpose:

Engineering efficient methods for living systems to transfer electrical energy to non-living systems, at relevant size scales, continues to challenge our knowledge of materials and biology. Successful design and engineering to achieve such interfacial structures would enable the development of novel systems that utilize the compact power source, specific sensing capability, and rapid response time of cells in a direct readout platform. Our goal is to enable signal transduction between cells and inorganic materials, using controlled electron transport as the energy transfer mechanism. We envision using the cell as a living battery, providing a set of environmental signals to trigger synthetic biological networks that divert intracellular electron transport pathways to inorganic extracellular structures. Conversely, changing electron influxes could guide cellular responses. It is challenging, however, to precisely engineer nanostructured materials to achieve controllable catalytic or electronic properties and connect them with biological energy sources. Our approach to this problem is to engineer protein scaffolds, taking advantage of the native recognition, selectivity and self-assembly properties of these nanoscale building blocks as well as their native intracellular localization patterns. We are using a type III secretion system (T3SS) needle protein from *Salmonella enterica*, PrgI, as a template for metal nanowire synthesis for biosensing and bioenergy applications. Our strategy is transformative as there are few examples of devices that interface live cells with micro/nano-circuitry to extend the native functionality of biological systems. This research is highly exploratory in nature and without precedence, but if successful could provide the foundation for new bio-interfaced systems that enables direct electronic powering and communication with cells. The work is in collaboration with University of California-Berkeley.

Structural Changes of Self-Assembled Lead Sulfide, Polystyrene Thin Films under Extreme Pressures using in situ High Pressure Small Angle X-Ray Scattering

173869
Year 1 of 1
Principal Investigator: M. Pepple

Project Purpose:

The focus of this project is the investigation of lead sulfide (PbS) nanoparticles under extremely high pressure to study the formation of new structures and characterize their various properties. The synthesis and implementation of nanocrystalline PbS semiconductors, or quantum dots, is a topic of interest in the telecommunications and optoelectronics industry due to their tunable optical properties in the near-infrared and infrared region of the spectrum. Some of the most promising applications for densely packed nanocrystalline solids include field effect transistors, devices for the emission of light, and photodetectors.

As with any colloidal synthesis, achieving monodisperse nanoparticles of the desired size and shape on a consistent basis is a requirement for nearly every device in which they could potentially find application. Just like other quantum dots, designing a cost-effective method of synthesis that results in a consistently high product yield and high quantum yield is essential. Finally, the issue of stability in air is also of concern for implementing PbS nanoparticles into various devices, as the particles oxidize over time. Solving these issues requires a thorough understanding of how the structure, orientation, and free energy of the nanoparticles respond to changes in pressure during assembly.

With only a handful of scientific articles published on the pressure directed assembly of nanoparticles, it is a topic of recent interest in the field of nanoparticle research. The successful completion of this work will provide pioneering insight into the properties of PbS nanoparticle superlattices and how they react in the presence of polymer. The work advances the science toward implementing the materials into devices such as optical triggers and sensors. The work is in collaboration with New Mexico State University.

Summary of Accomplishments:

Polymer nanocomposite films consisting of polystyrene (PS) and PbS quantum dots, as well as pure PbS quantum dot films were synthesized for the purpose of investigating the pressure directed assembly (PDA) of the nanomaterials and the interactions of polystyrene and the quantum dot superlattice under pressure. Samples were compressed using a diamond anvil cell (DAC) to pressures greater than 15 GPa and studied using x-ray synchrotron radiation in order to show the changes in the d-spacing of the superlattice with respect to pressure. Absorption characteristics were investigated with ultraviolet visible spectroscopy (UV/Vis), while structure and long range ordering of the lattice were studied using small angle x-ray scattering (SAXS) as well as grazing incidence small angle scattering (GISAXS). Particle size was examined with transmission electron microscopy (TEM). These inquiries into size, structure, and interactions were performed in order to gain a baseline understanding of the interplay between nanoparticles and a simple polymer in a composite system and how the composite systems can be composed in future experiments.

Now that a degree of information about the formation of long range Pb- polystyrene superlattice order on silicon substrates is known, it will be more amenable to experiment with a variety of materials, such as block copolymers, azoles, and thiophene. Additionally, other quantum dots can be employed. The experiments that use a diamond anvil cell represent some of the most cutting edge and exotic research that has been performed on nanoparticles.

Significance:

The knowledge gained from high pressure SAXS can provide insight on how physical and external phenomena can influence the structure and behavior of nanoparticles and the corresponding superlattice. Using the interactions of PbS with polystyrene of various weight percentages and densities can be used as a template for how to anticipate the interplay of the ligand capped nanoparticles in the neighborhood of 5 nm in diameter with nonpolar polymers; we can begin to understand these binary system in further detail. With this knowledge, science can move forward to experiment with nanoparticle-polymer superlattices of more practical use like superlattices that contain flexible or conductive polymers with potential use in a number of optoelectronic devices.

The Development of a Novel AlGaN Defect Detection, Localization, and Analysis Methodology

176400
Year 1 of 2
Principal Investigator: M. A. Miller

Project Purpose:

The aluminum gallium nitride (AlGaN) material system has great potential in light-emitting diodes (LEDs), laser diodes (LDs) and high electron mobility transistors (HEMTs). Increasing device efficiency or reliability through better understanding and control of defects would benefit a number of applications including biosensing, secure local communications, high frequency power amplifiers, and high voltage switches. Understanding the nature and effects of electrically active defects in AlGaN is crucial to overcoming materials challenges limiting optoelectronic device efficiency, reliability, and lifetimes. The materials challenges in wide bandgap AlGaN stem from non-native substrates, the need for wide-ranging AlGaN compositions in one device, poor p-type doping, spatial non-uniformities, and non-radiative point defects. Interpretation of defect signals can be difficult in conventional methods (electroluminescence, photoluminescence, cathodoluminescence, etc.) due to poor 3D spatial resolution, threading dislocation densities, the wide-bandgap itself, or limited access to the active region. To address the limitations of existing defect characterization capabilities, we plan a novel integration and development of a methodology comprised of laser-based localization techniques and deep level optical spectroscopy (DLOS). Together, they can be used to understand how the optical and electrical properties of spatially localized defects influence the radiative and electrical transport properties of AlGaN materials. This new approach will couple the 2D localization and wavelength-dependent characterization of electrically active defects with deep-level defect state identification to establish a comprehensive capability for III-nitride materials defect characterization. The methodology will bolster in-house AlGaN development and leverage future industrial collaborations. The major technical challenges are correlating laser-based localization techniques, which historically target extended defects, with DLOS point defect information and integrating DLOS into the laser scanning microscope to provide spatial mapping of the deep-level defect states, a toolset not yet commercially available. At Sandia, we have the unique opportunity to leverage Sandia-developed laser-based localization techniques and the DLOS technique and expertise that pioneered nanoscale depth-resolved DLOS for application to InGaN-based devices.

Room Temperature Solid State Deposition of Ceramics

177962
Year 1 of 3
Principal Investigator: P. Sarobol

Project Purpose:

The ability to integrate ceramics with other materials has been limited due to high temperature (>800 °C) ceramic processing. Recently, researchers demonstrated a novel process to fabricate ceramic films at room temperature (RT). In this process, sub-micron sized ceramic particles are accelerated by pressurized gas, impacted on the substrate, deformed, and form a dense film under vacuum. This process eliminates high temperature processing, thereby enabling device integration, in which ceramics can be deposited on metals/plastics/glass. However, knowledge in fundamental mechanisms for ceramic particle deformation and bonding to form dense films are needed and are essential in advancing this technology.

In this work, a combination of experimentation and atomistic simulation will be used to determine deformation/bonding behaviors of sub-micron sized ceramic particles; these are the fundamental steps needed to explain coating formation in the deposition process. High purity alumina particles with nominal sizes of 0.3µm and 3.0µm were examined. Particle characterization showed that the 0.3µm particles were relatively defect-free single crystals whereas 3.0µm particles were highly defective single crystals or particles contained low-angle grain boundaries. Absence/presence of defects play a role in particle deformation mechanisms. The 0.3µm-alumina particles exhibited ductile failure. In situ compression experiments showed 0.3µm particles deformed plastically, fractured, and became polycrystalline. Moreover, dislocation activity was observed during compression. These 0.3µm particles exhibited large accumulated strain (2-3 times those of 3.0µm particles) before first fracture. In agreement with the findings from experimentation, atomistic simulations of nanoalumina particles showed dislocation slip and significant plastic deformation during compression. In contrast, the 3.0µm-alumina particles exhibited brittle fracture. In situ compression experiments showed 3.0µm particles fractured into pieces without observable plastic deformation in compression. The knowledge gained will be used to inform alumina coating deposition parameters and particle-particle bonding in consolidated coatings.

Novel Cathode Materials for Large-Scale Electrical Energy Storage

177964
Year 1 of 3
Principal Investigator: D. F. Sava Gallis

Project Purpose:

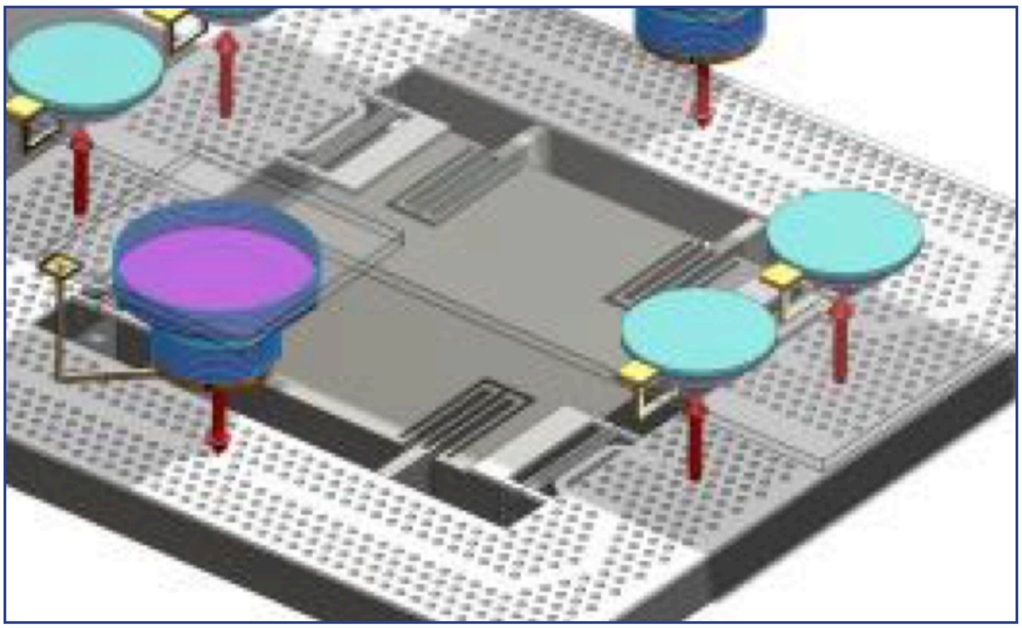
Environmental concerns and the limited resources of fossil fuels, in conjunction with energy security needs, have increased the importance of renewable technologies (wind and solar) in the electrical energy landscape. Since renewable energy sources are intermittent, integration with the grid requires reliable energy storage solutions to tailor power generation and supply to demand. Electrical energy storage is well equipped to balance the demand and supply, however, very few technologies can meet the cost-performance targets required for widespread implementation. Current electrochemical technologies for large-scale storage suffer several limitations: modest cycle life and efficiency (lead acid batteries), low charging rates and efficiency (Na-S, Na-metal halide), and prohibitive costs (Li-ion batteries).

This project focuses on the development of two different novel materials systems for Na-ion batteries (NIB) and redox flow batteries (RFB): 1) hybrid organic-inorganic redox- active metal-organic frameworks (MOFs) and 2) novel polyanion materials, based on naturally occurring sodium-rich minerals. The built-in features of the proposed systems can mitigate the shortcomings of existing materials through longer cycle life and enhanced energy density and efficiency.

The use of MOFs as cathode materials has not yet been evaluated in the context of NIB and RFB because, unlike Sandia, most battery research facilities do not have in-house materials synthesis capabilities. Therefore, this project is uniquely equipped to address the relevance of these highly tailorable platforms to emerging battery technologies. The cutting-edge nature of this study is multifold: 1) it targets the rational design of materials with predetermined features: redox-active MOFs and novel polyanion materials based on naturally occurring sodium minerals, 2) addresses fundamental scientific questions centered on the mechanism for ion insertion/extraction and correlation with the electrochemical performance, 3) combines a multidisciplinary approach via materials synthesis and characterization expertise and battery design and testing, and 4) expands the MOFs research portfolio at Sandia.

NANODEVICES AND MICROSYSTEMS

The Nanodevices and Microsystems Research Foundation supports Sandia's mission by performing creative, leading edge, and high-impact R&D. Its objective is to foster a bold, vibrant, groundbreaking, science and technology base of world-renown as a means to developing the critical and differentiating technical capabilities that will be needed in the future to support Sandia's national security missions. The Nanodevices and Microsystems Investment Area seeks proposals that 1) increase our understanding of physical phenomena across the nanoscale to microscale, 2) develop innovative nanoscale and microscale devices, 3) achieve new methods of integration, and 4) realize novel microsystems-based complex systems.



Drawing of an innovative Nano-Optomechanical Systems-Based MEMS Accelerometer that yields up to two orders of magnitude better resolution than current state-of-the-art MEMS inertial sensors with the same footprint. (Project 159256)

NANODEVICES AND MICROSYSTEMS

Electrically Tunable Metamaterials for Agile Filtering in the Infrared

158826
Year 3 of 3
Principal Investigator: I. Brener

Project Purpose:

Multispectral infrared imaging systems use multiple detector arrays and static filters that increase their weight, cost, and complexity. Such systems could be greatly improved through the incorporation of fast, pixilated, electrically tunable filter arrays that are tightly integrated with focal plane arrays. Previous attempts at tunable infrared (IR) filters have used Fabry-Perot cavities, photonic crystals or other multi-stacks in conjunction with microelectromechanical systems (MEMS), mechanical or temperature tuning approaches. None of these approaches can provide microscale, thin, high optical performance, and electrically tunable IR filter arrays.

In this project, we created compact semiconductor-based tunable infrared filters using electrically tunable planar metamaterials. We have shown that the spectral response of infrared planar metamaterials is greatly influenced by coupling to high mobility electron sheets or intersubband transitions in semiconductor heterostructures, placed within 200 nm of the metamaterial resonators. We intend to extend these concepts to electrically tunable filter arrays in the infrared (3-12 microns) by: 1) optimizing this spectral shift through the use of gated InSb/InAs doped layers and heterostructures of the In-Ga-Al-Sb-As material system and 2) design, modeling and fabrication of new matched metamaterial nano-resonators that couple efficiently to these heterostructures. Ultimately, we envision a monolithic integration of these III-V based metamaterial filters with III-V based IR focal plane arrays.

This project combines cutting-edge research in the areas of metamaterials, nanophotonics and semiconductor physics in order to provide a compact solution that will impact many mission areas at Sandia. It plays well into the strengths of Sandia, leveraging investments at the Microsystems and Engineering Sciences and Applications Facility and the Center for Integrated Nanotechnologies. This combination of bandgap engineering, devices physics, metamaterial design, and nanofabrication has never been tried before and hence has risks spanning from basic science to device integration. The team assembled to work in this project has world-class track record in the areas needed for successful completion.

Summary of Accomplishments:

We fine-tuned the two viable ways for spectral tuning metamaterials using voltage controlled coupling phenomena:

1) Coupling to epsilon-near-zero modes: we designed tunable IR filters using complementary metamaterials and optimized for the different thickness layers so that we get optimal coupling and tuning.
2) Coupling to intersubband transitions (IST): we developed a forward bias scheme that is able to tune the IST and therefore the spectral response. We demonstrated strong coupling at telecom wavelengths using III-Nitride heterostructures.

Significance:
If successful, this project could enable a new generation of infrared imaging systems ranging from compact night vision systems to satellite borne multispectral imagers. As such, this technology could have a direct impact on several DOE and national security missions.

Refereed Communications:
A. Benz, S. Campione, M.W. Moseley, J.J. Wierer, Jr., A.A. Allerman, J.R. Wendt, and I. Brener, "Optical Strong Coupling between Near-Infrared Metamaterials and Intersubband Transitions in III-Nitride Heterostructures," to be published in *ACS Photonics*.

S. Campione, A. Benz, M.B. Sinclair, F. Capolino, and I. Brener, "Second Harmonic Generation from Metamaterials Strongly Coupled to Intersubband Transitions in Quantum Wells," *Applied Physics Letters*, vol. 104, p. 131104, 2014.

S. Campione, A. Benz, J.F. Klem, M.B. Sinclair, I. Brener, and F. Capolino, "Electrodynamic Modeling of Strong Coupling between a Metasurface and Intersubband Transitions in Quantum Wells," *Physical Review B89*, p. 165133, April 2014.

Y.D. Sharma, Y.C. Jun, J.O. Kim, I. Brener, and S. Krishna, "Polarization-Dependent Photocurrent Enhancement in Metamaterial-Coupled Quantum Dots-in-a-Well Infrared Detectors," *Optics Communications*, vol. 312, pp. 31-34, 2014.

A. Benz, I. Montaño, J.F. Klem, and I. Brener, "Tunable Metamaterials Based on Voltage Controlled Strong Coupling," *Applied Physics Letters*, vol. 103, p. 263116, 2013.

A. Benz, I. Montaño, J.F. Klem, and I. Brener, "Voltage Tunable Strong Coupling with Planar Metamaterials: From Fundamentals to Optoelectronic Devices," presented at *Metamaterials*, 2014, Copenhagen, Denmark, 2014.

A. Benz, S. Campione, S. Liu, I. Montaño, J.F. Klem, M.B. Sinclair, F. Capolino, and I. Brener, "Monolithic Metallic Nanocavities for Strong Light-Matter Interaction to Quantum-Well Intersubband Excitations," *Optics Express*, vol. 21, pp. 32572-32581, December 2013.

A. Benz, S. Campione, S. Liu, I. Montaño, J.F. Klem, A. Allerman, J.R. Wendt, M.B. Sinclair, and I. Brener, "Strong Coupling in the Sub-Wavelength Limit using Metamaterial Nanocavities," *Nature Communications*, vol. 4, p. 2882, November 2013.

GaN Unipolar Optical Modulators

158830
Year 3 of 3
Principal Investigator: G. A. Vawter

Project Purpose:

The purpose of this project is to create a new class of optical data modulator with high bandwidth operation at high temperature in order to bypass the limitations of existing modulator technology. Conventional optical modulators change transmitted light intensity by modulating the interband (electron to hole, e-h) absorption energy and are made from InGaAsP/InP materials at telecom wavelengths (~1.5 µm). The small band-gap, long carrier-recombination lifetime and smearing of the e-h energy separation versus carrier density limit the operating temperature, saturation power, and recovery time of the modulation. We are using the extremely fast phonon-assisted relaxation times (~100 fs) and the high density-of-states of the intersubband (ISB) transitions (electrons in the conduction band) in GaN/AlN quantum well (QW) structures to improve saturation power, recovery from saturation, and operating temperature in optical intensity modulators operating at ~1.5 µm.

Summary of Accomplishments:

We demonstrated the first electro-optic waveguide modulator using GaN/AlGaN multi-quantum wells with ISB transitions in intimate contact with a GaN optical waveguide layer. The modulator displays, as much as 6 dB optical extinction, over a 40-volt bias swing. This key result enables future development of high-speed photonics for harsh environments. As a critical stepping stone, we also developed a means of growing smooth low-temperature GaN by metal organic chemical vapor deposition (MOCVD) on top of the multi-quantum well layers. Conventional growth methods require very high temperatures, which caused destruction of the desired ISB absorption. For low temperature growth we had to develop pulsed mode MOCVD.

Our physics models of ISB transitions and complex band structure of these polarized III-Nitrides materials has been used to predict a loss of free-carrier population in the quantum wells for particular Al-content, thickness, and doping of the waveguide cladding layers. Using this information we have created new modulator designs adapted to the non-intuitive band structure characteristics of the III-nitrides.

Additionally, we have demonstrated that SiNx deposited films can act to suppress disordering-induced quenching of the ISB absorption, adding to our capability for integration of modulators with non-absorbing interconnect waveguides.

Significance:

This work establishes Sandia as a III-nitride photonics leader and enables ultrafast photonic devices in harsh environments. By leveraging experimental understanding of the dynamical intersubband transitions in III-nitrides, and forging new methods of quantum-well intermixing and high-speed optical modulator fabrication, we make possible sophisticated new microsystems such as chip-scale radio frequency spectrometers and high-power mm-wave photonic links relevant to DoD interests and Defense Advanced Research Projects Agency. Further, III-nitride photonics integrated circuits offer operation at high-power and in severe-temperature environments, space and avionics, where the overhead of cooling has prevented utilization of photonics. This work provides unique, pioneering technology, enabling completely new approaches to signal processing.

Intrinsically Radiation-Hard Nonvolatile Memory: SnO2 Memristor Arrays

159056
Year 3 of 3
Principal Investigator: E. J. Garcia

Project Purpose:

We investigated SnO_2-based memristors to create inherently radiation-hardened, ultra-dense, non-volatile memory (NVM). Radiation-hardening-by-design is an effective solution that is based on redundancy and implemented in layout and architecture; however, it comes with the penalties of strict design constraints, lower performance (>1 Moore's Law generation) and higher cost (10,000 times more than its commercial counterpart). An inherently radiation-hardened, ultra-dense, non-volatile memory device compatible with complementary metal-oxide- semiconductor (CMOS) is key to relaxing design constraints and accelerating progress in radiation-hardened CMOS.

The memristor is a new type of memory device that has the potential to combine the best characteristics of the hard drive, RAM and flash in terms of density, access speed and power, and resistance to radiation effects. Excellent switching times of ~10 ns, memory endurance of >10E9 cycles, and extrapolated retention times of >10 years have been reported. Importantly, memristors are inherently radiation-hardened since information is stored as a structural change and not as electronic charge. Although different material systems have been investigated for memristors, SnO_2 has received little attention even though it is resistant to displacement and ionizing damage and has excellent electronic properties. Furthermore, SnO_2 can be deposited on flexible surfaces.

This project builds on relevant work and technologies, and US-Mexico collaborations to make a unique and inherently radiation-hardened NVM based on SnO_2 memristors. The project will combine the intrinsic radiation resistance of both the memristor structure and SnO_2 to make inherently radiation-hardened NVM. SnO_2-based memristor memory arrays will be fabricated on silicon wafers and tested for radiation hardness for the first time. Standard CMOS input/output (I/O) electronics and microsystems will be integrated with the memristor arrays to show NVM functionality. Moderately complex functionality of pre- and post-irradiated memristor arrays with peripheral electronics will be demonstrated. The work is in collaboration with the University of Texas at El Paso.

Summary of Accomplishments:

This project examined the efficacy of using SnO_2 thin films for resistive-switching applications and integrating these devices with CMOS and MEMS. Technology for creating SnO_2-based discrete memristor devices on silicon was developed. Furthermore, a technology for fabricating crossbar memristor arrays was also developed. Extensive materials and electrical characterizations of the discrete Ti/SnO_2/Au devices were performed to study the electroforming and current flow mechanisms. Unipolar resistive switching was observed and it was discovered that three current flow regimes exist in the high resistance state. A crossbar architecture was developed to increase device density and ease of I/O. Although endurance was limited to a few cycles, resistive switching showed proof of concept of the technology. Research was performed to discover and exploit new functionality obtained by integrating memristors with microelectromechanical systems (MEMS) structures. An invention disclosure was submitted related to the memristor technology.

Significance:

This project furthered our means to develop new capabilities in achieving radiation-hardened electronics using a very different technology (SnO_2 thin films) that may have intrinsic radiation resistant properties. This was an activity that could potentially affect the entire DOE complex in terms of where radiation hardened circuitry is required, such as nuclear weapon systems and satellite applications. This work will provide a path for integration of MEMS with the associated radiation hardened circuitry needed for sensing and control of the microsystem.

Refereed Communications:

S. Almeida, "Integration of Memristors with MEMS for Dynamic Displacement Control," doctoral dissertation, University of Texas at El Paso, 2013.

A. Talukdar, S. Almeida, J. Mireles, E. MacDonald, J.H. Pierluissi, E. Garcia, and D. Zubia, "Unipolar Resistive Switching and Current Flow Mechanism in Thin Film SnO_2," in *Proceedings of the TechConnect World Innovation Conference and Expo*, Washington, DC, 2014.

Coupling of Quantum Dots to Nanoplasmonic Structures

159184
Year 3 of 3
Principal Investigator: I. Brener

Project Purpose:

Quantum-dot lasers are extremely attractive because of their compact size, high spectral selectivity, ultra-low power consumption, and increased modulation bandwidth. To fully exploit the unique properties of quantum dots, such as atomic-like spectra, ultrahigh charge carrier concentrations, and wide spectral tenability via the quantum size effect, it is crucial to investigate the dynamics of photon-quantum dot interactions in sub-diffraction resonant cavities. Due to the diffraction limit of traditional optical systems, light confinement comparable to the physical size of quantum dots is extremely difficult. In addition, integration of quantum dots into a stable sub-diffraction cavity is a major technical challenge in the development of quantum-dot lasers. The research will attempt to demonstrate a quantum-dot laser by creating a novel plasmonic nanocavity structure embedded in a giant-quantum dot (g-QD)-doped polymer film such as poly(methyl methacrylate) (PMMA) or poly(lauryl methacrylate) (PLMA).

Plasmonic structures suffer from high ohmic losses. To overcome this issue, we foresee a hybrid plasmonic structure to demonstrate stimulated emission of g-QDs in a sub-wavelength cavity. Investigation of the interaction between colloidal g-QDs and a periodic plasmonic nanostructure was chosen as an initial step towards designing the subwavelength cavity. This work provides insight into the strong interactions between spontaneously emitted photons and resonant plasmonic modes. With the knowledge of how g-QDs behave in sub-wavelength apertures, and further study, we will design a sub-wavelength plasmonic cavity to demonstrate stimulated emission. These results are an important step towards realizing a quantum dot based plasmonic coherent source. This work is in collaboration with New Mexico State University.

Summary of Accomplishments:

We have investigated, through numerical study, a modified hybrid plasmonic structure that focuses the pump beam into sub-wavelength apertures through the excitation of surface plasmons (SP) waves. The integration of quantum dots into a stable sub-wavelength plasmonic cavity has proven to be exceptionally technically challenging. The outcome of this project has provided great insight into quantum dot/plasmon interactions and has further elucidated what is known about light-matter interactions in a nanoscale environment. Additionally, simulation of a novel structure could provide the necessary information to realize a plasmon assisted colloidal quantum dot based nanolaser.

Significance:

This work provides insight into the strong interactions between spontaneously emitted photons and resonant plasmonic modes. With the knowledge of how g-QDs behave in sub-wavelength apertures, and further study, we will design a sub-wavelength plasmonic cavity to demonstrate stimulated emission. These results are an important step towards realizing a quantum dot based plasmonic coherent source. If successful, the research could significantly impact the DOE and national security missions by enabling ultracompact and low-threshold, light sources that could be integrated into numerous nano-and microsystems such as chem-bio and atom-chip sensors. New functionalities could be enabled in the integration of electronics and photonics, solid-state lighting, energy conversion, ultra-high density storage, and high-resolution imaging and lithography. New understandings of light-matter interactions in nanostructures would impact other mission critical areas such as energy harvesting.

Refereed Communications:

J.L. Briscoe, S.-Y. Cho, and I. Brener, "Part-Per-Trillion Level Detection of Microcystin-LR using a Periodic Nanostructure," to be published in *IEEE Sensors Journal*.

Applications of Microwave Frequency Nano-Optomechanical Systems: Oscillators, Circuits, and Sensors

159256
Year 3 of 3
Principal Investigator: M. Eichenfield

Project Purpose:

Nano-optomechanical systems (NOMS) can simultaneously localize optical photons and microwave-frequency phonons to volumes thousands of times smaller than the volume of the smallest human cell — volumes limited only by the diffraction of the two waves. At this level of localization, the light-matter interaction becomes almost unimaginably strong, with each photon exerting forces on the matter containing it larger than 10 times the weight of that matter. This enables a fully engineerable and scalable platform for light-matter interactions with strengths previously attainable only when trapped atoms, trapped ions, and quantum dots interact with light from external, macroscopic cavities. This Truman Fellowship research project broadly investigates novel NOMS-based chip-scale devices using NOMS to develop sensors and transducers with unprecedented sensitivity and resolution.

Novel acousto-optic interactions were explored in aluminum nitride, a piezoelectric thin film with a relatively high degree of optical transparency. The piezoelectric nature of this optically transparent material yields the ability to directly and efficiently generate and detect the microwave-frequency phonons that participate in or result from an optomechanical interaction. This has not been done before because of the extreme challenge involved in integrating efficient electromechanical transducers with optomechanically optimized nanoscale photonic structures. The use of a NOMS displacement sensor was investigated as backbone of a novel microelectromechanical systems (MEMS) accelerometer and vibratory Coriolis gyroscope. These inertial sensors will have orders of magnitude better sensitivity than their state-of-the-art electrically sensed counterparts, giving them performance normally associated with much larger sensor packages but with the size, weight, and power consumption of a MEMS platform.

Summary of Accomplishments:

Noteworthy accomplishments for this Truman Fellowship have been in two major areas: generation and optical detection of microwave frequency acoustic beams and optomechanical inertial sensors.

<u>Generation and optical detection of microwave frequency acoustic beams</u>:
We have — for the first time — generated Gaussian focused beams of acoustic Lamb waves at microwave frequencies using advances electrode design, fabrication, and characterization techniques. We have developed the fundamental theory of focused beam propagation, using a very intuitive theoretical formulation of the solutions to the wave equation in thin plates. We also developed analytical and numerical tools for designing complex electrode shapes that produce these focused beams. We built the first demonstration of such devices, operating at 2 GHz. Finally, we developed a state-of-the-art scanning laser Doppler vibrometer that could reconstruct the propagation of the focused acoustic beams and allow comparison to the underlying theoretical and design tools we developed.

<u>Optomechanical inertial sensors</u>:
We began building a revolutionary platform for miniature inertial sensors using nano-optomechanical systems as the displacement sensors. We have shown from theoretical first principles that this system will have up to

two orders of magnitude better resolution than the current state of the art in MEMS inertial sensors for both accelerometers and gyroscopes. We have also developed advanced packaging techniques that should allow the systems to operate in environments relevant to national security, as well as challenging commercial applications (such as in oil and gas exploration). We have built all of the component pieces and have begun the process of assembling the technologies together into the first engineering development unit.

Significance:

The nano-optomechanical inertial sensing platform that we are developing is extremely diverse in the application space it can impact. It will certainly enhance navigation in small size, weight, and power (SWaP) constrained systems. We believe this technology will ultimately see insertion into myriad inertial measurement and inertial reference units that have large impact in national security. Sandia has executed four Work for Other contracts from national security customers in the last year based on this technology.

Refereed Communications:

M. Eichenfield and B. Homeijer, "Nano-Optomechanical Massive MEMS Accelerometer," presented at the *DARPA QUASAR Conference*, Pensacola, FL, 2014.

M. Eichenfield and B. Homeijer, "Nano-Optomechanical Massive MEMS Accelerometer," presented at the *DARPA QUASAR Conference*, Long Beach, CA, 2014.

M. Eichenfield and B. Homeijer, "Nano-Optomechanical Massive MEMS Accelerometer," presented at the *AFRL CSTAR Industry Day Conference*, Pensacola, FL, 2014.

Defect Localization, Characterization, and Acceleration Factor Assessment in Emerging Photovoltaic and Power Electronic Materials

164183
Year 3 of 3
Principal Investigator: B. B. Yang

Project Purpose:

Next-generation photovoltaic technologies, such as microsystems-enabled photovoltaics (MEPV) that are under development at Sandia, promise to produce affordable solar energy. The rapid adoption and continued investment in such technologies depends on demonstrated reliability and quantifiable longevity. The long-term reliability of these new devices, however, is untested and the failure mechanisms are not well understood. We seek to fill this gap by being the first to adapt certain microelectronics failure analysis techniques, such as thermally induced voltage alteration, for MEPVs. We will also use accelerated testing to examine the effects of electrical, light, and temperature stresses. The findings will demonstrate new characterization tools for these technologies and establish their readiness for further investment and rapid adoption.

MEPVs are relatively immature compared to their traditional silicon-based counterparts. As such, there is a weaker understanding of the physics behind performance degradation and device failure. This uncertainty makes the development of a reliability model and exploration of in situ monitoring techniques inherently risky. The findings of the degradation mechanism may not relate to monitoring techniques that can be practically implemented. Additionally, while microelectronics failure analysis concepts apply to these materials systems, they must adapt to different requirements, such as scale over resolution and foreign materials in the device and its packaging. Much of the investment risk lies in the success of the failure analysis tools, progress in understanding the physics of failure, and the successful development of a reliability model. This project will decrease the risk associated with future investments in these technologies by providing techniques to understand failure mechanisms and quantify reliability performance.

Summary of Accomplishments:

This project examines failure analysis techniques to perform defect localization and evaluate MEPV modules. Complementary metal-oxide-semiconductor (CMOS) failure analysis techniques, including electroluminescence (EL), light-induced voltage alteration (LIVA), thermally induced voltage alteration (TIVA), optical beam induced current (OBIC), and Seebeck effect imaging (SEI) were successfully adapted to characterize MEPV modules. The relative advantages of each approach are reported. EL can be used to evaluate cell performance and identify thermal damage sites associated with avalanche breakdown. LIVA can be used as a rapid screening tool in a manufacturing setting when multiple laser scanning directions are implemented. Both SEI and TIVA are effective at troubleshooting electrical contacts. OBIC is best suited for high-resolution evaluation of MEPV cell performance.

The effects of exposure to reverse bias stress, light stress, and thermal stress were also explored. MEPV was found to have good resilience to all three stress factors. Reverse bias stress did not result in breakdown until 75 volts. Only minor increases in reverse bias leakage current were observed after prolonged exposure to sub-breakdown voltage stress. Significant changes in electrical characteristics were not observed after extended exposure to photons at 405-nanometer wavelength at a power concentration of 75-times that of air mass 1.5. No degradation in efficiency was observed after mild thermal cycling.

These results form a basis for further development of failure analysis techniques for MEPVs of different materials systems or next-generation, multi-junction MEPVs. The development of failure analysis and defect localization tools in this project can be broadly applied to facilitate process development of microsystems-based photovoltaic technologies. The incorporation of additional stress factors and testing parameters could be used to develop a reliability model to generate lifetime predictions for MEPVs as well as uncover opportunities for future design improvements.

Significance:

The microsystems-based approach to photovoltaics is a promising avenue to new portable power generation technologies with high power density by weight. Early supporters of these technologies consist of entities operating in defense and space applications. Since reliability and surety is important to these potential customers, early work in failure analysis and reliability for MEPV is a crucial investment to facilitate its adoption. The tools and capabilities developed in this project will also decrease development time of new iterations of MEPVs, thereby accelerating MEPV maturation into a high-impact technology.

Refereed Communications:

B.B. Yang, J.L. Cruz-Campa, G.S. Haase, P. Tangyunyong, M. Okandan, and G.N. Nielson, "Stress Factor Assessment for Microsystems-Enabled Photovoltaics," in *Proceedings of the 40th IEEE Photovoltaic Specialists Conference (PVSC)*, pp. 1305-1309, Denver, CO, 2014.

B.B. Yang, J.L. Cruz-Campa, G.S. Haase, E.I. Cole, Jr., P. Tangyunyong, M. Okandan, and G.N. Nielson, "Comparison of Beam-Based Failure Analysis Techniques for Microsystems-Enabled Photovoltaics," in *Proceedings of* the *2013 International Symposium for Testing and Failure Analysis (ISTFA)*, pp. 369-375, San Jose, CA, 2013.

B.B. Yang, J.L. Cruz-Campa, G.S. Haase, E.I. Cole, Jr., P. Tangyunyong, P.J. Resnick, M. Okandan, and G.N. Nielson, "Failure Analysis Techniques for Microsystems-Enabled Photovoltaics," *IEEE Journal of Photovoltaics*, vol. 4, pp. 470-476, January 2014.

Nano-Structured Silicon Phononic Crystals with Metal Inclusions for ZT Enhancement Proof-of-Concept

164672
Year 3 of 3
Principal Investigator: C. M. Reinke

Project Purpose:

Most published research on improvement of the thermoelectric figure of merit, ZT ($ZT = (S^2*sigma/k)T$, where S, sigma, and k are the Seebeck coefficient, electrical conductivity, and thermal conductivity, respectively) has largely focused on only one of its components, with the hope that the other two remain favorable. However, due to the interdependent nature of the problem, efforts to reduce k by incoherent phonon scattering inadvertently create electron scattering with a corresponding reduction in sigma, and efforts to increase sigma via doping typically decrease in S in accordance with the Mott relationship. We will circumvent these issues by addressing all three parameters of ZT simultaneously using nano-structured phononic crystals (PnCs). The engineered scattering of phonons using PnCs reduces k, while metal inclusions increase the sigma of the PnC. Additionally, metallic nanoparticles will be implanted to engineered the electronic band structure at the semiconductor-metal interfaces in a manner that increases S, thus increasing the overall ZT.

Efforts to extend previous research in thermal conductivity reduction using PnCs to high-temperature, high-ZT devices were not funded, with questions raised regarding whether the relative reduction in k remains constant at higher temperatures, would sigma be enhanced in a semiconductor-metal PnC (rather than semiconductor-air) while maintaining the reduction in kappa, and can S be enhanced using low-dimensional metallic inclusions. The first question will be answered by measuring the reduction in k relative to an unpatterned slab of the same thickness as the temperature is increased, and the second will be addressed by measuring the S, sigma, and k of a Si-W PnC using an existing thermal equilibrium test bench. The third question will require careful introduction of metallic nanoparticles into the PnCs using focused-ion beams or ion implanter. All three tasks are supplemented by the theoretical expertise developed at Sandia in PnC design and thermal conductivity calculations for periodic nanoscale materials.

Summary of Accomplishments:

The work represents a comprehensive study of the enhancement of thermoelectric ZT in Si-based microscale PnCs and examines a relatively low-cost method for creating high-ZT materials. The first measured reduction of the thermal conductivity of microscale Si-air PnCs at elevated temperature is reported here, suggesting a persistent role for coherence in PnCs at in high-temperature applications. A modified Callaway-Holland model was developed for the prediction of thermal conductivity in micro-scale periodic devices, and represents the most comprehensive and accurate model reported to date. This model also enables the exploration of the crossover between the continuum and quantum regimes of thermal transport. Additionally, by matching the experimental data using the threshold mean free path parameter, this technique provides information about the phonon mean free path of the measured samples, which was absent in previous models. A highly flexible, suspended-island measurement platform was developed that can measure the electrical and thermal conductivities and Seebeck coefficient of a device concurrently, with high accuracy and minimal systematic error. The predicted ZT enhancement factor of 5 as compared with bulk Si reported in this work for Si-W PnCs is the highest reported value of any complementary metal-oxide-semiconductor (CMOS) compatible Si-based device and demonstrates the power of PnCs to decouple the conductivities and enhance both simultaneously.

The information learned here opens up a new class of thermoelectric materials and devices, potentially enabling efficient chip-scale thermoelectric cooling and cost-efficient waste heat scavenging.

Significance:

Given the pervasive need for thermal management in all types of systems, it is clear that this work could impact several key areas of interest for Sandia. Possible applications range from near-junction cooling of focal plane arrays to thermal management in radar systems. Additionally, several proposals for follow-on funding have come out of this project, including a whitepaper on thermal rectification. The potential exists for proposals to Advanced Research Projects Agency-Energy or other agencies for waste heat recovery applications. Future studies could address topics such as electronic band bending at nanoscale metal-semiconductor interfaces, simultaneously engineering of electrical conductivity and Seebeck, and non-symmetric phonon propagation.

Refereed Communications:

S. Alaie, D.F. Goettler, K. Abbas, M F. Su, C.M. Reinke, I. El-Kady, and Z. C. Leseman, “Conductivity of Thin Films and Nanostructured Materials with Consideration of Contact Resistance,” *Review of Scientific Instruments*, vol. 84, p. 105003, 2013.

M.G. Baboly, M.F. Su, C.M. Reinke, S. Alaie, D.F. Goettler, I. El-Kady, and Z.C. Leseman, “The Effect of Stiffness and Mass on Coupled Oscillations in a Phononic Crystal,” *AIP Advances,* vol. 3, p. 112121, 2013.

Gate-Controlled Diode Structure to Investigate Leakage Current and Early Breakdown in Graded InGaAsP/InP Junctions

164676
Year 3 of 3
Principal Investigator: D. Leonhardt

Project Purpose:

The scope of the project is to understand the primary leakage current mechanisms in graded InGaAs/InAlAs pn junctions operating under large electric fields. First, the work involves an investigation of the dominant mechanisms of leakage current generation and conduction. Second, the work will identify the location of the leakage current in the device, and the relative contributions to the leakage coming from the device perimeter (surface states) versus area (bulk material). Third, an electrostatics model is required to identify the location of the maximum electric field within the device, and predict the magnitude of the leakage current for different layer thicknesses and doping densities. Last, the project attempts to identify new material combinations with potential for high breakdown voltage, low leakage current, and high mobility devices.

Summary of Accomplishments:

Band-to-band tunneling was determined to be the dominant leakage current mechanism occurring at large reverse biases. Shockley-Read-Hall (SRH) generation was determined to be the primary mechanism for leakage current at small reverse biases. The SRH was found to be coming from the perimeter of the device (surface states) for square devices less than 100 µm on a side. The SRH comes from the area (bulk) of the device in larger devices.

An electrostatics model of the device showed that the largest electric field in the device occurs at the InGas/graded InAlAs interface. Band-to-band tunneling is most sensitive to the maximum electric field and, therefore, the InGas/graded InAlAs interface is the location of the source of the tunneling leakage current. The model predicts that an addition of donor doping in the graded layer, or a reduction in the doping density in the InAlAs will decrease the leakage current by several orders of magnitude.

Lastly, several new material combinations (lattice matched to commercially available substrates) are identified that could potentially result in several classes of devices with improved voltage breakdown, switching speeds, and radiation tolerance.

Significance:

The findings that resulted from this work address the long-standing problem of large leakage currents in III-V compound semiconductor devices. The III-V devices are used in a variety of national security and defense applications including lasers, infrared detectors, and radiation tolerant transistors. The insights gained from determining the mechanisms of leakage current in InGAs/InAlAs diodes has allowed future work to be focused and new device designs proposed that could result in significant reductions in leakage current in future III-V devices.

Active Plasmonics from the Weak to Strong Coupling Regime

165702
Year 2 of 3
Principal Investigator: G. A. Keeler

Project Purpose:

Plasmonics focuses on the manipulation of light using metallic nanostructures and promises to transform the field of optoelectronics, which has traditionally relied upon light guiding in dielectrics and semiconductor-based devices. Most nanoplasmonics efforts have examined passive structures with static, geometry-defined responses. We will demonstrate, for the first time, a range of active plasmonic devices based on guided surface plasmons coupled with electrically controlled compound semiconductor structures operating at near-infrared (NIR) wavelengths. We expect these active devices to fundamentally alter the photonics landscape and push the frontiers of nanoscale optics.

The primary scientific question examined in this project is how light-matter coupling changes when light is confined to the nanometer scale in the form of plasmons. Experimental tests of our theoretical understanding will be performed using test devices such as modulators, amplifiers, and emitters that bring about various degrees of plasmon coupling (weak to strong). Plasmonic modulators and amplifiers will be based on semiconductor quantum wells that can be forward or reverse biased to achieve gain or loss through relatively weak plasmon-exciton coupling. Laser integration represents a more complex hybrid system, wherein the plasmonic structure will be strongly coupled within the optical cavity of a vertical-cavity surface-emitting laser (VCSEL), with plasmon interactions occurring in a high-field environment.

To date, there have been no demonstrations of efficient electrical modulation and amplification techniques for NIR guided plasmons. Plasmon integration within a laser cavity represents another exciting new area of study, with significant complexity at the nanoscale. Active plasmonic devices have the potential to impact a wide range of applications. Sandia is uniquely positioned to fully explore active plasmonics technologies and rapidly resolve fundamental scientific and technological uncertainties, thereby potentially enabling mission customers to leverage the technology through follow-on activities.

Minority Carrier Lifetime Characterization and Analysis for Infrared Detectors

165703
Year 2 of 3
Principal Investigator: E. A. Shaner

Project Purpose:

Infrared detector performance is degraded by carrier recombination and dark current generation. The nBn device architecture, comprised of two n-type semiconductors sandwiching a barrier layer, has experimentally proved its superiority over mercury cadmium telluride (MCT) and InSb. Both parasitic generation-recombination current and perimeter currents are completely suppressed in optimized designs. However, the fundamental dark current diffusing from the absorber limits its performance to a level only marginally better than MCT. To dramatically reduce the dark current by another order of magnitude requires a new absorber material with long carrier lifetimes at mid-wave infrared (MWIR) and even longer lifetimes in the long-wave infrared (LWIR). We will study dark current and minority carrier lifetime in nBn absorbers such as InAsSb, as well as InAs/InAsSb superlattice material systems, and correlate measurements with growth conditions and crystal structure. Our goal is to develop an understanding of lifetime limiting mechanisms in these materials and work towards improvements that will impact detector performance.

The overall goal of this research effort is to characterize and understand dark current generation, the impact of defects on detector performance, and to explore solutions to these issues using either bulk or superlattice absorbers. We will focus primarily on minority carrier lifetime since material quality is the primary driver for improved performance. To fully understand an immature material system such as InAs/InAsSb, many different structures with varying layer composition and doping must be characterized over a wide range of temperatures. While basic material studies such as this can lead to significant device improvements, they are not typically called for in external program announcements that are more often concerned with demonstration devices.

Electrically Injected UV-Visible Nanowire Lasers

165704
Year 2 of 3
Principal Investigator: G. T. Wang

Project Purpose:

There is strong interest in minimizing the volume of lasers to enable ultracompact, low-power, coherent light sources. Nanowires (NWs) represent an ideal candidate for such nanolasers as stand-alone optical cavities and gain media, and optically pumped NW lasing has been demonstrated in several semiconductor systems. Electrically injected NW lasers are needed to realize actual working devices but have been elusive due to limitations of current methods to address the requirement for NW device heterostructures with high material quality, controlled doping and geometry, low optical loss, and efficient carrier injection. We will demonstrate electrically injected NW lasers emitting in the important UV to visible wavelengths. Our approach to simultaneously address these challenges is based on high quality III-nitride NW device heterostructures with precisely controlled geometries and strong gain and mode confinement to minimize lasing thresholds, enabled by a unique top-down NW fabrication technique developed at Sandia that provides maximum design flexibility. Our approach applies novel strategies for addressing these issues and leverages our combined expertise in III-nitride NW fabrication and characterization, nanodevices, and semiconductor laser modeling. Theory and modeling will be closely integrated with experiments to help design and demonstrate NW heterostructures with minimal lasing thresholds and to understand and predict the properties and physics from these nanolasers. Successful demonstration of a working III-nitride NW laser would enable diverse new functionalities in the integration of electronics and photonics, chem-bio sensing, imaging, ultra-high density storage, nanolithography, lighting, and quantum information. This project seeks to perform a proof-of-concept demonstration in electrically injected NW lasers.

Efficient Heat Removal from Power-Semiconductor Devices using Carbon Nanotube Arrays and Graphene

165705
Year 2 of 3
Principal Investigator: M. P. Siegal

Project Purpose:

Efficient heat removal from semiconductor-based power electronics is becoming increasingly important, especially with the growing investment in renewable energy sources that requires advanced power electronics to interface with the electric grid. For example, excessive temperature reduces performance and causes failure in Si-based power-switching devices such as insulated gate bipolar transistors (photovoltaic-inverters). This problem is exacerbated as voltage, current, and switching-frequency scale to increase grid efficiency. This led to the pursuit of wide-bandgap SiC and GaN for next-generation power electronics. However, their advantages are obscured by reduced performance and lifetime that occur with increased temperature. To fully achieve these material gains, the thermal resistance of the system must be reduced. Therefore, this project targets the large thermal-resistance occurring at the device die/package boundary where standard thermal-interface-materials (TIM) (e.g., metal-loaded epoxies) with thermal conductivity ~1 W/m-K, act as a thermal bottleneck that can mitigate performance or even cause failure.

We seek to eliminate the TIM heat-transfer bottleneck from high-power devices to enable efficient cooling for improved device performance and reliability by creating all-carbon TIM cooling strategies to meet present/future needs. Carbon nanotubes (CNTs) and graphene can have thermal conductivities > 10x that of metals. We will synthesize high-quality, vertically aligned CNT arrays directly onto a metal package that directly bonds to the device die in order to reduce TIM resistance by 10 - 100X. While this alone will reduce the existing thermal bottleneck, we will incorporate graphene sheets onto the top of device surfaces to act as an ultimate heat spreader. By then making direct thermal contact between a graphene heat spreader and CNT-TIM in a flip-chip architecture, and with the assistance of fundamental studies of phonon transfer through each new material and interface, 1,000X improvements over state-of-the-art TIM technology are obtainable, potentially rendering irrelevant the device substrate thermal conductivity, and lead to a new paradigm for high-power device performance via thermal management.

Fabrication and Characterization of a Single Hole Transistor in p-type GaAs/AlGaAs Heterostructures

165706
Year 2 of 3
Principal Investigator: L. A. Tracy

Project Purpose:

One of the leading candidates for a solid-state quantum bit is the spin of a single electron confined in a semiconductor. Coherent control of individual electron spins has already been demonstrated in quantum dots. These groundbreaking experiments utilized high-mobility 2D electron systems in GaAs/AlGaAs heterostructures grown via molecular beam epitaxy (MBE). The major source of decoherence in such experiments is coupling between electron spins and nuclear spins in the host GaAs semiconductor. It has been suggested that hole spins in GaAs would be better suited for such experiments due to a lesser coupling between hole and nuclear spins. Recent experiments already show that the coherence time for hole spins in GaAs quantum dots are at least one order of magnitude longer than that of the electron spin.

Building on recent successes in the growth of high-mobility 2D hole systems (2DHS) via carbon doping of (100) oriented GaAs/AlGaAs heterostructures at Sandia, we seek to fabricate and characterize single hole transistors, looking towards eventual applications in the area of quantum computing. This work will leverage Sandia's unique, world-class capabilities in MBE growth of GaAs/AlGaAs heterostructures and expertise in low-temperature measurements.

To date, experiments looking at the possibility of using spins in semiconductors as quantum bits have primarily focused on electron spins. It was only recently suggested that hole spins in GaAs might provide better coherence times. One of the main reasons that there are relatively few experiments on holes in GaAs, as compared to electrons, is the difficulty of growing high-quality 2DHS that can be used to fabricate stable-hole nanostructures (such as quantum dots). However, recent advances in growth of 2DHS via carbon doping provide a new possible route to obtaining material of comparable quality to current high-mobility 2D electron systems in GaAs.

Optical Polarization-Based Genomic Sensor

165707
Year 2 of 3
Principal Investigator: R. Polsky

Project Purpose:

Optical fluorescence-based DNA assays are commonly used for pathogen detection and consist of an optical substrate containing DNA capture molecules, binding of target DNA sequences, followed by detection of the hybridization event with a fluorescent probe. Though fluorescence detection can offer exquisite signal-to-background ratios with high specificity, vast opportunities exist to improve current optical-based genomic sensing approaches. For instance, photobleaching, whereby fluorescent probes transition to a dark state under prolonged excitation, necessarily limits detection sensitivity. Furthermore, fluorescence detection requires relatively intense, narrow band excitation light sources, as well as expensive dichroic/band pass optical filters to isolate signal whose alignment tolerances may preclude deployment in rugged environments. Finally, particularly sensitive applications necessitate costly detectors to attain sufficient sensitivity, further decreasing overall robustness. Thus, there is a clear need to explore alternative optical sensing paradigms to alleviate these restrictions.

Bio-templated nanomaterial synthesis has become a powerful concept for developing new platforms for biosensing, as the biomolecule of interest can act as part of the sensing transducer mechanism. We will explore innovative genomic sensing methodologies based on interactions between light and nanoparticle assemblies. Rod-shaped, noble metal nanoparticles (nanorods) have been shown to strongly interact with light in a resonant fashion. This interaction can be many thousand-fold larger than fluorescent dyes, and does not suffer from photobleaching. However, the full potential of this phenomenon has yet to be realized. We will use nucleic acid hybridization as a means to link metal nanorods end-to-end, in order to create particle assemblies that are predicted to display unique properties for sensing specific genomic sequences. We will characterize the nanorod-DNA assemblies in complex media and explore the tunability of the optical properties of gold nanorod assemblies via dissimilar aspect ratios and widths and varying coupling geometries via DNA tertiary structures. Finally, we will synthesize nanorods exploring various surfactants to modulate binding strength of surfactant and DNA probe.

Programmable Piezoelectric RF Filters

165708
Year 2 of 3
Principal Investigator: C. Nordquist

Project Purpose:

We are exploring micromechanical modulation of distributed piezoelectric transducers to create the first widely tunable acoustic radio frequency (RF) filters, which will revolutionize RF filters. Currently, high quality factor (Q>1000) reconfigurable filters cannot be achieved because of the difficulty in tuning acoustic resonators and the large size of electromagnetic resonators. The planned programmable high-Q filter will dramatically reduce size, weight, and power for RF systems and will adapt to evolving performance requirements.

We are combining modeling and experiment to explore the fundamental coupling mechanisms in microelectromechanical systems (MEMS)-based piezoelectric modulation switches that serve as the fingers of an acoustic filter. Varying the distance between the MEMS switch finger and the substrate from nanometers to micrometers changes the electric field in the piezoelectric film, which in turn modifies the electromechanical transduction of the signal into and out of the filter. Switching individual fingers tunes the effective width and pitch of the transducer and reflector gratings, controlling the filter center frequency, coupling, and band shape. Additionally, designing the filter to avoid contact of the fingers with the piezoelectric film will reduce damping and increase Q.

Achieving this result requires meeting challenges in acoustic device modeling, microelectromechanics, and integration. In particular, the influence of surface contamination, roughness, stress, and charge state on the transduction must be understood by modeling, designing, fabricating, and characterizing a robust switchable element and filters. Also, the synthesis of the filter response must be modeled and refined using coupling-of-modes modeling and optimization.

This project is expected to enable a new class of programmable filters, advance the state-of-the-art, and enable new, smaller, and more efficient RF systems. This is the first attempt towards integrating a MEMS switch as a finger in a piezoelectric filter, and it presents novel science and engineering opportunities with high risk and high potential reward.

Computational and Experimental Characterization of Aluminum Nitride-Silicon Carbide Thin Film Composites for High Temperature Sensor Applications

165711
Year 2 of 2
Principal Investigator: B. Griffin

Project Purpose:

A number of important energy- and defense-related applications would benefit from sensors capable of withstanding extreme temperatures (>300 °C). Examples include sensors for automobile engines, gas turbines, nuclear and coal power plants, and petroleum and geothermal well drilling. Military applications, such as hypersonic flight research, would also benefit from sensors capable of 1000 C. Silicon carbide (SiC) has long been recognized as a promising material for harsh environment sensors and electronics. Yet today, many advanced SiC microelectromechanical systems (MEMS) are limited to lower temperatures because they are made from SiC films deposited on silicon wafers. Other limitations arise from sensor transduction by measuring changes in capacitance or resistance, which require biasing or modulation schemes that can withstand elevated temperatures. We circumvented these issues by developing sensing structures directly on SiC wafers using SiC and aluminum nitride (AlN, a high temperature capable piezoelectric material), thin films.

Summary of Accomplishments:

We demonstrated the first-ever aluminum nitride/silicon carbide based MEMS on SiC wafer process, coined XMEMS. We tested multiple device types, including ultrasonic transducers and contour mode resonators, successfully demonstrating their operation even after an exposure to a 935 °C anneal.

Significance:

Through this work, we were able to form a high temperature materials compatible process that allowed for survivability at extreme temperatures (up to 935 °C). We expect this work to enhance research in high temperature capable electronics and to enable missions in energy and national defense.

Refereed Communications:

B.A. Griffin, S.D. Habermehl, and P.J. Clews, "High Temperature Microelectromechanical Systems using Piezoelectric Aluminum Nitride," in Proceedings of *the IMAPS International Conference and Exhibition on High Temperature Electronics*, Albuquerque, NM, 2014.

B.A. Griffin, S.D. Habermehl, and P.J. Clews, "Development of an Aluminum Nitride-Silicon Carbide Material Set for High-Temperature Sensor Applications," presented (invited) at *SPIE DSS: Sensors for Extreme Harsh Environments*, Baltimore MD, 2014.

Development of a MEMS Dual-Axis Differential Capacitance

165823
Year 2 of 3
Principal Investigator: B. Griffin

Project Purpose:

Reduction of drag over a surface, due to both viscous skin friction and pressure separation effects, is an essential component of the effort to increase vehicle efficiency. Currently, there is no method for time resolved, direct measurement of wall shear stress at the spatial and temporal scales of turbulent flow structures inside model testing facilities. Indirect methods require extensive in situ calibration, and rely on inferred relations to produce a measurement. Direct sensors can circumvent these issues. Direct sensors based on microelectromechanical systems (MEMS) technology benefit from many favorable scaling effects which reduce overall measurement error, and retain spatial resolution while measuring small-magnitude forces. To prevent spatial averaging the sensor length scale needs to remain under 20 viscous wall units, where a typical wall unit can be on the order of 10 µm for a turbulent boundary layer. This scale sensor is achievable with MEMS. Prior designs at the University of Florida have yielded sensors that both measured static or dynamic shear stress and achieved a noise floor of 14.9 µPa with 102 dB of dynamic range. Previous sensors have been constrained to single axis sensing, carrying concerns over accuracy due to alignment in testing and multi-directional flow effects. Presently, there are no sensors capable of compliant dual-axis sensing at the microscale. A MEMS-based differential capacitance floating element shear stress sensor capable of sensing force inputs in two orthogonal in-plane directions will be developed. Differential capacitance sensing schemes using interdigitated multi-finger designs have been found able to achieve suitable levels of minimum detectable shear stress and dynamic range. By allowing for compliance and subsequent detection in two directions, a vector measurement of shear forces tangential to the surface will be produced. This work is in collaboration with the University of Florida.

In Situ Techniques to Characterize Creep and Fatigue in Freestanding Metal Thin Films

166154
Year 2 of 3
Principal Investigator: B. Boyce

Project Purpose:

Thin film mechanical properties are of critical importance in micro/nano-electromechanical systems (MEMS/NEMS). Despite increasing interests and potentials of thin-film metals as the materials of MEMS/NEMS devices, their mechanical properties have been explored much less than silicon, of which diverse mechanical properties such as Young's modulus, fracture strength, and fracture toughness as well as mechanical stability such as fatigue and creep characteristics have been comprehensively studied and established. However, silicon has limitations in some important application areas. Its high resistivity (typically larger than 10 micro-ohm-m) makes it difficult to be used in microswitches. Its relatively low optical reflectivity provides very limited opportunities in optical applications such as micromirrors. Recently thin-film metals such as aluminum have been noted as a great alternative in such applications where low electrical resistivity or high optical reflectivity is critical. However, in spite of their potential, their poorly known mechanical properties and reliability characteristics remain a big hurdle. Typically, thin-film metals tend to grow with much smaller grain size than their bulk counterparts, so are expected to provide higher mechanical strength and stability. In this study, we are developing an on-chip test method to examine the high temperature behavior of deposited metal films.

In collaboration with Carnegie Mellon, this new test technique enables the study of thin film creep and fatigue using MEMS design, processing and test methods. Initial prove-in work is performed on aluminum thin films. Once established, we aim to apply these tests to develop high strength multilayer thin-film metal stacks. Diverse applications for these materials are possible: 1) as low creep/fatigue materials in microrelays and micromirrors, 2) as damage-tolerant materials in extreme radiation environments [Misra, 2007] (e.g., in nuclear reactor walls), 3) as high-temperature high-strength materials, and 4) for x-ray focusing [Mitsuishi, 2010].

Decoupling Superconducting Transmon Qubits from their Quantum Bus/Readout Resonators to Enable Scaling

172334
Year 2 of 3
Principal Investigator: R. M. Lewis

Project Purpose:

Superconducting qubits have made great strides in coherence time, gating, and algorithms. However, to achieve real scalability, more is required. We will study the problem of coupling and decoupling a transmon, a popular type of superconducting qubit, from its host resonator, which serves the dual role of as a bus connecting qubits together, and a readout channel. The transmon couples to its host resonator via its electric-dipole moment. We plan to use a characteristic of quantum mechanics to null the dipole moment and decouple the transmon. In doing so, we hope to study a variety of physics associated with multi-qubit operation, control, and readout.

Reduced Dimensionality Lithium Niobate Microsystems

173126
Year 1 of 3
Principal Investigator: M. Eichenfield

Project Purpose:

Next-generation optical and radio frequency (RF) communications components require unprecedented bandwidth, low power, efficiency, and small size. Because of its superior piezoelectric coupling, low acoustic/optical loss, high nonlinear optical susceptibility, and optical transparency over broad wavelengths (350 to 5200 nm), Lithium Niobate ($LiNbO_3$) has found widespread use in RF filters, laser frequency doublers, and acousto-optic (AO) devices. We plan to develop a new class of acoustic, optical, and AO devices with orders of magnitude improvements in bandwidth, power consumption, efficiency, and size enabled by reducing the dimensionality of $LiNbO_3$ structures. By micromachining $LiNbO_3$ into suspended structures where the thickness and in-plane features are on the order of, or much smaller than, the acoustic/optical wavelength, the already outstanding piezoelectric and optical properties of $LiNbO_3$ can be significantly enhanced, with corresponding improvements in device performance. We will demonstrate these theoretical performance benefits in a novel AO modulator. Several scientific and technical problems must be solved including the realization of suspended $LiNbO_3$ structures with the desired small features, optical and acoustic properties and the modeling and co-design of AO structures in strongly anisotropic materials.

We will utilize Sandia's unique and extensive microfabrication and ion beam facilities to realize thin $LiNbO_3$ membranes with precisely controlled nanoscale features, a significant challenge for this brittle anisotropic material. We will use our experience in finite-element, plane-wave expansion, and finite-difference time-domain modeling to explore and simultaneously optimize the acoustic and optical device properties in this highly anisotropic media, where the piezoelectric and optical coefficients and wave velocities vary considerably with the material cut and propagation direction. Using this platform, we will demonstrate the co-confinement and coherent phase matching of acoustic and optical waves in an AO photonic/phononic crystal waveguide, enabling high diffraction efficiency (>80%), low power (< 10 mW), and operation at frequencies in excess of 1 GHz - surpassing current AO devices.

The Anatomy of the Minority Carrier — Atomic Cluster Interaction in Semiconductors

173127
Year 1 of 3
Principal Investigator: B. L. Doyle

Project Purpose:

This project will eventually use the nanoImplanter (nI) to produce a single heavy-ion-induced collision cascade, or defect clusters, in pn diodes, simulating cascades made by primary knock on atoms recoiled by neutrons, and then launch carriers into these clusters using scanned and highly focused light ions also from the nI. The ion beam induced charge (IBIC) signal produced by each light ion is expected to map regions of lower charge collection efficiency (CCE), and thereby reveal details of the shape of the cascade and the physics of recombination of carriers that interact with the cluster. The current plan is to use 200 keV Bi+2 to initiate the cascade, and 100 keV Li+1 for the scanned IBIC. The nI utilizes all electrostatic lenses and scanners, so both of these ions will focus and steer identically, and the cascade-cluster that is produced by the Bi will be centered in the area scanned by the Li. This year, we performed scanned IBIC experiments on the Pelletron uBEAM using He^{+} ions of energies from 300-750 keV on several pn diode candidates, and with different preamplifiers. The lowest noise recorded was 1.25 keV using a Linear Systems DPAD5 diode that had its passivation removed and an Amptek A250 preamp mounted inside the uBEAM end station. Such low noise values are critical to the experiment so that the arrival of a single Bi ion can be detected, and that the contrast in the Li IBIC signal is adequate to measure the anticipated small changes in CCE. The DPAD5+A250 combination was engineered into a compact unit that fits in the cooled and instrumented stage on the nanoImplanter, and experiments on the nI will start the first quarter of FY 2015. The comparison of results with carrier transport and recombination codes provide improved understanding of the carrier-cluster recombination physics and may potentially lead to improved parameterization of carrier recombination used by Qualification-Alternatives-to-the-Sandia-Pulsed-Reactor (QASPR) Program.

Seebeck Enhancement via Quantum Confinement in MOSFETs: Towards Monolithic On-Chip Cooling

173128
Year 1 of 3
Principal Investigator: I. F. El-Kady

Project Purpose:

We will utilize quantum confinement effects in 2D electron (2DEG) and hole (2DHG) gases in metal-oxide-semiconductor field-effect transistor (MOSFET) structures to enhance the Seebeck coefficient (S) and subsequently the thermoelectric figure-of-merit ZT given by (S^2*sigma/k)T; where sigma and k are the electrical and thermal conductivities, respectively. Due to the inherent difficulty of improving S, most published attempts focused on reducing k to improve the overall ZT. The fundamental problem with this approach is that electrical and thermal conductivities are interrelated: attempts to reduce k by incoherent phonon scattering often inadvertently also scatter electrons, resulting in a concurrent reduction in sigma and hence minimal overall gains in ZT. Here, we delaminate the electrical and thermal paths, and suggest a route by which all three components of ZT are optimally modified.

The uniqueness of our approach is based on decoupling the electrical and thermal paths to address all three components of ZT by using an inversion-mode MOSFET structure. The existence of source/body and drain/body barrier potentials acts to isolate the MOSFET body electrically, leaving the high sigma inversion channel as the only viable electrical path. By operating the MOSFET under strong inversion, a 2DEG (2DHG) is realized where quantum confinement effects prevail, leading to an enhanced electronic density of states near the Fermi level, hence boosting S. In this arrangement, the thermal conductivity will be dominated by the phonon population propagating through the MOSFET's body. Thus, if realized in a low-k semiconductor material, such as SiGe, the overall predicted thermoelectric performance is very promising and could enable the realization of highly efficient, integrated on-chip cooling. Because of the lack of SiGe-complementary metal-oxide-semiconductor (CMOS) capabilities at Sandia, we intend to use Si-based systems to demonstrate the quantum confinement physics. At the same time, we also intend to validate these predictions in SiGe nanowires fabricated at the Center for Integrated Nanotechnologies in a cylindrical MOSFET system with a wrap-around gate.

Beyond Moore's Law through 3D-IC Fabrication

173129
Year 1 of 3
Principal Investigator: D. B. Burckel

Project Purpose:

The goal of the research is to develop 3D integrated circuits (ICs) at both the device and system levels, and furthermore to apply these circuits to hybrid technologies such as complementary metal-oxide-semiconductor (CMOS)/photonic and CMOS/biological applications. Today's ICs are fabricated using top down techniques on planar surfaces. Scaling areal transistor density has continued to increase IC performance, but requires increasingly expensive lithography equipment. An approach using 3D fabrication has been identified to extend effective areal density, but current methods for 3D fabrication at the sub-micron scale are rare, typically not CMOS-compatible and lack high-volume manufacturing scalability.

Recently, we invented and demonstrated membrane projection lithography, a microfabrication technique where directional deposition through a suspended, patterned membrane was used to create micron-scale 3D metamaterials. By generalizing this fabrication approach to include patterned etch and patterned ion implantation, combined with blanket processes such as oxidation, dielectric deposition and planarization, we will provide a first-of-its-kind approach to 3D-IC fabrication.

Creation of 3D circuits will transform devices, systems and technologies:
<u>Devices</u>: Fabrication in 3D enables higher transistor packing density, new geometries for devices such as power transistors, and the possibility of making radiation hardened CMOS on non-silicon on insulator (SOI) substrates.

<u>System</u>: 3D-ICs will be more difficult to reverse engineer while providing new topologies for interconnect/signal routing, improving signal integrity and RC delay.

<u>Technologies</u>: For the first time, hybrid technologies where biological cells or photons are interfaced directly to CMOS control/sensing electronics are possible with a mature 3D-IC platform. In order to realize these benefits, we need an entirely new fabrication paradigm capable of creating complex 3D structures in a sub-micron CMOS compatible platform and addressing issues of thermal budget, device isolation, interconnect strategies, and 3D topography-induced stress.

A New Approach to Entangling Neutral Atoms

173130
Year 1 of 3
Principal Investigator: G. Biedermann

Project Purpose:

We will pursue the development of a new technique for entangling neutral atoms that will show feasibility of significant metrological gains. A successful outcome will directly impact the emerging field of "quantum sensing" and position us to lead future work. The principal motivation for harnessing entanglement in the context of quantum sensing is the superior scaling of sensitivity with atom number, N, when compared with classical sensing (e.g., N versus sqrt(N), respectively). While the advantage with a small number of atoms is moderate, it reaches an order of magnitude improvement with only 100 atoms. Neutral atoms are the most compelling candidate for quantum sensing with entangled systems because they have been broadly shown to make exceptional sensors of time, radio frequency fields, static magnetic and electric fields, gravity, and Casimir-Polder forces. However, the fidelity of entangling two atomic qubits is thus far limited to 75%, a number unsuitable for entangling many atoms. Our new Rydberg-dressed approach offers the potential to surpass this fidelity.

A Rydberg-dressed approach to entanglement in neutral atoms can realize high fidelity and long-lived coherence in free-fall interferometers, an unprecedented achievement. Entangling neutral atoms currently uses resonant excitation to a Rydberg level, allowing atoms to interact via electric dipole-dipole coupling. The primary limit to fidelity is the thermal motion of the atoms that causes the exciting laser beams to imprint random phases on the quantum states and thereby degrade the coherence of the entangling interaction. However, by employing adiabatic evolution induced by a laser tuned off-resonance from a high-lying Rydberg level, the coherence is much more robust. Two-qubit entanglement with fidelities near 99% should be achievable with technology already in place. In addition, the interaction of atoms in highly excited Rydberg states allows for unique entangling operations beyond two-qubits that are not easily accessible in other technologies. We anticipate multi-faceted impacts in both quantum sensing and computation.

Fundamental Scaling of Microplasmas and Tunable UV Light Generation

173131
Year 1 of 3
Principal Investigator: R. P. Manginell

Project Purpose:

Microplasmas utilize scaling to operate at atmospheric pressure and micron-scale dimensions. This generates unique microplasma device (MD) behavior, including high electron densities and the efficient creation of excimer states and intense ultraviolet (UV) emission down to 65 nm. Similar behavior in the macroscale would require low-pressure, high-frequency operation. However, the physics of microplasmas is relatively new and with few connections to modeling/theory. In particular, non-direct current microplasmas are relatively unexplored via modeling/theory, despite their enhanced electrode lifetimes and UV emission.

This project seeks to understand the fundamental physics of scaling and UV emission in MDs by a combined experimental-modeling approach. We will develop and publish for the first time experimentally validated fully kinetic models of MD in the DC (direct current) and non-DC realms. Published models, which have been restricted to DC operation, make many assumptions, including electron energy. Fully kinetic models implicitly calculate such physics, leading to more accurate results. Kinetic plasma modeling in complex geometries requires the specialized computational resources and expertise developed at Sandia. Deep UV measurements from MD are extremely challenging and require specialized tools and expertise that we are developing for this purpose. These tools will be useful for this project and others at Sandia and within the broader scientific community. This study will allow for the eventual development of useful MD applications like photonics (light sources for atomic and quantum physics, and laser gain media) and chemical ionization/detection. MD offer wavelengths less than 200 nm needed for many quantum/atomic and chemical applications, a range not easily amenable to solid-state light sources.

Zero-Power Wake-Up Device

173132
Year 1 of 2
Principal Investigator: R. W. Brocato

Project Purpose:

The purpose of the project is to fabricate an optimum pyroelectric demodulator component needed in a zero-power radio receiver. The pyroelectric demodulator is a microwave microelectronic component invented at Sandia. The Zero-Power Receiver is a microwave/radio frequency (RF) device that makes use of the pyroelectric demodulator for receiving radio signals using unpowered or ultra-low power electronics. The Zero-Power Receiver has an advantage over conventional radio-frequency identification (RFID) devices in that it can operate at much greater ranges than unpowered RFIDs. Modern unpowered RFID devices in commercial applications make use of semiconductor junction devices to detect and demodulate received RF signals. Commercial unpowered RFIDs have been limited to signals with enough received voltage to turn on a semiconductor diode. The pyroelectric demodulator, used in the Zero-Power Receiver, has no diode knee voltage because it has no semiconductor depletion region. It is a thermal device, not a semiconductor device. The pyroelectric demodulator is the key component needed to enable the Zero-Power Receiver. Hence, this project focuses on creating and optimizing the pyroelectric demodulator. To accomplish this, the project has four different goals. The first goal is to package, test, and characterize legacy devices produced in FY 2006 and FY 2007 that had previously been probe-tested but had never been successfully packaged. The second goal is to design, fabricate, and test pyroelectric demodulators using mesa structures of lead-zirconate tantalate (PZT). These first two goals were met in this fiscal year. The third goal is to prepare thinned, wafer-bonded lithium niobate substrates. The final goal is to design, fabricate, and test crystalline pyroelectric devices, using lithium niobate prepared from the third goal, and to design, fabricate, and test improved PZT devices.

Metal-Organic Framework Thin Films as Gas-Chromatography Stationary Phases for the Detection of Toxic Industrial Chemicals

173133
Year 1 of 2
Principal Investigator: D. Read

Project Purpose:

Toxic industrial chemicals (TICs) represent a large class of ubiquitous, highly volatile chemicals that pose a threat to human life and the environment though accidental or terrorist release. Example TICs include: chlorine gas, hydrogen cyanide, hydrogen sulfide, sulfur dioxide, and formaldehyde. The Department of Homeland Security, Defense Threat Reduction Agency, and National Counterterrorism Center have all identified TICs as a major area of concern for possible chemical attack. Current Sandia microfabricated gas-chromatography (µGC) columns are not suited to the detection of TICs due to their poor retention characteristics on traditional polymer sorbent materials. A need exists for a material that can fill this gap in chem-detection capabilities. One such class of candidate materials is that of metal-organic frameworks (MOFs). MOFs are crystalline materials containing inorganic clusters crosslinked by a rigid organic network. They are highly porous, thermally stable, and possess tunable chemical sorption affinity through modification of their chemical functionality and pore structure. MOFs have been demonstrated to be well suited for small molecule absorption.

The purpose of this project is to integrate surface-mounted metal-organic framework (SURMOF) materials with Sandia's current µGC columns to enable the portable detection of high-volatility analytes such as TICs (µGCs are necessary to meet the power and size requirements of a portable GC system). The use of SURMOFs as µGC-column stationary phases has not yet been demonstrated in the literature, constituting a new approach to address these challenging µGC separations. The successful integration of MOFs and µGCs would not only offer a valuable and innovative solution to this chemical detection crux, but would also further knowledge in the field of MOF research through the development of a method for quickly determining chemical/MOF sorption thermodynamic constants using gas chromatography instrumentation. In addition, a stationary phase for high-volatility analytes would dramatically expand the repertoire of detectable compounds for Sandia's various microanalysis systems.

A Space-Like Low-Energy Proton Test Environment to Rapidly Qualify Advanced Microelectronics for Flight Readiness

173134
Year 1 of 2
Principal Investigator: N. A. Dodds

Project Purpose:

For the past 30 years, space programs have predicted the rate of occurrence of radiation-induced errors in microelectronics using the same general set of testing and modeling methods. These methods have broken down in the past few years because, unlike older technologies, new highly scaled (sub 100 nm) technologies are so susceptible to charged particle strikes that now even low-energy protons are able to trigger errors through direct ionization. These protons are abundant in most space environments and, therefore, might dominate on-orbit error rates. New error rate prediction methods have been previously suggested to deal with this new mechanism, but they are impractical because implementing them requires over one year per integrated circuit (IC). To enable the reliable use of cutting-edge ICs in space, we aim to create a space-like proton test environment in which the on-orbit error rate caused by this mechanism could be determined through a one-hour test. This environment will first be designed through computer simulations and will then be built, characterized, and used to investigate the contribution of this mechanism to on-orbit error rates. If successful, this R&D will enable spacecraft designers to rapidly quantify the risk of using cutting-edge ICs in space radiation environments, allowing higher performance systems to be constructed.

Multifunctional Integrated Sensors (MFISES)

173269
Year 1 of 3
Principal Investigator: B. D. Homeijer

Project Purpose:

Self-powered autonomous sensor systems would be a great benefit for many national security applications, including border and infrastructure security, and soldier health monitoring. Large channel count wireless arrays on structures such as pipelines and autonomous sensors are just two applications where replacing a battery is either impractical or dangerous. The applications are vast and most previously suggested solutions are specific to the given application. This work is focused on developing self-powered multifunctional sensor nodes to achieve generic sensing platforms suitable for wireless network integration and real-time monitoring in a range of applications such as unattended ground sensing, infrastructure monitoring, and soldier health monitoring. The architecture of the node includes: 1) devices and electronics to harvest, manage, and store electrical energy, 2) a multifunctional sensor, 3) a low-power microcontroller, and 4) low-power communications.

This research is focused on the sensor and energy harvester components. The projected sensor nodes will provide pivotal enabling technology in the emerging technologies of autonomous wireless sensor networks. Current sensor node technologies are cumbersome by wiring requirements to meet power demands, limited in deployment duration by expendable power sources, and are designed to measure only a single parameter. Incorporating onboard multi-functional energy scavenging with a multi-functional sensor would greatly increase the utility and potential deployment space of the sensing networks. In addition, sensor node manufacturing based on high-volume integrated circuit (IC) and microelectromechanical systems (MEMS) technologies can greatly reduce the cost and size of the sensor nodes. Finally, the broad functionality and self-contained design will enable the use of the sensors in a broad range of applications while providing measurement data on important parameters for real-time sensing. Potential applications for this work include remote chemical sensing, real-time structural health monitoring, and many other areas. The work is in collaboration with Stanford University.

Chemical Vapor into Liquid (CViL) Encapsulation of Microorganisms for Hazardous Agent Detection

173339
Year 1 of 3
Principal Investigator: J. C. Harper

Project Purpose:

To detect chemical and biological threats both on and off the battlefield, development of portable, robust detection systems capable of real-time identification of these threats is essential. Living cell-based sensors have proven effective as sensitive and specific detectors, capable of near real-time detection. However, living cell-based sensors require frequent replenishment with new cells due to cellular sensitivity to the ex-vivo environment. To make cell-based devices practical for implementation, cells must be encapsulated in a biocompatible matrix that protects cells from environmental stresses, maintains biological sensing functions, and allows cellular interaction with the sensing environment. Silica materials have promising potential as encapsulation matrices, with advantages such as biological inertness, mechanical stability, simple room temperature processing, and tunable material and chemical properties. However, traditional, aqueous sol-gel routes are cytotoxic to cells, limiting their use for biosensor design.

To generate stable biosensing components, living cells need to be encapsulated in silica matrices that allow cellular interaction with molecules of interest, while maintaining cell viability. In collaboration with the Tartis Laboratory at New Mexico Tech, we will use a novel sol-generating chemical vapor into liquid (SG-CViL) process to encapsulate genetically engineered *S. cerevisiae*, *E. coli*, and B-lymphocytes in porous, nanostructured silica shells as model biosensing components. This process minimizes cell contact with cytotoxic reaction constituents, allows precise control of reaction parameters, and facilitates incorporation of components, such as polyethylene glycol, that enhance silica gel biocompatibility. These factors make SG-CViL attractive as an encapsulation strategy for biosensor design. This work focuses on characterizing cell-silica biocomposites, assessing encapsulated cell activity, and optimizing cell-silica biocomposites for particular sensing functions. Successful development of SG-CViL will be a significant step in designing biosensors that use cells as the sensing unit, potentially leading to devices capable of detecting multiple threat agents at very low concentrations.

Piezoelectric Nano-Optomechanical Systems

173496
Year 1 of 3
Principal Investigator: M. Eichenfield

Project Purpose:

The field of nano-optomechanical systems (NOMS) investigates the properties of photon-phonon interactions confined to nanoscale volumes, as well as the potential applications of these interactions. Optomechanical crystals (OMCs) are man-made metamaterials that allow both light and sound vibrations to be confined within the nanoscale volume, where they strongly interact. Experiments on OMCs have been used to test quantum limits and study the quantum effects in mechanical systems due to their exquisite sensitivities to mechanical motion. However, many potentially groundbreaking applications of these systems are still outstanding.

An area that is only beginning to be explored in this field is photon-phonon-charge interactions in NOMS using optically transparent piezoelectric materials, such as aluminum nitride and lithium niobate. Previous devices were fabricated using silicon and silicon nitride, which are not piezoelectric. However, Sandia has developed new capabilities in the micromachining of piezoelectric thin films, and these capabilities could and should be used to study optomechanics in piezoelectric materials.

In addition to more standard photon-phonon interactions, piezoelectric NOMS also include electromechanical piezoelectric interactions, essentially coupling the internal charge distribution of the material to the light and mechanical vibrations. The dynamics of these kinds of systems are largely unexplored and offer myriad possibilities for study of their fundamental properties and potential applications.

Creating piezoelectric NOMS devices is extremely worthwhile goal, but it is also an extremely challenging one. To make these devices, one needs to precisely fabricate nanoscale systems in materials like lithium niobate and aluminum nitride, which are difficult to fabricate and still experimental compared to more standard CMOS materials. Moreover, there are theoretical, numerical, and experimental challenges to solve to design and test such devices. The work is in collaboration with University of New Mexico.

Defect Characterization in Low Bandgap Materials

173665
Year 1 of 2
Principal Investigator: E. A. Shaner

Project Purpose:

New infrared (IR) focal plane arrays composed of III-V detector elements, which employ band gap engineering techniques such as nBn and strained-layer superlattices (SLS), have recently demonstrated performance improvements over current HgCdTe (MCT) technology, such as improved detection at higher operating temperatures. The III-V materials are less costly to fabricate and can be produced with greater uniformity than MCT, making them better suited for many applications employing IR focal plane arrays (FPAs), especially those requiring larger format, higher sensitivity, and better operability.

The purpose of this effort is to conduct research into specific generation-recombination and dark current producing mechanisms of modern III-V material systems to aid in minimizing their impact on device performance. The nBn device architecture has experimentally proved its superiority over MCT and InSb and we understand its optimization parameters well. However, the fundamental dark current diffusing from the absorber limits its performance to a level only marginally better than MCT. We will utilize deep level transient spectroscopy (DLTS) to quantify the defects existing in these materials. Under the project, we will study defects in nBn absorbers such as InAsSb, as well as GaSb/InAsSb and InAs/InAsSb strained layer superlattice (SLS) material systems and correlate measurements with growth conditions and crystal structure.

Electric Field Control in Vertical and Lateral GaN-Based Power Transistors for Enhanced Breakdown Voltage

176307
Year 1 of 1
Principal Investigator: R. Kaplar

Project Purpose:

Significantly improved power electronics are required to facilitate energy efficiency in the United States, especially as more renewable energy sources are brought online. Due to its higher critical breakdown electric field, gallium nitride (GaN) has theoretically superior performance compared to both conventional silicon (Si) and emerging silicon carbide (SiC) technologies. However, realizing this potential in a practical device has been severely hampered by the significant deviation of the electric field distribution from that of an ideal planar junction. Without proper electric field control, the theoretical potential of GaN for power devices will not be realized. Such concepts are well known in the Si power device world, and electric fields are routinely controlled and indeed intentionally manipulated in this mature technology, which has allowed the creation of "superjunction" devices that exceed the ideal planar-junction performance. It is the purpose of this project to implement several field-control schemes in GaN power devices, to gain experience with the practical challenges of power device fabrication, and to build a foundation in GaN power devices at Sandia. This project will leverage Sandia's extensive experience in GaN epitaxial materials growth, obtained through many years of work as the lead national laboratory focused on solid-state lighting. Likewise, Sandia has extensive expertise in the design and simulation of semiconductor devices that will be applied to GaN power electronics. Moreover, the Microsystems and Engineering Sciences Application (MESA) microfabrication facility is an exceptional resource that will be extensively utilized for the project. A number of unique approaches to electric field control, including low n-type doping, integration of n- and p-type regions, resistive field plates, and lateral variation of doping, will be implemented. While these and other techniques are widespread in the Si world, such concepts have barely begun to influence GaN power devices.

Summary of Accomplishments:

We achieved controllable n-type doping in GaN, with the electron density $n < 10^{16}$ cm^{-3}. This represents the state-of-the-art in the field and is sufficient to fabricate vertical Schottky or PiN diodes with breakdown voltages exceeding 5 kV. We examined GaN growth on native GaN substrates obtained from three different vendors, and observed significant differences in the properties of the epilayers on the three types of substrates, even when the epilayers were grown during the same run. This implies a significant impact of substrate on carrier density and other material and device properties. We also successfully integrated p-type layers doped in the mid-10^{17} cm^{-3} range with our low-doped n-type drift layers, as needed for PiN diode fabrication. Numerical simulations of guard-ring field-termination structures demonstrated the effectiveness of such structures in improving the breakdown voltage of vertical diodes. Breakdown voltage showed greater sensitivity to guard ring spacing than width. For lateral power HEMTs, we simulated several field-control approaches including the use of discrete external resistors and a continuous internal resistive field plate to produce a more uniform electric field within the device and a commensurately higher breakdown voltage. The simulations demonstrated that the ideas work, and a technical advance was filed. Resistive films suitable for fab implementation of the idea were grown and characterized, and Ohmic contacts were demonstrated on several of these films. Analytical approximations as well as simulations suggested that the RC time constant introduced using this approach may undesirably slow switching time, so a second approach was also derived analytically and was simulated, which flattens the electric field and increases breakdown voltage through the introduction of a laterally graded charge profile. This approach was also shown to be viable. Initial measurements to understand field-induced reliability issues were also performed on lateral High Electron Mobility Transistors (HEMTs). The electric field-control schemes created, particularly for lateral HEMTs, represent the state-of-the-art.

Significance:

Achieving low n-type doping in GaN is a hurdle involving both epitaxial growth and defect physics, and this project represents a scientific approach to this problem. The project has laid the foundation for a GaN power device capability at the Labs, and provides the knowledge and experience needed for fabrication of efficient GaN power electronics devices. GaN power devices have numerous potential applications to national security missions, chiefly due to their ability to increase the power density of power converters (commonly referred to as size, weight, and power, or SWaP) as well to enable operation in extreme environments. Such devices will likely find application in the incorporation of renewable energy sources (solar, wind) and large-scale energy storage necessary to address the issue of renewable source intermittency in the electric grid. Other applications include electric vehicles, aircraft, and ships (both for civilian and military applications), as well as more efficient power management for lower power (but numerous and energy-consuming) applications such as home appliances and computers.

Combining Interferometric Lithography with Membrane Projection Lithography

179753
Year 1 of 1
Principal Investigator: D. B. Burckel

Project Purpose:

The goal of this small footprint research project was to establish a baseline process for using interferometric lithography (IL) to perform resist patterning. By successfully developing this methodology, we can then combine interferometric lithography with membrane projection lithography to create a wide range of artificial dielectric materials. In addition to enabling the creation of artificial dielectrics with sub-micrometer inclusions, developing a generic IL capability at Sandia will allow us to explore a wide variety of 1-D, 2-D, and 3-D structures with micron-scale periodicity.

Summary of Accomplishments:

We successfully created interference fringe patterns using the laser setup. This is the necessary first step to establishing interferometrically patterned structures.

Significance:

We now have an interferometric lithography setup at Sandia. We anticipate many potential energy storage, catalysis and sensing research to emerge out of this capability, with applications that could have significant potential impact to DoD and DHS customers.

RADIATION EFFECTS AND HIGH ENERGY DENSITY SCIENCES

The Radiation Effects and High Energy Density Sciences Investment Area seeks to advance science and engineering in the areas of radiation effects science, high energy density science, and pulsed power science and enabling technologies.

The goal of the radiation effects sciences area is to ensure that engineered systems are able to operate as intended in radiation environments they encounter. Researchers are developing new radiation-resistant materials and technologies and creating technology to generate extreme radiation environments. They are advancing materials, switching, power flow, and engineering to build reliable pulsed power systems.

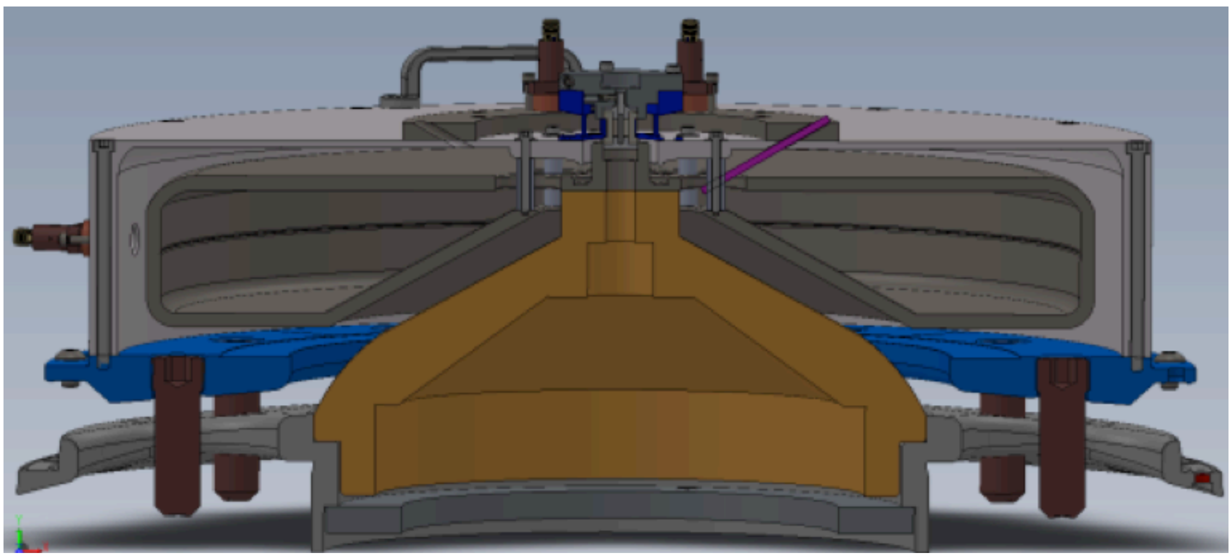


Diagram of an experiment-ready Load Current Multiplier designed for use on Z hardware. Dynamic material properties experiments on the Z Facility obtain equations of state data for materials at multi-megabar pressures with unprecedented precision. (Project 165740)

RADIATION EFFECTS AND HIGH ENERGY DENSITY SCIENCES

Fundamental Studies on Initiation and Evolution of Multichannel Discharges and their Application to Next-Generation Pulsed Power Machines

158858
Year 3 of 3
Principal Investigator: J. Schwarz

Project Purpose:

Future pulsed power systems may rely on linear transformer driver (LTD) technology. The LTDs will be the building blocks for a driver that can deliver higher current than the Z machine. The LTDs would require tens of thousands of low inductance (<85nH), high voltage (200kV DC) switches with high reliability and long lifetime (>>10^4shots). Sandia's Z machine employs 36 megavolt class switches that are laser triggered by a single channel discharge. This is feasible for tens of switches but the high inductance and short switch lifetime, associated with the single channel discharge, are undesirable for future machines.

Thus, the fundamental problem is how to lower inductance and losses while increasing switch lifetime and reliability. These goals can be achieved by increasing the number of current-carrying channels. The rail gap switch is ideal for this purpose.

Although those switches have been extensively studied, each effort has only characterized a particular switch. There is no comprehensive understanding of the underlying physics that would allow predictive capability for arbitrary switch geometry. We will study rail gap switches via an extensive suite of advanced diagnostics in synergy with theoretical physics and advanced modeling. Design and topology of multichannel switches as well as discharge dynamics will be investigated. This involves electrically and optically triggered rail gaps and multisite switch concepts.

This research is aimed at gaining a full understanding of the underlying physics that drives the behavior of either optical or electrical triggered rail gap switches. The biggest risk factors are the complexity of the modeling and the fact that some triggering techniques may turn out to be cost prohibitive on a large-scale machine. The research has tremendous payoff since it will provide a comprehensive understanding and predictive capability of high repetition rate, high reliability, and long lifetime switches which is an enabling technology for a realistic pursuit of next-generation pulsed power fusion machines.

Summary of Accomplishments:

We have developed an advanced high voltage (HV) test stand for development of next-generation switches. HV switching is the essence of pulsed power. Lower inductance switches could allow more compact LTD components, which could enable cost effective drivers for applications ranging from material science to fusion. The switch testbed we developed can accept a wide variety of switches and has a built-in suite of advanced diagnostics. The system is also fully self-contained and easily movable so that it can serve as a resource for Sandia. Recently, this test stand has been used to develop the first-ever 200kV DC-charged rail switch with which we were able to reduce the overall circuit inductance of an LTD brick from formerly 135nH to 85nH, a 30% reduction. This switch employed dry air with moderate hold-off pressures that is a great benefit in terms of environment, safety and health concerns (historically those switches have been using SF_6) and will allow for scalability to large pulsed power machines. Optical diagnostics have also led to a new understanding of rail switch dynamics.

In preparation for fielding a laser-triggered option, we investigated the interaction of fiber transported laser beams when focused on various metal electrodes. As part of this study, we developed a new method for measuring the size of laser generated plasma plumes.

Furthermore, we have succeeded in running fully kinetic 3D full-scale particle-in-cell (PIC) simulations at realistic switch geometries and pressures. These runs are very complex and track up to 18 “particle species” in dry air. We also continued the development of a free space nonlinear laser beam propagation code. This code includes: diffraction, group velocity dispersion, third order dispersion, self-focusing, plasma defocusing, multiphoton ionization, multiphoton absorption, self-phase modulation, beam splitting, Raman effects, avalanche ionization, and more.

Significance:

Low inductance, long-lived switches are the key component in lower cost, high power, pulsed power machines. We gained a new understanding of multichannel switching which could lead to improvements for future pulsed power machines (e.g., Thor). The newly developed test stand will also serve as a great resource for Sandia.

More research is needed, but ideas for production line switches already exist.

A New Capability to Model Defects in InGaAs and InGaP Alloys

158860
Year 3 of 3
Principal Investigator: A. F. Wright

Project Purpose:

Because point defects can degrade the performance of semiconductor-based electronic and optoelectronic devices, they have been studied for the past 50 years using a wide variety of experimental techniques. In spite of this effort, significant knowledge gaps remain to the extent that density functional theory (DFT) calculations are being used to obtain many of the defect characteristics (formation energies, energy levels in the gap, thermal diffusion processes, and athermal diffusion processes) needed to develop atomistic models of gain degradation and recovery in radiation-hard group-III/group-V (III-V) devices at Sandia. Currently, DFT capabilities exist to compute defect characteristics in binary III-V semiconductors such as GaAs. However, a direct application of these capabilities to an III-V alloy (such as InGaAs) is not feasible because defect characteristics are sensitive to nearby group-III site occupations (Ga or In), which vary with location in an alloy. The objective of this project is to develop a new capability that can provide point defect characteristics with DFT-level precision in an alloy and to use this capability to obtain the characteristics of the As interstitial in InGaAs. The most important element of this new capability is a "cluster expansion," which yields the formation energy of a defect at an arbitrary location in the alloy (i.e., for an arbitrary set of nearby group-III site occupations {GA or In}). There are two challenging aspects to developing cluster expansions for defects in InGaAs: 1) defects in semiconductors can have a multitude of charge states and configurations, both of which carry technical challenges, and 2) based on our prior investigations of the As interstitial in GaAs, we expect the As interstitial to be highly mobile in InGaAs because of both thermal and athermal diffusion processes.

Summary of Accomplishments:

This project has developed a new theoretical capability which can be used to advance understanding of defects in semiconductor alloys, including the time dependence of their thermal and carrier-induced diffusion rates for which there is currently no information available from experiments. Specifically, the new capability enables kinetic Monte Carlo (KMC) simulations of defect diffusion in semiconductor alloys with DFT accuracy by pioneering the development of cluster expansions of DFT formation energies of stable and metastable defect states and of defect diffusion saddle points. The cluster expansions involve alloy sites near the defect, and innovative new techniques were developed in this project for both identifying the most important nearby alloy sites and mitigating the effects of the sites further away from the defect, which are not explicitly included in the cluster expansion. The new capability was demonstrated by performing KMC simulations of the thermal diffusion of a -1 As interstitial defect in an $In_{0.5}Ga_{0.5}As$ alloy. The simulations yield a time-dependent diffusion rate, which arises from the large (>1 electron volt) variation in the defect formation energy with respect to the nearby alloy site occupancies, and hence, to the location of the defect in the alloy. In addition to studying defect diffusion, we also examined the effect of alloying on the thermodynamic energy levels of the As interstitial in a variety of different configurations. The mean levels (averaged over the alloy configurations from which the cluster expansions were derived) were similar to those found for the As interstitial in GaAs, while the standard deviations were on the order of 0.1 electron volt).

Significance:

Recently, the material of choice for radiation-hard electronic devices has begun to shift from silicon to III-V semiconductors such as GaAs, InAs, and their InGaAs alloys. Computer codes being developed to help qualify radiation-hard devices for short-pulse neutral irradiation currently presume that defect diffusion rates do not change with time and, thus, do not fully capture physical processes that can arise in advanced radiation-hard devices. The new capability that has been developed in this project can be used both to understand these processes and to enable their inclusion in these codes.

Investigate Emerging Material Technologies for the Development of Next-Generation Magnetic Core Inductors for LTD Pulsed Power Drivers

158861
Year 3 of 3
Principal Investigator: D. L. Huber

Project Purpose:

The use of magnetic cores in linear transformer drivers (LTDs) creates a significant risk to the success of realizing next-generation pulsed power drivers. Costs are extremely high and fabrication schedules are not aligned to forecasted requirements due to materials utilized and complex manufacturing methods. A breakthrough research and development effort focused on the utilization of emerging advanced high performance materials for this critical pulsed power component is required to assure that product performance, cost, and availability meet the requirements of this critical pulsed power driver component.

This project aims to design and synthesize a novel material for a pressing need in pulsed power technology. The use of iron nanoparticle composites as magnetic core inductors (e.g., for transformer cores) has been discussed in the literature recently, but has never been realized. There are a number of scientific hurdles to the creation of this material that must be overcome. First, we must devise new synthetic methods to produce iron nanoparticles of the appropriate size (estimated to be 10-20 nm) to optimize performance. Second, we must disperse these particles into an appropriate non-magnetic matrix material, such as a polymer, to create the desired nanocomposite. Finally, we must better understand the structure-property relationships in these magnetic nanocomposites at a basic physics level, as the structural details will determine the performance of this class of materials.

Summary of Accomplishments:

We have developed a new material for transformer applications based on a matrix-free nanocomposite. The material represents a significant improvement over current materials in cost, scalablility, and performance. Significant improvements are seen in hysteretic losses and susceptibility. This new material is expected to replace the amorphous alloys currently used in high frequency applications. As economies of scale develop, the material could be much more broadly applied to high efficiency transformers.

While much of the work here was of a fundamental nature, an effort was made to look forward to developing a scalable method for creating this material. Reactions were expanded to the 100g levels to allow engineering scale parts to be made and tested. Detailed plans were made to allow expansion to the multi-kilogram level, and a concept developed to allow scaling to the ton level.

Significance:

The material developed here may potentially impact the pulsed power research in the DOE, with its significant national security implications. This is also an enabling technology for fusion energy production that can provide energy security. The work also developed new chemistry and materials engineering.

Time-Dependent Resistivity of Millimeter-Gap Magnetically Insulated Transmission Lines Operated at Megampere/ Centimeter Current Densities

164759
Year 3 of 3
Principal Investigator: B. T. Hutsel

Project Purpose:

Magnetically insulated transmission lines (MITLs) are commonly used in the final stages of pulsed power systems to transfer power at high voltage and current to the physics package load. Future pulsed power systems, which will deliver greater power to the load, will require MITLs to transfer power at greater voltage and current. Minimizing current loss within the MITL will be a critical design issue for these larger pulsed power systems.

This research will investigate current loss in a MITL at megampere/centimeter lineal current densities due to gap closure. Gap closure occurs when plasma forms within the MITL anode-cathode gap providing a conductive path for current to be shunted away from the load, resulting in reduced power transferred to the load.

Current loss within a MITL will be characterized as a function of gap distance, peak current, peak voltage, and pressure in the MITL gap. Surface chemistry will be considered and gap closure will be investigated relative to vacuum surface conditions and MITL-electrode cleaning procedures. In addition to experimental results, a theoretical model of gap closure will be developed with the aid of particle-in-cell (PIC) simulations.

This research will extend existing knowledge of MITL behavior at high lineal current densities. The main technical challenges include quantitatively characterizing the vacuum surface conditions to determine their effect on MITL current loss. Development of a theoretical model of gap closure though combination of experiment results and PIC simulations will aid in the design of MITLs used in future pulsed power machines.

A systematic study focused on gap closure, combined with new simulation capabilities, has yet to be performed. The experiment will yield a more thorough understanding of gap closure within a MITL. Results from characterizing MITL performance at high current densities will aid in designs of future pulsed power accelerators necessary to extend high energy density physics (HEDP) research.

Summary of Accomplishments:

An experiment platform was designed to study vacuum power flow in MITLs. The experiments conducted quantified the current loss in a millimeter-gap MITL with respect to vacuum conditions in the MITL for two different gap distances, 1.0 and 1.3 mm. The current loss for each gap was measured for three different vacuum pump-down times. As a ride-along experiment, multiple shots were conducted with each set of hardware to determine if there was a conditioning effect to increase current delivery on subsequent shots.

The experiment results revealed large differences in performance for the 1.0 and 1.3 mm gaps. The 1.0 mm gap resulted in current loss of 40%-60% of peak current. The 1.3 mm gap resulted in current losses of less than 5% of peak current. Classical MITL models that neglect plasma expansion predict that there should be zero current loss, after magnetic insulation is established, for both of these gaps. Results indicated that the vacuum pressure or pump-down time did not have a significant effect on the measured current loss at vacuum pressures between $1e^{-4}$ and $1e^{-5}$ Torr. Additionally, there was not repeatable evidence of a conditioning effect that reduced current loss for subsequent full-energy shots on a given set of hardware. It should be noted that the experiments conducted likely did not have large loss contributions due to ion emission from the anode due to the relatively small current densities (25-40 kA/cm) in the MITL that limited the anode temperature rise due to ohmic heating. The results and conclusions from these experiments may have limited applicability to MITLs of high current density (>400 kA/cm) used in the convolute and load region of the Z which experience temperature increases of >400 ºC and generate ion emission from anode surfaces.

Significance:

Experiment results will aid in the design of powerful next-generation pulsed power accelerators that may play a key role in several DOE missions. The future accelerators will continue to support development of clean energy systems through nuclear fusion research. The accelerators will also continue support of the nuclear stockpile and military needs of the country. Pulsed power machines are used to produce the extreme pulsed radiation environments necessary to certify that our nuclear weapons will operate as intended, and to predict their behavior without actual testing.

Nonequilibrium Electron-Ion Dynamics under Extreme Conditions via Time-Dependent Density Functional Theory

165731
Year 2 of 2
Principal Investigator: R. J. Magyar

Project Purpose:

Successful approaches for materials properties at extreme conditions, led by density functional theory based molecular dynamics (DFT-MD), lack both time-dependent electronic processes and energy transfer between electrons and ions, making them unsuitable for several applications in high energy density science. Among these is x-ray Thomson scattering (XRTS), for which interpretation of the signals limits a powerful diagnostic approach and electron ion equilibration, which depends crucially on the transfer of energy between electrons and ions.

We will address both of these phenomena by extending the machinery of time-dependent density functional theory (TDDFT) to extended systems. TDDFT is capable of accurately modeling the energy transfer between electrons and ions. We will study XRTS by calculating dynamic structure factors that may be directly compared with experiments. This will facilitate temperature measurements off the Hugoniot on next-generation pulsed power machines. We will also study systems with different initial electron and ion temperatures to determine the rate at which energy flows between these degrees of freedom. These rates are vital for accurate simulations of non-equilibrium plasmas especially at temperatures of several eV where degeneracy affects the accuracy.

Summary of Accomplishments:

This project created a capability to simulate electron dynamics within the time-dependent density functional framework. This capability enables the simulation of optical response, dielectric functions, stopping powers, and x-ray Thomson scattering signals for matter under a wide range of conditions and with many fewer physical assumptions than previous methods.

The electron dynamics is simulated through a Crank-Nicholson propagation of a set of initial KS wave functions with fixed Mermin temperature-dependent weights. The use of an iterative solver facilitates the practical solution of the time integration. This algorithm is implemented in a standard plane-wave projector-augmented wave code and may be implemented in other similar codes.

The accomplishments include careful testing of time-integration schemes and ensuring that the unitary aspect of time evolution is preserved. Several fundamental challenges for simulation under extreme conditions were found and future work remains to address some of these more formally. Serendipitously, it was found that the methods used for electron dynamics might lead to more scalable electronic structure molecular dynamics calculations. To illustrate these capabilities, we have performed stopping power simulations on aluminum (Al) and beryllium (Be) at room and several eV temperatures. We also calculated the XRTS response of Al and Be under these conditions and compression. To validate our efforts, we have simulated the optical response of a sodium dimer and bulk silicon. Several post-processing tools were created to enable the analysis of complex simulation results.

We learned that coupling classical nuclear dynamics to electron dynamics is challenging to do accurately as this decomposition violates correlations in the underlying coupled electron-nuclear wave function. We developed a code that is capable of this coupling and we are currently investigating the accuracy of this model. We discovered that adiabatic effects play a role in high velocity stopping simulations.

Significance:

Tools developed in this effort can provide stopping powers of ions under ambient and extreme conditions. The ability to simulate these quantities impacts inertial confinement fusion efforts as well as equation of state work.

Refereed Communications:

R.J. Magyar, "Large Systems," presented at the *TDDFT Gordon Conference 2013*, Biddeford, ME, 2014.

R.J. Magyar, "Density Functional Theory of Extreme Environments," presented at the *Sanibel Symposium on Computational Chemistry*, St. Simmons, GA, 2014.

L. Shulenburger, "Quantum Mechanical Calculations at High Pressure beyond Kohn-Sham: Opportunities and Challenges," presented at the *Gordon Conference on High Pressure Physics*, Biddeford, ME, 2014.

Electrical Breakdown Physics in Photoconductive Semiconductor Switches (PCSS)

165732
Year 2 of 3
Principal Investigator: A. Mar

Project Purpose:

Advanced switching devices with long lifetime will be critical components for linear transformer drivers (LTDs) in next-generation accelerators. LTD designs employ high switch counts. With current gas switch technology at ~$10e^3$ shot life, a potential game changer would be the development of a reliable low-impedance (<35nh) optically triggered compact solid-state switch capable of switching 200kV and 50kA with $10e^5$ shotlife or better. Other potential applications of this technology are pulse shaping programmable systems for dynamic material studies, efficient pulsed power systems for biofuel feedstock, short pulse (10 ns) accelerator designs, and sprytron replacements in nuclear weapons firing sets.

Optically triggered photoconductive semiconductor switch (PCSS) devices have been developed at Sandia for very fast switching of electrical power. Low-cost PCSS devices are highly reliable and very compact. High-gain GaAs PCSS are triggerable by low energy semiconductor lasers through a fiber and have demonstrated lifetimes >$10e^8$ cycles with 20A per filament. The shot life of PCSS is predominately dependent on the switched charge as opposed to the switched voltage, as was evident in high-power PCSS demonstrations up to 220kV and 8kA. Therefore, the current can be scaled without sacrificing lifetime by initiating multiple parallel filaments in multiple parallel devices. This project will develop PCSS switching modules capable of 200kV (DC) and 20kA current that can be stacked in parallel to achieve hundreds of kA with $10e^5$ shot lifetime.

The scaling of PCSS designs to switch megavolt and 10s-100s kiloamp systems will be supported by developing an improved model of the electrical breakdown physics in the device, which impacts filament diameter, peak current density, packing density (spacing), and optical trigger energy, the key parameters for scaling PCSS-based systems to the megaampere regime. Sentaurus device process modeling will also be employed to optimize the contact structures in the PCSS device for reliability.

Z-Pinch X-Ray Sources for 15-60keV

165733
Year 2 of 3
Principal Investigator: D. Ampleford

Project Purpose:

The purpose of this project was to develop higher photon energy x-ray sources than are currently available on the Z machine. By using emission lines produced by inner-shell ionization, we are able to create high photon energy x-ray sources (>15 keV) that are brighter than those that can be produced by typical thermal K-shell line emission. In experiments, we have demonstrated the ability of z-pinches to produce 22 keV line emission using K-alpha radiation from a silver wire array z-pinch. We have developed methods capable of diagnosing x-ray emission on Z up to 1 megaelectron-volt and have been developing a Faraday cup to characterize energetic electrons in experiments on Z. Simulation tools are being developed to model energetic electrons within z-pinch plasmas and have provided insight into the mechanisms that allow intense emission from inner-shell emission lines.

Implementing and Diagnosing Magnetic Flux Compression on Z

165736
Year 2 of 3
Principal Investigator: R. D. McBride

Project Purpose:

The Z Pulsed Power Facility offers a unique platform for producing very large magnetic fields (10s - 100s MGauss) coupled to very high energy density (HED) plasmas (>>1 Mbar). These extreme states of magnetized matter offer many rich and exciting phenomena for scientific inquiry. One interesting and potentially important way to achieve very high magnetic field intensities on Z is through magnetic flux compression. An axially aligned, pre-imposed seed field, B_{z0}, can be trapped and compressed (amplified) by a fast (100-ns) imploding liner, where the implosion is driven by the azimuthal field, B-theta, of the Z accelerator's power pulse. Flux compression can, in principle, amplify seed fields of ~30 T to more than 10,000 T (100s of MGauss). This phenomenon is exploited by the magnetized liner inertial fusion (MagLIF) concept currently under development at Sandia. However, our ability to compress flux remains unclear due to poorly understood physics. For example, the Nernst Effect (a thermo-electromagnetic effect) can cause significant flux loss in the presence of strong temperature gradients. The Nernst Effect is included in higher-order magneto-hydrodynamic theory, but the physics needs to be validated experimentally. Clearly, developing diagnostics to measure these compressed fields is required to assess whether or not adequate compression is achieved.

Producing and diagnosing such intense magnetic fields on Z is nontrivial. We, therefore, plan to evaluate and test on Z the most promising diagnostic methods that have been proven to work on smaller-scale facilities. These methods include Zeeman spectroscopy, miniaturized "micro" B-dot loops, and Faraday rotation.

Evaluation of Warm X-Ray Bremsstrahlung Diodes on Z

165738
Year 2 of 3
Principal Investigator: V. Harper-Slaboszewicz

Project Purpose:

The purpose of the project is to create a new type of warm x-ray bremsstrahlung source that could be fielded on the Z accelerator. Enhanced capability to understand and simulate nuclear weapons effects has become increasingly important as the stockpile is updated and data from previous underground test becomes less relevant. Warm x-ray simulation sources have been developed at Defense Threat Reduction Agency (DTRA) facilities and on the Saturn simulator to support these studies. However, the intensity and exposure volume available with existing simulators is not sufficient to access all relevant exposure conditions. The Z facility has much greater current capability than the existing simulators and, therefore, should be able to drive higher intensities and exposure volumes than existing sources. However, the drive voltage and pulse shape on Z are incompatible with present bremsstrahlung sources. Innovative bremsstrahlung diode designs will be required to produce a usable source on Z. This project will develop the technical basis for a massively parallel bremsstrahlung diode that is scalable to Z.

High Pressure Pre-Compression Cells for Planetary and Stellar Science

165739
Year 2 of 3
Principal Investigator: C. T. Seagle

Project Purpose:

Hydrogen (H_2) and helium (He) are the most abundant elements in the universe and occur in a variety of extreme environments, both natural and man-made. Mixtures of hydrogen and helium exhibit an extraordinary degree of non-ideality; the volume of the mixture is not the sum of the individual components. The relative "simplicity" of hydrogen and helium would suggest theoretical calculations of the properties of the mixture would be quite accurate; however, major discrepancies in predicted properties exist between different calculation methodologies. Few experimental data are available on the mixture, particularly at high compression. A detailed experimental study of the mixture will provide invaluable data to benchmark theoretical studies and enhance predictive capability. Applications for the data exist in several scientific disciplines including fusion research, stewardship science, and the interpretation of stellar and Jovian oscillations, which depend on the equation of state of the constituent material.

H_2-He mixtures are extremely difficult to study in laboratory settings at conditions relevant to planetary interiors because of low initial density, mixing properties, and high compressibility of the gases. In shock wave experiments, thermal pressure effects that become significant as the shock strength increases limit the maximum compression. One method to overcome these issues and obtain shock data for H_2-He mixtures at higher compressions is to precompress the mixtures prior to dynamic loading. For the gases, this precompression substantially decreases the initial compressibility and results in very different loading paths than typically achieved. We will quantify the non-ideal mixing behavior and equation of state of H_2-He mixtures under shock loading, at conditions relevant to stellar and planetary interiors, by developing and utilizing precompression to achieve higher density states than previously possible. Difficult challenges in the development of precompression for dynamic studies exist. If successful, results of this project will gain access to regions of phase space not previously explored.

Assessment of Load Current Multipliers to Increase Load Magnetic Pressures for Dynamic Materials and Fusion Experiments

165740
Year 2 of 2
Principal Investigator: T. J. Awe

Project Purpose:

Dynamic material properties (DMP) experiments on the Z Facility obtain equation of state (EOS) data for materials at multi-megabar pressures with unprecedented precision. Z's ultra-high (I~26 MA) current and advanced pulsed shaping capabilities provide a world-class platform for shock and isentropic compression experiments, yet important phase transitions remain inaccessible. A new enabling technology, the load current multiplier (LCM), will allow Z to deliver ~40% higher current to long-pulse DMP loads with minimal alteration to the generator architecture. Forty percent higher current could also increase the x-ray energy radiated from z-pinches by a factor of two, and increase fusion neutron yields in inertial confinement fusion (ICF) experiments by a factor of 4 (I^4 scaling) or more.

LCMs increase the efficiency of electromagnetic energy coupling between a high-impedance generator and a low-impedance load by forcing current to pass through the load twice. Using an LCM on Z-DMP experiments could nearly double the measurable pressure along the principal isentrope, enabling first-time access to a host of multi-megabar phase transitions. While recent experiments have demonstrated current multiplication in medium-scale pulsed-power facilities (~1 MA/100 ns and ~5 MA/2 µs), LCM performance under the more challenging conditions (lower generator inductance, higher voltage, ultra-high and fast-rising current) of the Z Facility remains uncertain.

Summary of Accomplishments:

An experiment-ready LCM design has been proposed which couples to the 31 cm convolute, and incorporates standard load hardware that accommodates short circuit loads, imploding ICF liners, and DMP experiments. The proposed LCM design includes solutions to a variety of technical challenges. For example, the central extruder of the LCM is difficult to fabricate. Based on a number of considerations including cost, gap uniformity, ease of handling and installation, and high voltage performance, the geometry of the extruder was simplified, and the walls were thickened to enable fabrication of a two piece extruder that could then be robustly mechanically connected by welding. A second technical challenge that has been addressed is the large number of LCM electrical contacts located in regions of high current density and large electric field strength. Knife-edge techniques are used throughout the design and have been shown effective at similar current density to avoid early high voltage breakdown and non-thermal plasma formation. Finally, the design accommodates B-dot and VISAR based current diagnostics, as well as access for diagnosis of plasmas formed in the Z and LCM convolutes.

For the first time, we have simulated the coupling of an ideally performing LCM to realistic load physics relevant to targets fielded on the Z machine. These simulations suggest that an experimental series to evaluate the performance of the LCM should include a non-imploding rod, large initial diameter imploding liner, or rectangular coaxial load. These targets, in conjunction with an LCM, have the possibility of generating otherwise unachievable pressures and velocities relevant to both the dynamic materials program and the inertial confinement fusion program at the Z Facility. Future work on this topic should be focused on the experimental evaluation of loss mechanisms in both the 31cm convolute and the LCM convolute, as empirical models do not currently exist.

Significance:

Higher generator currents could provide new regimes of performance (magnetic pressures or x-ray yields) for all pulsed-power-driven loads including those for dynamics materials, weapons effects, secondary assessment and inertial confinement fusion. If successful, this work is relevant to DOE strategic needs in nuclear weapons stewardship (enhances accelerator and load yields for weapons physics and effects experiments), and energy security (decreases the cost of future z-pinch-driven inertial fusion energy sources).

Radiation Susceptibility of Memristive Technologies in Hostile Environments

165741
Year 2 of 3
Principal Investigator: M. L. McLain

Project Purpose:

Memristor technologies show great promise as a next-generation nonvolatile memory with high endurance (one trillion cycles), long retention (>10 years), and low power (<1 pJ switching). In order to use memristive technologies in harsh radiation environments, it is necessary to understand the radiation susceptibility in all possible radiation environments. Currently, it is unknown how memristor technologies will operate in a high dose rate or neutron environment, and the radiation response in a total dose, proton, or heavy ion environment is not well understood. In this project, we will use a combined theoretical-experimental effort to probe the radiation response of memristor devices currently being fabricated by Hewlett Packard (HP) and Sandia's Microsystems and Engineering Sciences Application (MESA) Fab. We will then apply what we learn to discover other possible radiation-resistant memristive materials that are candidates to be inserted into the memristor fabrication process at MESA. Sandia is in a unique position to study the radiation susceptibility of potential radiation-hardened memristive technologies because of a cooperative research and development agreement (CRADA) that has provided us with knowledge of HP's proprietary, leading-edge memristive-memory design. If successful, this work will lead to an enhanced understanding of what governs the radiation tolerance of memristive materials. This will enable the discovery of a radiation-hardened memristive technology to be used in future radiation applications.

The essence of this work is to understand the physics and material properties that lead to radiation-hardened memristors. We will use state-of-the-art radiation test facilities to investigate, for the first time in some cases, the radiation response of memristor devices. The physics of the observed response will have to be fully understood to advance Sandia's knowledge to a point at which the next generation of rad-hard circuits can be fabricated. Because there are many unknowns associated with memristors, it may be difficult identifying the primary feature contributing to the radiation hardness of the device.

Exploring New Frontiers in Wave-Particle Physics in Nonstationary, ICF-Related Plasmas

165746
Year 2 of 3
Principal Investigator: P. Schmit

Project Purpose:

The purpose of this project is to develop new tools and models that enhance our understanding of important kinetic processes in inertial confinement fusion (ICF) experiments. Kinetic effects are identified here as any relevant target physics requiring detailed knowledge of the dynamics of individual charged particles in a fusion plasma. For both historical and practical reasons, the theoretical treatment of the plasma physics of ICF experiments typically adopts a simpler, hydrodynamic picture of the fusion plasma, either ignoring or approximating any background kinetic effects. While the hydrodynamic approach is far more computationally tractable than fully resolved plasma kinetics in integrated ICF simulations, the validity of the underlying transport, burn, and radiation models — three critical components of any simulation — relies on the satisfaction of a long and stringent list of assumptions about the overall target physics. Given the plethora of assumptions these models presume, it is no surprise that integrated simulations are often overly optimistic and/or quantitatively incorrect.

Therefore, in this project we will develop new theoretical and numerical tools to elucidate potentially important physics missed by traditional ICF multiphysics codes. Particular attention will be given to the kinetics of superthermal ions, the charged particles primarily responsible for fusion in the target, within their global environment. Substantial progress has been made in the development of a fully 3D particle code capable of resolving the kinetics of these ions in a wide variety of scenarios. This code will provide extensive new insights into problems relating to reactivity depletion, mix effects, magnetic confinement, and numerous other outstanding problems in ICF. Development and use of other existing codes and models will enhance and diversify the investigation of target kinetics beyond the problems mentioned explicitly in this abstract. Progress will be accelerated by new and ongoing collaborations with staff researchers and students at Sandia, Los Alamos National Laboratory, the Naval Research Laboratory, and Princeton University.

The PI is a Sandia Truman Fellow.

Fiber Optic Streak Spectroscopy of Gas Cells in Extreme Radiation Environments

170977
Year 2 of 3
Principal Investigator: K. M. Williamson

Project Purpose:

An enduring component of Sandia's core mission is to ensure our nation's security in a rapidly changing technological environment. An imminent challenge to this mission is the impact of system-generated electromagnetic pulse (SGEMP) on the performance and reliability of nuclear weapons and satellite systems. The physical mechanisms involved with coupling high-energy radiation into, and damaging, critical system components are being studied at Sandia.

These experiments utilize high-intensity x-rays from z-pinch radiation sources on the Z machine to ionize a specialized gas cell. Indirect sensing of this nonthermal plasma was being conducted with only a B-dot sensor that results in a highly averaged measurement of the changing magnetic fields. The purpose of this research was directed at the creation of a new diagnostic and analysis technique that will enable more refined characterization of this plasma that is critical for accurate modeling and simulation of SGEMP.

A major step toward understanding SGEMP is to create a spectroscopic diagnostic and analysis technique with the ability to directly measure plasma emission and create a temporally resolved map of the current density in the plasma. A shielded fiber optic probe was inserted into the gas cell to collect photon emission from the plasma. Multiple gas cells were fielded for each experiment. The location and pressure of each cell was varied to produce a range of plasma characteristics. Six SGEMP plasma spectra with clear continuum and line emission were captured from three shots with varied pressures and cell geometry. Analysis of these data could provide the critical electron temperature and density history needed to more accurately simulate the SGEMP phenomenon.

Wavelength Conversion Arrays for Optical and X-Ray Diagnostics at Z

173189
Year 1 of 3
Principal Investigator: E. J. Skogen

Project Purpose:

This project is focused on the development of a chip-scale linear array of visible-to-infrared wavelength conversion circuits that meet the needs of the experiments conducted at Z machine.

Optical diagnostics play a central role in dynamic compression research. A visible-to-infrared wavelength converter is the missing link that would enable construction of novel measurement system for dynamic materials experiments at Z machine. Currently, streak cameras are employed to record temporal and spectroscopic information in single event experiments. Streak camera equipment costs limit the experimental versatility and limited readout elements constrain the tradeoff between temporal resolution and time duration.

This project is solving the limitations that streak cameras impose on dynamic compression experiments while reducing both cost and risk by utilizing standard high-speed digitizers and commercial telecommunications equipment. The missing link is the capability to convert the set of experimental (visible/x-ray) wavelengths to the infrared wavelengths used by telecommunications equipment. Previous wavelength converter efforts target infrared-to-infrared conversion, not conversion from the shorter visible wavelengths of interest here, and therein lies the difficulty. The materials used to construct the devices to convert from visible or x-ray to infrared is not necessarily the same; therefore, new integration techniques must be devised. There has never been a chip-scale demonstration of visible-to-infrared wavelength conversion technology needed here. In pursuing this avenue of research, we must innovate to overcome several key challenges.

We must find new ways of integrating the optoelectronic components that form the converter, a photodiode and electroabsorption modulator, as it is of crucial importance to limit radio-frequency parasitics in the integration. Additionally, we must push the state-of-the-art in photodiode design, as it will set the dynamic range and the bandwidth of the converter. Similarly, the modulator design and fabrication must be pushed, as its characteristics will determine the efficiency and signal integrity.

Investigating Laser Preheat and Applied Magnetic Fields Relevant to the MagLIF Fusion Scheme

173190
Year 1 of 3
Principal Investigator: A. J. Harvey-Thompson

Project Purpose:

The magnetized liner inertial fusion (MagLIF) concept is a potentially promising inertial confinement fusion scheme for achieving ignition and burn using a pulsed power driver. The scheme involves imploding a cylindrical liner filled with a dense, gaseous deuterium fuel with the Z generator. The fuel is preheated with an external energy source, in this case the Z-beamlet laser, and magnetized with an external magnetic field to modify the plasma transport properties and achieve relevant fusion conditions at stagnation. Knowing how electron thermal transport is modified by magnetization and how well laser energy can be absorbed by the fuel is important for determining the requirements for MagLIF.

The conditions in MagLIF-relevant plasmas are less well studied than tokamaks and high energy density plasmas, to which they are intermediate in parameters. The modification of plasma transport properties via magnetic fields is a fundamental problem that can be studied in a scaled manner on intermediate scale facilities, such as large lasers. The recently realized ability to magnetize large (>1cm^3) volumes of plasma with large (10 T) magnetic fields on the Omega-EP (extended performance) Facility at the Laboratory for Laser Energetics and at Sandia allows the effects of magnetization to be determined on plasmas that are of higher density, temperature, and volume and over longer timescales than have been achieved previously. Magnetizing the plasma is expected to affect both the temperature time history of the plasma and the laser energy deposition within the plasma, both of which are relevant to MagLIF and have not been studied previously at these conditions.

Creating the Foundation of Next-Generation Pulsed-Power-Accelerator Technology

173191
Year 1 of 3
Principal Investigator: B. Stoltzfus

Project Purpose:

In this effort, we are creating the foundation for the world's largest and most powerful pulsed-power accelerator. It will use next-generation technology and know-how that will allow Sandia to maintain its role as the world's leader in pulsed-power accelerator physics.

Nuclear weapons play a critical role as part of the global security strategy pursued by the US. The 2010 Nuclear Posture Review reiterates the continuing need to maintain a safe, secure, and effective nuclear deterrent. The Review also outlines a "path to zero" for nuclear weapons. Hence, the number of weapons in the stockpile will continue to decline. As the stockpile shrinks, the requisite deterrent value of each weapon increases. This, in turn, drives the critical new challenge of increasing our confidence in the reliability and effectiveness of each weapon.

The weapons are constantly changing as components age and are upgraded through life extension programs. While standard engineering practice calls for field testing new or revised products, the 1992 decision to end underground testing precludes full system tests for nuclear weapons. A key challenge for the NNSA and its laboratories is to certify that our weapons will work in the absence of such tests. This is accomplished through a variety of science and engineering projects, which include the study of radiation effects science (RES) and high energy density science (HEDS).

The goal of RES is to develop the understanding needed to certify that our nuclear weapons will operate as intended in the extreme pulsed radiation environments they may encounter during the stockpile-to-target sequence. Some threat environments can be simulated with fidelity, but others can only be approximated or not simulated at all. Today's laboratory x-ray sources lack the fluence, exposure volume, and energy-spectrum coverage to reproduce many of the radiation threats our weapons may encounter.

An ion-Neutron electron-Gamma SIMulation System for Radiation Testing of Optical Components for Weapons Systems - NGSIM-O

173192
Year 1 of 3
Principal Investigator: B. L. Doyle

Project Purpose:

The NGSIM-O project is developing a capability on the Ion Beam Laboratory (IBL) Tandem accelerator facility to quantify the performance degradation of optical components when exposed to hostile radiation environments. The Qualification Alternatives to the Sandia Pulsed Reactor (QASPR) program has demonstrated the utility of using high-energy ions and electrons to simulate the displacement damage and ionization in electronics caused by neutrons and gamma rays at fluxes previously only available on SPR-III and HERMES-III (much larger historical facilities, now retired.) This year, the instrumentation in the QASPR-II and III endstations has been modified to enable the diagnostics of optoelectronic components. We performed ion-only exposures (MeV C, Si, and Ge) on laser-illuminated GaAs rad-hard photovoltaic (PV) diodes, and measured the degradation of the induced photocurrent. Plots of charge collection efficiency (CCE) vs. the 1-MeV-equivalent-neutron-fluence of the ions matched similar measurements made on the Annular Core Research Reactor (ACRR). In addition, our experiments agree with theoretical results derived from a Taylor expansion of a modified Hecht CCE theory for a partially depleted PV. These results also suggest that the PV can be made more radiation hard by lowering the concentration of the GaAs(Si) doping thereby fully depleting the GaAs. The development of a new NGSIM-O irradiation capability at Sandia will be the first of its kind to experimentally measure the response of optical devices to mixed neutron and gamma irradiations that are independently adjustable in time and magnitude.

Next-Generation Multi-Scale Plasma Codes

173193
Year 1 of 2
Principal Investigator: M. Martin

Project Purpose:

Our predictive simulation capability for the modeling of pulsed-power-driven targets such as imploding solid liners for magneto-inertial fusion and wire-array z pinches as radiation sources is severely limited through the labs exclusive use of resistive magneto-hydro-dynamic (RMHD) codes for the design of experiments. All of the codes (ALEGRA, HYDRA, etc.) used for the design and analysis of our experiments on the refurbished Z machine depend upon free parameters that are not a physical quantity. These parameters are tuned to experimental results and limit our predictive capability. Our planned solution is the implementation of an implicit quasineutral extended MHD (XMHD) model that correctly treats the transition from collisionless to collisional plasma while maintaining the correct solution in the asymptotic RMHD limits and while being computationally feasible for 3D simulation. Key to the development of this capability is the creation of asymptotic preserving semi-implicit time integration schemes which are stable and accurate for explicit hydrodynamics advanced with iterative-Riemann solvers compatible with tabular equations of state coupled to stiff implicit source terms which can vary on timescales fourteen orders of magnitude faster than the explicit pieces. In the first year of the project, we have developed the Riemann solver capability and explored time integration approaches that meet these goals. We have also developed a linear wave code compatible with our tabular constitutive relations. This code allows us to test each wave family independent of the other using realistic plasma parameters in the XHMD model. Year two will focus on applying these advances to a fully integrated 3D XHMD code and the modeling of pulsed power loads.

Modeling of Non-Local Electron Conduction for Inertial Confinement Fusion

173868
Year 1 of 3
Principal Investigator: L. Lorence

Project Purpose:

The work is in collaboration with the University of Wisconsin-Madison. This research will advance modeling of nonlocal electron conduction for direct drive inertial confinement fusion (ICF) target implosions. Current capability involves multigroup diffusion based theory of "diffusing" higher order moments of the electron distribution function to simulation nonlocal electron thermal conduction. In this research, a new Implicit Monte Carlo-Discrete Diffusion Monte Carlo (IMC-DDMC) numerical algorithm, developed for x-ray transport, will be used to efficiently simulate nonlocal electron conduction. The details of applying this hybrid transport-diffusion theory to electron physics with its electromagnetic fields are not obvious. However, the efficacy of the hybrid IMC-DDMC method for computationally efficient transport of x-ray photons appears promising. This study seeks to apply this advanced numerical method to electron physics. One goal would be to more accurately include the effects of electric and magnetic fields in this theory. The result would be improved modeling of nonlocal electron conduction, an important ICF phenomenon for target implosions.

The work will involve advanced modeling of nonlocal electron conduction in the multidimensional radiation hydrodynamics simulation code, DRACO.

IMC-DDMC is a new method that has yet to be applied to electron physics. It has the potential to allow for more accurate simulation for nonlocal electron conduction especially those encountered in high energy density type problems where very steep temperature gradients are found. Furthermore, DDMC is not being use in production codes as of yet.

Technical challenges include the theory dealing with a zero current condition in kinetic theory without invoking full Maxwell's equations. Furthermore, numerical robustness in the method will need to be developed. Finally, the IMC-DDMC model will need to hold up to current electron thermal transport models. Model development of a 1D spherical IMC-DDMC model is in progress.

Cavity Electron Density Measurements within Pulsed Radiation Environments

177967
Year 1 of 3
Principal Investigator: K. S. Bell

Project Purpose:

The purpose of the project is to create a fiber optic based diagnostic that is able to measure the line-integrated electron density as a function of time and chord position within a plasma with highly limited diagnostic access that is driven by the Z Facility at Sandia. In order to successfully collect relevant data, the diagnostic should be malleable enough to couple to remote spaces within an experiment on the Z machine, robust enough to survive the harsh driving radiation and electromagnetic interference, have a fast time response (nanosecond), and sensitive enough to extend the measurement below $1e^{16}$ electrons per cubic centimeter. Of these, the most challenging aspect will be extending the measurement to low densities using a fiber optic system. Additional challenges exist in the interpretation of the measurement due to the possibility of several complex conditions existing within the plasma under study. These could include large currents (kiloamperes), significant electric and magnetic fields, wide electron temperature distributions (including relativistic electrons), and neutrals. The initial design will incorporate existing 1550 nanometer wavelength laser and fiber optic technology, with a focus on developing novel analysis techniques to extend the diagnostic sensitivity beyond the nominal factor of 1/200 of a fringe for fiber optic based interferometry. It is also possible for the plasma to be emitting light with the same frequency as the probe beam that would pollute the signal and increase the background noise making the analysis more complex. Therefore, this project will require significant benchmarking, analysis, and modeling to correctly interpret the measurement.

NEW IDEAS

The New Ideas Investment Area aims to position Sandia to anticipate and respond to national security challenges (both now and in the future) by supporting high risk new ideas that have the potential to be transformational; for example, those with long time horizons, potentially high but as yet uncertain mission impacts, or nascent research in a new field that may in the future become transformational for our mission. It is intended to support leading-edge research that is outside Sandia's current research focus areas, but that may lead to breakthroughs in science and technology that could profoundly impact our national security mission.

A representation of a transcranial direct current stimulation (tDCS) device. Research at Sandia indicates that tDCS can improve both associative memory and working memory performance. These findings indicate that tDCS could be a powerful tool to enhance training, enabling trainees to encode and recall information more effectively. (Project 165715)

NEW IDEAS

Exploring the Possibility of Exotic Ground States in Twisted Bilayer Graphene

165713
Year 2 of 3
Principal Investigator: T. Ohta

Project Purpose:

We will examine the electronic properties of doped twisted bilayer graphene (TBG) in a search for exotic ground states in this material. The following specific scientific questions will be addressed via our leading capability in this emerging material: 1) can van Hove singularities (vHs) be engineered in TBG? and 2) can exotic ground states, or perhaps superconductivity, be induced by filling electrons up to, and leveraging these vHs?

The ramifications of superconductive graphene are far reaching. As its charge carriers are readily manipulated at cryogenic temperatures using the field effect (FE), gate-tunable superconductive elements equivalent to three-terminal switches may be realized. Importantly, such a simple switching function is currently missing for superconductor circuitries envisioned for exascale supercomputers.

Superconductivity in graphene has not been experimentally observed despite numerous predictions of its existence. The theoretical predictions have suggested the emergence of exotic ground states at vHs residing >2eV from the charge neutrality point. These energies are inaccessible using atypical FE structures. TBG, in contrast, has additional low-energy vHs, which are accessible by FE-gating. They evolve as a natural consequence of the two-graphene sheets being misaligned. Consequently, TBG provides an exciting medium to explore the possibility of superconductivity in graphene.

The search for superconductivity is a high-risk endeavor in a low-dimensional material. TBG, however, is an emerging class of graphene whose electronic dispersion offers promise towards this end, even though its precise dispersion remains a topic of debate. Building on our leading expertise in TBG, we will strive to engineer the vHs to induce exotic ground states. Our approach is the first of its kind.

Best Case Outcome: Gate-tunable superconductivity, a disruptive technology, will greatly simplify the hardware of superconductor-based supercomputers.

Closing the Nutrient Utilization Loop in Algal Production

165714
Year 2 of 3
Principal Investigator: T. Lane

Project Purpose:

Despite widespread interest in electric modes of transportation, the environmental impact assessment (EIA) projects that liquid fuels will provide more than 90% of US transportation energy through 2035, and few alternatives are on the horizon for aviation transport. Biofuels look well positioned for this role, but face daunting challenges in scale-up and sustainability. Biofuel production from algae biomass is a compelling solution for sustainable domestic production of fuels. However, recent studies suggest that replacing 10% of the domestic fuel supply with algae would require a doubling of nitrogen and phosphorus fertilizer usage. Unlike ammonia, phosphate is a non-renewable resource, and a peak in worldwide production is expected as early as 2030. Thus, without significant technological progress to recycle these major nutrients, expansion of algal biofuels to commodity scale can be expected to catalyze a food versus fuel crisis.

We will close the nutrient-recycling loop by harnessing remineralization processes, the biological conversion of organic forms of nutrients to inorganic forms. We will develop a novel, cost-effective process for remineralization of phosphate and nitrogen from oil extracted algal biomass and the conversion of these nutrients into forms that are captured and amenable for use as nitrogen and phosphate sources. To facilitate separation of the remineralized nutrients from the bulk phase, we will induce the co-precipitation of ammonium and phosphate as struvite (NH_4MgPO_4). Converting nutrients to solids is a low-energy means of recovering the bulk of the phosphorous and a portion of the nitrogen with maximum transportability. The remainder of the nitrogen will be recovered as ammonium. To identify scale-up concerns, we will develop models that relate the phosphate remineralization enzyme kinetics, mixing and precipitation kinetics. Our planned nutrient recycling method is conceptual, and this project will generate proof of principal.

Testing the Effects of Transcranial Direct Current Stimulation on Human Learning

165715
Year 2 of 2
Principal Investigator: L. E. Matzen

Project Purpose:

Training a person in a new knowledge base or skill set can be extremely time consuming and costly, particularly in highly specialized domains such as the military and the intelligence community. Recent research in cognitive neuroscience has suggested that a technique called transcranial direct current stimulation (tDCS) has the potential to revolutionize training by enabling learners to acquire new skills faster, more efficiently, and more robustly (Bullard, et al., 2011). In tDCS, a small region of the brain is stimulated with a weak electrical current (1-2 milliamps) via an electrode placed on the scalp. This current makes the neurons in the vicinity of the stimulation either more or less likely to fire, depending on the polarity of the electrical field. Although tDCS has been used for over 50 years, recent advances in technology have created a surge of new applications (Utz, et al., 2010). Some researchers suggest that tDCS devices will be widely available to the public in the near future (Peck, 2007). Most of the research in this rapidly developing field has been focused on medical applications, such as treating migraines or assisting with rehabilitation of brain injuries. However, tDCS has many potential applications with implications for national security and those applications have received little attention to date.

Although tDCS has the potential to have a major impact on human performance, particularly in the area of training, the research on tDCS' effects in this area is in its infancy. In this project, we intend to study the effects of tDCS on three types of memory that are crucial for training: working memory, semantic memory, and associative memory. This work would significantly advance the science in this area, including our understanding of the potential for technical surprise, and could position Sandia on the cutting edge of research into the training applications of tDCS.

Summary of Accomplishments:

In this project, we tested the effects of tDCS on two different types of memory performance: associative memory and working memory. Associative memory refers to memory for the relationships between multiple pieces of information and working memory refers to the amount of information that can be held in mind and processed at one time. Both types of memory are vitally important for education and training. We conducted two, double-blind, sham-controlled studies to test the effects of tDCS on working memory and associative memory. We found that tDCS can improve working memory performance and that, under certain conditions, this improvement can transfer to other tasks. This indicates that tDCS can enhance general cognitive abilities. In the associative memory experiment, we found that tDCS can improve recall performance by about 50%. tDCS also showed the largest benefits on the associative memory tasks that were most difficult.

Taken together, the two experiments in this project provide strong support for the idea that tDCS can improve cognitive performance. This has potential applications in numerous national security domains. Most national security problems involve an element of human performance and human decision making, leaving open the possibility for human error. There are also many domains in which people must learn complex skills or how to use extremely complex tools, whether those tools are hardware, software, or systems. Our research, combined with other ongoing research in this area, indicates that tDCS has the potential to improve human cognitive performance and to help people learn information faster and remember it better.

Significance:

This research has contributed to our basic understanding of the brain's memory systems and the cognitive effects of tDCS. Our findings have profound implications for training applications of tDCS. If tDCS can be used to improve general cognitive abilities, such as working memory capacity and fluid intelligence, it could have a dramatic impact on the speed at which people are able to learn new information or skills, or on their overall cognitive performance in tasks that place a high burden on working memory or adaptive reasoning. tDCS has the potential to impact numerous national security domains through improving human performance.

Refereed Communications:

L. Matzen, "Using Recordings of Brain Activity to Predict and Improve Human Performance," presented (invited) *Emerging Trends Symposium*, Washington, DC, 2013.

Searching for Majorana Fermions in Topological Superconductors

165717
Year 2 of 2
Principal Investigator: W. Pan

Project Purpose:

The goal of this project is to search for Majorana fermions (MFs), a new quantum particle in a topological superconductor; that is, a new quantum matter achieved in a topological insulator proximitized by an s-wave superconductor.

MFs, predicted in 1937 by the Italian theorist Ettore Majorana, are electron-like particles that are their own anti-particles. MFs are shown to obey non-Abelian statistics and, thus, can be harnessed to make a fault-resistant topological quantum computer. Over the last decade, searching for MFs has mainly been focused on the exotic 5/2 fractional quantum Hall effect (FQHE). With the arrival of topological insulators, new schemes to create MFs have been proposed in hybrid systems by combining a topological insulator with a conventional superconductor. Compared to FQHE, this new approach of creating MFs is promised to be more versatile and the requirement of material quality is less stringent. Since 2008, a global race has been on to realize yet-elusive MFs in low dimensional semiconductor systems.

In this project, we will follow the theoretical proposals made by Lutchyn, Sau, Das Sarma, Fu and Kane to search for MFs in 1D topological superconductors. One-dimensional (1D) topological superconductor will be created inside of a quantum point contact (with the metal pinch-off gates made of conventional s-wave superconductors such as niobium) in a 2D topological insulator (such as inverted type-II InAs/GaSb heterostructure).

Results from this project will help to create a science-based knowledge foundation for creating, controlling, manipulating, and exploiting quantum particles in building 21st century technology. Sandia is the ideal place to perform the proposed research, which requires expertise in the high quality molecular beam epitaxy (MBE) growth of type-II InAs/GaSb heterostructures, sophisticated device fabrication of semiconductor nanostructures, and ultra-low temperature quantum transport measurements, rarely found together in a single place.

Summary of Accomplishments:

We discovered giant supercurrent states in a superconductor-InAs/GaSb bilayer-superconductor junction with critical quantum well (QW) width through transport measurements. The induced superconductivity seems to exist both in the edge channels and the bulk of the bilayer. Moreover, the bulk supercurrent states are unexpectedly strong in the temperature — magnetic field parameter space, contrasting to the conventional expectation that only an exponentially weak supercurrent is expected in such a thick junction. This robust proximity induced superconductivity provides an ideal platform for studying MF physics. Also, in this sample, new features, such as the concurrence of differential resistance peaks near the superconducting gap and the fluctuations, are interesting and expected to inspire further in-depth studies.

Moreover, we observed that the transport across the Ta-InAs/GaSb-Ta junction depends largely on the interfacial transparency, exhibiting distinct zero-bias behaviors. We have also achieved high quality MBE growth of InAs/GaSb bilayers. Our InAs/GaSb bilayer sample was grown by molecular beam epitaxy on a

GaSb substrate. The thickness of GaSb and InAs quantum well layers was 5.0 nm and 10.0 nm, respectively. The bilayer was sandwiched by two AlSb barrier layers. Conventional photolithography and wet chemical etching processes were utilized for device fabrication. Au/Ti (200/10 nm thick) electrodes were deposited by an e-beam evaporator to connect the InAs/GaSb bilayer at the four corners of the mesa. Superconducting Ta electrodes are directly sputtered on top of it to form a Ta-bilayer-Ta junction. The DC I-V of the sample was measured with DC voltage or current sources and digital multimeters in a two-terminal configuration. For differential resistance measurements, a small AC current was summed with the DC current then feeds to the junction, the AC voltage response of the sample was measured by the standard lock-in technique. All measurements were carried out in dilution refrigerators.

Significance:

The research results in this project could have significant near-term impact and provide interesting new science direction for quantum transport field in solid state physics. Sandia's unique combination of capabilities and expertise has enabled these accomplishments.

Refereed Communications:

W. Pan, "New Quantum Transport Results in Type-II InAs/GaSb Quantum Wells," presented (invited) *10th International Conference on Computational Methods in Sciences and Engineering*, Athens, Greece, 2014.

W. Pan, "Electron Transport Studies in Type-II InAs/GaSb Heterostructures," presented (invited) *8th Joint Meeting of Chinese Physicists Worldwide (OCPA8)*, Singapore, 2014.

Single Atom Deposition

173135
Year 1 of 1
Principal Investigator: G. Biedermann

Project Purpose:

A new generation of optoelectronic devices are being intensely investigated that will set new noise and size limits and perform functions beyond the capability of classical (Maxwell equation) light. An important example is a single quantum dot source for quantum key distribution (QKD), quantum computing, and single-photon generation. For these applications, precise placement of the quantum dot at the center of a microcavity is essential. Presently, one only accomplishes this with yield unacceptable for wafer-level production. Limitations come from density, flux, or spatial uncertainties from a classical source.

We will seek a quantum leap in improvement by developing cold atom sources for device fabrication. We aim to experimentally demonstrate, with optical tweezers, single cesium atom deposition as a proof-of-principle study. Significant modeling will also be performed to evaluate utility and design future placement sources.

The experimental effort will demonstrate trapping, deposition, and detection of single cesium atoms on a substrate, an unprecedented achievement. This is the simplest demonstration of the control that is required to place individual atoms at precise locations and will provide information for other elements that can be cooled and trapped. Mastering these cesium-placement techniques will open the door to using a different atom, or molecule, species as well as placement on more useful substrates such as a photonic crystal. Future candidates include Erbium. Erbium lasers at a desirable wavelength and can be laser-cooled for loading into optical tweezers. The theoretical investigation will model a forward-looking improved cold atom source for deterministically placing single atoms. Future work could also use a microfabricated lens array to create an array of tweezers for wafer-scale patterning of single-atom deposition.

Summary of Accomplishments:

We have theoretically and experimentally investigated the possibility of single atom deposition using laser-cooled sources. In our theoretical work, we investigated an atom source composed of out-coupling from a Bose-Einstein condensate in a trap. A model was developed for these devices. To illustrate its application, a two-well system is studied. The results show interesting and possibly useful differences between operation with coherent (phased-locked) and incoherent (unlocked) population transfer between levels in the two wells. The two modes of operation are governed by interplay among scattering, energy renormalizations and coupling between wells. In parallel, we have experimentally investigated the possibility of controlled deposition of single cesium atoms onto surfaces using optical tweezers. We have measured the rate limit for translation of single atoms in optical tweezers and have constructed an apparatus for deposition of single atoms on a sapphire substrate for future work.

Significance:

Our simulation shows a difference between conventional tunneling and the more effective coherent tunneling possible with a coherent source. Our simulation also demonstrates viability of our model as design tool for 'Atom-tronics' that is important for wafer scale single-atom deposition. Future work could employ our approach to determine the Casimir-Polder interaction of a single atom probe with a surface. This work is focused on the deterministic design and discovery of new materials and chemical assemblies with novel structures, functions, and properties. It could potentially promote cybersecurity knowledge and innovation, secure communications, and cryptography.

Active Control of Nitride Plasmonic Dispersion in the Far Infrared

173137
Year 1 of 1
Principal Investigator: E. A. Shaner

Project Purpose:

We plan to investigate the tailorability of plasmonic structures in nitride-based materials for far infrared (IR) applications. The 2D electron gas (2DEG) in the GaN/AlGaN material system, much like metal-dielectric structures, is a patternable plasmonic medium. However, it also permits for direct tunability via an applied voltage.

While there have been proof-of-principle demonstrations of plasma excitations in nitride 2DEGs, exploration of the potential of this material system has thus far been limited. We recently demonstrated coherent phenomena such as the formation of plasmonic crystals, strong coupling of tunable crystal defects to a plasmonic crystal and electromagnetically induced transparency in GaAs/AlGaAs 2DEGs at sub-THz frequencies. In this project, we will explore whether these effects can be realized in nitride 2DEG materials above 1 THz and at temperatures exceeding 77 K.

The critical initial step in this endeavor is to observe strongly coupled under-damped plasmonic excitations in multi-component nitride-based plasmonic structures. This scientifically driven research would pave the way for the development of sensor and waveguiding technology at frequencies compatible with existing far-IR sources like quantum cascade lasers.

Nitrides are a relatively immature plasmonic material system, and fundamental questions concerning their potential as a reconfigurable plasmonic medium remain open. In comparison to mature III-V materials such as GaAs/AlGaAs structures, electron scattering rates are higher in nitride 2DEGs. Electron scattering contributes significantly to plasmon damping. We anticipate that the capability of operation above 1 THz will compensate for the contributions from electron scattering mechanisms to plasmon damping. However, this needs to be demonstrated conclusively.

Summary of Accomplishments:

Along with collaborators, we theoretically demonstrated that opening of plasmonic bandgaps in gallium nitride (GaN) based high-mobility electron transistors is possible using realistic material parameters.

We developed suitable fabrication processes for GaN devices and fabricated devices at the Center for Integrated Nanotechnology (CINT). Subsequent electrical characterization demonstrated that the devices are functional and should give rise to reasonable terahertz (THz) photoresponse based on our past experience in other material systems.

Significance:

The THz portion of the spectrum is useful in certain applications for see-through imaging at short range and chemical fingerprinting. In addition, THz is important to material science as it allows probing of charge carriers at time scales shorter than the scattering time. Our work in this effort aims to elevate the temperature and frequency at which novel plasmonic effects in 2D electron channels can be obtained which may benefit these areas in the future. This work could potentially be used in spectroscopic components of sensor systems for national security applications.

Refereed Communications:

M. Karabiyik, R. Sinha, C. Al-Amina, G.C. Dyer, N. Pala, and M.S. Shur, "Dispersion Studies in THz Plasmonic Devices with Cavities," in *Proceedings of SPIE*, vol. 9102, 2014.

Exploring Revolutionary Thermoelectric Performance via Quantum Confinement

173139
Year 1 of 2
Principal Investigator: M. P. Siegal

Project Purpose:

Theory has long predicted a dramatic enhancement of thermoelectric (TE) properties through quantum confinement for nanomaterial geometries. While small performance improvements have been achieved by size reduction, the improvements so far have resulted from reducing thermal conductivity via enhanced phonon scattering. The potential to improve the electronic properties via quantum confinement remains untapped due to the challenges of growing nanomaterials with the high quality needed to achieve the requisite properties.

Rather than struggling to optimize the growth of TE nanomaterials to achieve the necessary dimensionalities, we will take a new approach. We will start with easier-to-grow, high-quality films and employ a novel subtractive approach to create nanochannels of high-quality, intrinsically connected TE materials engineered to enhance TE properties via quantum confinement. Sandia is uniquely positioned to perform this research with a confluence of expertise and capabilities in TE materials growth, ion beam irradiation, structural characterizations, and thermal/electrical measurements on nanostructured materials. The immediate impact of successfully demonstrating high figure of merit ZT (performance) TE's will be profound for the scientific community with high-profile publications.

We will study $Bi_{1-x}Sb_x$, which theory predicts a doubling of ZT with achievable 65-nm dimensions. Ion-beam parameter selection for optimal nanostructural features (dimension, interfacial-sharpness) will be guided by modeling and characterization using Sandia's state-of-the-art transmission electron microscopy (TEM) facilities. Correlating the nanostructures with resulting TE properties will provide deep scientific insight as we progress toward revolutionary TE performance.

Synthetic DNA for Highly Secure Information Storage and Transmission

173140
Year 1 of 3
Principal Investigator: G. Bachand

Project Purpose:

Protection of information is one of the greatest challenges to our nation's security and will continue to be for the foreseeable future. In particular, digital storage and transmission has proven increasingly susceptible to compromise, necessitating the development of disruptive technologies to secure highly sensitive information. The use of synthesized DNA to store digital information with high capacity and low maintenance was first reported in a 2013 paper in *Nature*. This proof-of-concept system represents a novel paradigm for information storage, particularly as DNA can be stably stored for tens of thousands years. This system, however, also offers the ability to transmit information in a highly secure biomolecule, as opposed to an encrypted digital format. We will apply the general premise of information storage in DNA, but focus on developing a fundamentally novel approach for transmitting encrypted data within DNA constructs. Our approach will specifically borrow from nature's means of translating genomic information into functional units to encrypt data in a highly secure manner. The idea of writing and securing digital data in DNA has been proposed in the scientific community primarily based on a binary language. Here, as in living organisms, we propose to use a "triplet codon," (i.e., three adjoining DNA nucleotides) to develop more than 1089 (i.e., 64 factorial) individual 64-character libraries that can be used for data encryption. The design will involve synthetic DNA constructs consisting of: 1) a "lock" securing the DNA from being "read" by anyone lacking authorization, 2) a "translation key" sequences that specifies the language for decoding the encrypted data, and 3) the encrypted data itself. In addition, this approach will allow us to use "nonsense" code sequences, mimicking the intron/exon structure found in genomic DNA. If successful, our proposed storage mechanism may be widely applied toward highly secure, information storage/transmission (e.g., classified documents) in a synthetic nanoscopic biomolecule.

Probing Small-Molecule Degradation to Counter Enzyme Promiscuity

173142
Year 1 of 3
Principal Investigator: S. Rempe

Project Purpose

Enzymes that degrade specific small molecules could save lives by neutralizing threats from chemical agents in the blood or environment, but promiscuous interactions with other molecules typically limit their effectiveness by blocking the enzyme active site. An obvious solution is to re-engineer the enzyme to enhance catalytic fidelity, but lack of understanding about how enzymes discriminate between molecules remains a formidable challenge to this approach. Our recent work in collaboration with University of Texas at Austin (UT) suggests a new approach and a model system for understanding enzyme specificity. Asparaginase enzymes catalyze degradation of asparagine, which forms the basis of medical treatment. Competition by other abundant molecules interferes with asparagine decomposition, thus, hindering enzyme efficacy. Asparaginase is advantageous as a model degradation enzyme because variants that demonstrate different binding affinities and catalytic rates can be compared. Our preliminary work suggests that the mechanism of molecular specificity in asparaginase depends on a different set of chemical interactions than previously speculated. We will leverage Sandia's strengths in molecular simulation and UT experimental expertise in asparaginase modification and functional assays to understand enzyme degradation of small molecules. Our simulations will probe how local properties of the asparaginase active site determine molecular binding affinities and free energy barriers to degradation, and predict mutations (tested experimentally) to tune catalysis to favor a specific molecule.

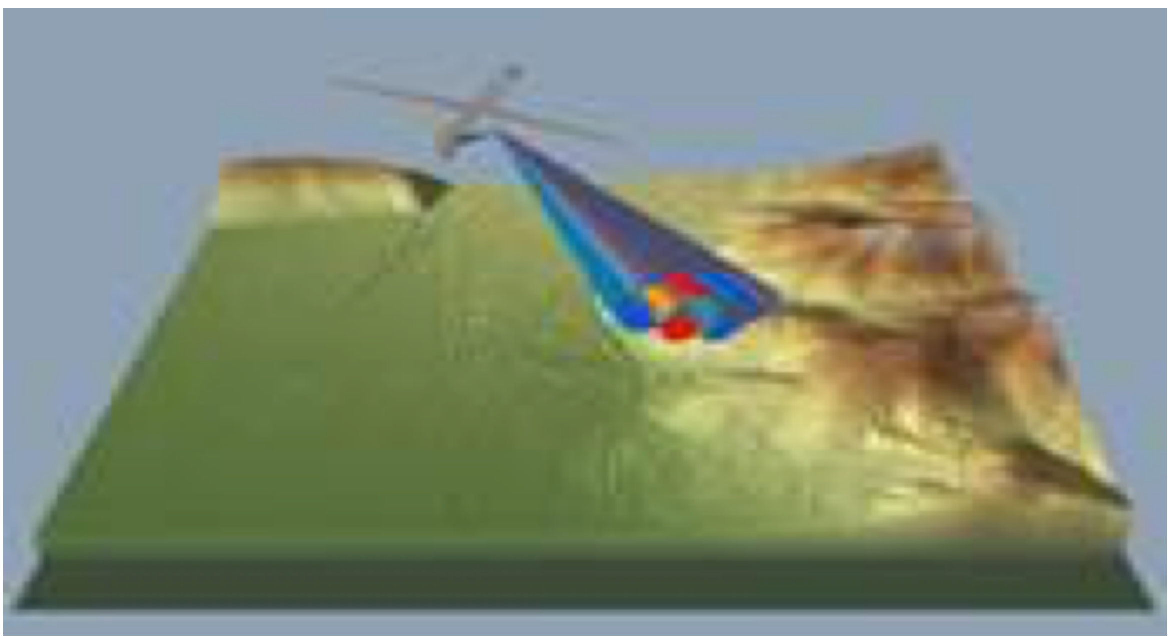
Our solution leverages Sandia's high performance computing capabilities, our extensive expertise in classical and quantum simulation, and an established collaboration for testing theory-generated hypotheses on modified enzymes that yields unique scientific insight. Few researchers possess this required combination of capabilities, or vision to pursue a model enzyme degradation process. Our experience suggests that a breakthrough in understanding small molecule degradation by a model enzyme is now attainable. This work will provide a new strategy for re-engineering enzyme active sites to favor degradation of specific molecules important for national security (e.g., chemical warfare agents).

DEFENSE SYSTEMS AND ASSESSMENTS

The Defense Systems and Assessments Investment Area (IA) delivers advanced science and technology solutions to deter, detect, track, defeat, and defend against threats to our national security. The work includes the development of innovative systems, sensors, and technologies for the nation's defense communities.

This IA seeks to draw upon Sandia's state-of-the-art ST&E capabilities through focused investments in three strategic program areas: Space Mission and Remote Sensing (SMRS), Information and Intelligence Technologies (ITT), and Integrated Domain Awareness and Prompt Response (IDAPR).

SMRS is focused on next-generation satellite flight and ground systems and future challenges facing the space community. The work supports the development of enabling technologies for revolutionary remote sensing and collection systems. IIT addresses the asymmetric threats arising from our nation's dependence on information networks and on anticipating disruptive capability and technology developments that threaten national security. IDAPR identifies enabling technologies that support precision knowledge, precision decisions, and precision response for the national security community.



Moving Target Detection and Location in Terrain using Radar (Project 158770)

DEFENSE SYSTEMS AND ASSESSMENTS

An Adaptive Web Spider for Multi-Modal Data

158747
Year 3 of 3
Principal Investigator: J. T. McClain

Project Purpose:

While search capabilities are improving with an increased number of utilities to locate documents and images on the Internet, the task to locate data continues to be manually intensive and relies on astute search abilities. Quickly and accurately locating information is most successful when the user has a priori knowledge about the relevant search terms and domain areas. Typically, the process to locate a document involves iteratively examining the URLs and web pages returned and modifying key terms to hone the search. Searching for images is limited to the metadata a person has associated with the image, and not the image itself. We will develop an intelligent web spider (aka crawler) to automate human search and browsing behavior on the Internet to significantly improve the speed, accuracy, and the comprehensiveness of an Internet search. Such a capability will accelerate the data gathering tasks, thus accelerating the intended information processing, review, or analysis objective.

Acknowledging the value of data content inherent to a picture and the value of the implications of recent advancements in data comparison for text and images is at the core of this innovative project idea. We plan to develop an intelligent web spider with the capability to examine both text and images within a web page or document, as well as the capability to adapt its search strategy, using machine-learning algorithms. If successful, this automated search capability will allow for more efficient, more accurate, and more comprehensive search results with minimal user intervention. The potential benefit can encompass Internet users across all domains, government industry, academia, and private industry.

Summary of Accomplishments:

This project has succeeded in demonstrating that combining images and text for purposes of information retrieval can improve performance, in some cases drastically, over text-only techniques. In addition, we have developed and tested a novel algorithm for fusing images and text using an image processing algorithm that describes images as bags of words, along with a bucket of models algorithm that utilizes two support vector machines (SVMs) built on text and fused image/text vectors. We have demonstrated that this algorithm outperforms a number of other approaches on an information retrieval task. In some cases, our algorithm drastically outperforms image-only and text-only approaches. Our conclusion is that fusing images and text is in all cases beneficial for performance on information retrieval tasks, and becomes even more critical as dataset complexity increases.

This project also developed an advanced, state-of-the-art intelligent web crawler, called Avondale. Avondale is capable of rapidly and accurately searching the Internet for specific information, while providing an advanced user interface for analyzing crawl results.

Significance:

"A picture is worth a thousand words" underlies the significance of data inherent in engineering drawings, photographs, presentations, equations, and more. The relevance of this capability to extend text-based searches with pictorial information spans across DOE and national security missions. Including images as Internet search cues and having them returned as pertinent search results could catalyze the efficiency and comprehensiveness of work done by the US government. This technology is a natural extension to current search capabilities and could potentially contribute to the information superiority required to protect our nation's critical infrastructure, environment, and citizens.

2-color nBn FPA

158754
Year 3 of 3
Principal Investigator: J. K. Kim

Project Purpose:
Traditional systems employ dual optic columns or beam paths that increase the size/weight/power and significantly limit sensor capability and/or mission duration. Two-color focal plane arrays (FPAs) that sense two wavelength bands in a single sensor are a natural and effective solution to this problem, but the current 2-color FPAs using HgCdTe technology compromise the resolution, quantum efficiency, and/or operability due to material and device architecture limitations.

Summary of Accomplishments:
We have developed a novel short-wave/mid-wave 2-color photodetector based on the nBn technology, which naturally lends itself to vertical stacking of short- and mid-wave absorbers with no loss in the pixel density, quantum efficiency, or operability. The bipolar design ensures perfect spatial co-registration between short- and mid-wave bands. We developed novel device design concepts and methods for fabricating 2-color nBn focal plane arrays with dry etching. We measured materials properties and device performance characteristics.

Significance:
Two-color sensing can be highly advantageous for numerous remote sensing mission areas. Event and target discrimination is enhanced because the complementary thermal signatures in the two bands help with disambiguation. Our work will enhance the performance of 2-color focal plane arrays. Our technology approach offers easier and lower-cost manufacturing, improved array uniformity and signal-to-noise characteristics, and operation at higher temperatures. When fully matured, this technology could ultimately provide a leapfrog advance in a wide range of infrared sensing applications contributing to national security.

Refereed Communications:
J.K. Kim, et.al, "Design and Performance of 2-color SWIR/MWIR nBn Photodetectors," presented at the *Military Sensing Symposium*, 2014.

J.K. Kim, et.al, "MBE and Material Characteristics of T2SL for IR Photodetection," presented (invited) at *International Conference on Molecular Beam Epitaxy*, Flagstaff, AZ, 2014.

Training Adaptive Decision Making

158764
Year 3 of 3
Principal Investigator: R. G. Abbott

Project Purpose:

Military personnel must make consequential decisions in complex situations where the outcomes of alternative actions cannot be anticipated with confidence, and changing circumstances may cause a good decision today to become a bad decision tomorrow. A recent Army Research Institute report stated, “The development of adaptive leaders has become a high priority for the Army; however, current research and practice related to adaptability is still in its infancy.” Adaptive decision making remains an ill-defined concept, with little certainty of what makes decisions more or less adaptive. Without a scientifically grounded, principles-based approach for engineering training solutions, military leaders must rely upon thoughtful intentions, and some measure of faith, that their solutions are producing the desired outcomes (i.e., personnel capable of making effective decisions despite ambiguous, continually changing conditions).

Sandia’s R&D addressing cognitive elements of training have focused on after action review (AAR). While valuable, AAR is inherently a retrospective approach, with inherent limitations. There is a need to expand the scope of these capabilities to include all phases of training, beginning with instructional design. A recent Sandia project undertook a series of experiments to identify the factors that underlie effective adaptive decision making. While the resulting model has accurately predicted behavior for laboratory tasks, further research is necessary to translate these findings into technologies ready for operational settings. This project provides the essential bridge to convert scientific accomplishments into operational impacts. If successful, adaptive decision making will be transformed from a nebulous, yet important, concept into a formally defined, measurable attribute of individuals and teams. Furthermore, a scientifically grounded foundation will emerge for engineering training technologies that assess the effectiveness of adaptive decision making, provide relevant performance feedback, and manipulate training content to improve decision making performance.

Summary of Accomplishments:

We explored applications of this research to benefit national security missions. Our development effort was guided by our research findings, which indicated that the critical factor in adaptive decision making is the ability to rapidly enumerate and evaluate possible courses of action. Our premise is that this ability is improved through training, by exposure to varied situations and responses to them. High-consequence environments provide significant challenges in providing training of this nature because the costs/consequences of incorrect decisions are too severe to allow trainees free exploration. As a result, computer simulations are used extensively to allow consequence-free exploration of tradeoffs.

We focused our efforts on DANTE, which is an UMBRA-based computer simulation of physical security scenarios for protecting high-value assets. DANTE provides artificial intelligence for computer agents who move and shoot autonomously. This high level of automation, combined with DOE supercomputing capacity, allows running hundreds of variations of a scenario very rapidly. However, if protective forces are trained to respond correctly to situations, running the scenarios is not enough — somehow the hundreds of runs must be condensed into insight that captures the available courses of action and consequences. Thus, analytics are equally important to data generation.

We addressed this need by developing data import from DANTE to the spatio-temporal analytic software developed under this project. This allows DANTE users to quickly visualize and summarize numerous scenario executions, so they can foresee likely outcomes of their actions, should they be placed in a similar situation. An example analytic is a visualization that overlays lines of fire from hundreds of runs onto a single visual. From this, the protective forces can identify the most lethal positions at the site and focus their efforts on controlling those positions.

Significance:

Our research is relevant to the core Sandia/DOE mission because it may help protective forces to guard high value DOE assets from possible destruction or diversion. This is an active area of research at Sandia as we seek to modernize our simulation and training capabilities.

A Complexity Science-Based Framework for Global Joint Operations Analysis to Support Force Projection

158765
Year 3 of 3
Principal Investigator: C. R. Lawton

Project Purpose:

The goal of this project is to develop a generic framework for analyzing Complex Enterprise Systems and Complex Adaptive Systems of Systems (CASoS). This framework and constituent functional decomposition, models, and analytical modules are intended to be domain agnostic (e.g., applicable to many complex enterprises). Through this research, we seek to provide a general, foundational framework for systematic, scientific, and explicit evaluation of strategic portfolios. A strategic portfolio consists of a set of systems that interact to accomplish missions that are important for maintaining security.

As an initial use case, we focused on the national defense enterprise that constitutes a complex enterprise system that coordinates the acquisition, planning, development and deployment of national assets to accomplish effective global force projection. The military is undergoing a significant transformation as it modernizes for the information age and adapts to include an emerging asymmetric threat beyond traditional cold war era adversaries. This current and future operating environment will require us to cast global force projection in the broader context of a CASoS. Office of the Secretary of Defense (OSD) must coordinate countless factors, over a short period of time, including civilian leadership objectives, budget limitations, and adaptive adversaries to determine the optimal trade-offs of resources and capabilities to accomplish national security missions.

Summary of Accomplishments:

This project leveraged the significant capability Sandia has developed in analyzing CASoS and SoS. We have used complex SoS engineering to develop an enterprise-modeling framework, which will enable OSD-level decision makers to better understand their enterprise. The complex adaptive system component of the hybrid-modeling framework analyzes the structure and dynamics of OSD. The framework incorporates three main subsystems: 1) US military industrial complex model (conventional and nuclear), 2) global threat model composed of a set of nation-states and non-state actors, and 3) OSD decision analysis system. The global threat model provides integrated modeling capability of international military and political developments. The US military industrial base model represents national scale military industrial complex entities. The decision analysis system is designed to explore parameter spaces to derive the best performing, lowest uncertainty options.

Significance:

Management of the DoD's enterprise dynamic constrained system has, for decades, relied on theory and best practices of public policy and procurement to maximize force projection. Techniques such as traditional large-scale, joint services war gaming analysis is no longer adequate to support program evaluation activities and mission planning analysis at the enterprise level because the operating environment is evolving too quickly. This project has resulted in new analytical capabilities that could address modernization of the DoD enterprise and maintain national security.

Refereed Communications:

C.R. Lawton, "A Model-Based Systems Engineering Framework for Evaluation and Improvement of Complex Enterprises," presented (invited) at the *International Federation of Operational Research Societies (IFORS) 2014 Conference*, Barcelona, Spain, 2014.

Quantitative Adaptation Analytics for Assessing Dynamic Systems of Systems

158767
Year 3 of 3
Principal Investigator: J. H. Gauthier

Project Purpose:

Our national security is built of dynamic system-of-systems (dSoS) — the military, homeland security, the nuclear weapons complex, and organizations and technologies therein. dSoS are collections of systems that interact and reconfigure over time in response to internal (e.g., budget) and external (e.g., threat environment) pressures. The problem is how to structure and manage a dSoS in an efficient and effective way, a way that maximizes multiple dSoS functional capabilities (with interdependencies) as missions and threats change and the collection of systems must be resized or reconfigured. This problem is of concern to many, including the US Army. Research on dSoS adaptability is lacking, but research in similar areas has centered on qualitative behavior — self-organization, learning, and emergence (e.g., Levin 2002, Macal and North 2010). Our project is novel because of the concentration on quantification, on general-purpose dSoS analytics, on national security dSoS, and on a new treatment of adaptation.

How to achieve more efficient and more effective national security dSoS, given budget pressures and constantly changing threat environments, is currently unknown. Our research focuses on the following topics: 1) quantitative adaptation metrics, 2) rules/decisions enabling successful adaptation, and 3) analytic tools that are useful and generally applicable to a variety of national security dSoS. This research will expand our knowledge of what constitutes effective dSoS adaptation in its many forms — flexibility, resilience, and robustness.

Summary of Accomplishments:

We completed derivation of equations for measuring adaptability in a system-of-systems (SoS) context. These equations are used to quantify the 15 different aspects of SoS adaptability; some of the equations can be used ab initio to assist in the design (both setup and operations) of adaptable SoS, and some can be used in simulations to capture time-based adaptability behavior. Of importance is that analysts and designers can now quantify differences in adaptability of different SoS designs. We developed a SoS adaptability index (SoSAI) that is an aggregation of an application-specific subset of the adaptability metrics. This construct allows the relative adaptability of different SoS designs to be compared using single composite adaptability values. We demonstrated that a subset of the adaptability metrics and SoSAI correlate with performance in a notional military deployment test case. This due diligence demonstrated that the adaptability metrics and equations actually can discriminate more adaptable SoS designs, and that these more adaptable designs can indicate better mission performance. As part of this effort, we developed software that is capable of assessing the adaptability of SoS. We developed a method for designing substitutability (one of the adaptability metrics) into a SoS. We also developed a new measure of SoS performance, called SoS availability or A_SoS that is used in the method. The method involves simulating a SoS and attempting to maximize A_SoS whenever systems need to be replaced (because of reliability or combat issues). The end result is a SoS designed with the most effective substitutability of systems.

Significance:

This work advances complexity science by developing an approach to incorporate adaptability into SoS. Using this approach, SoS can be designed to operate effectively under conditions of changing missions, under changing threat environments, and under changing natural environments. Thus, analysts and designers can now quantify the adaptability of vital national security SoS, such as those involved in a military deployment. Some of the adaptability metrics developed by this work also show promise in other national security areas, such as assessing supply chain integrity and determining representative sets of options in a combinatorial multi-objective optimization.

Ultra-Stable Oscillators for RF Systems

158768
Year 3 of 3
Principal Investigator: B. L. Tise

Project Purpose:

This project will leverage Sandia's microelectromechanical systems (MEMS) oven-controlled MEMS oscillator (OCMO) technology to create two new classes of high stability, low size weight and power (SWaP) radio frequency (RF) sources, create waveforms that leverage this stability, and recommend and test novel signal processing techniques made possible by the resultant sources.

Local oscillator (LO) instability affects RF system performance in a variety of ways — one chief mechanism is the inability to coherently integrate RF energy at a receiver past the point where RF phase is predictable. The advent of miniaturized, low power MEMS OCMOs could allow the device LO to remain coherent for a longer period of time and progressively become a smaller and smaller source of signal processing error. A device with a more stable LO is smaller due to the fact that it may transmit an equal amount of energy longer using a lower power output stage and with lower power batteries. In contrast, an instable LO may need to use a large, power hungry, and heat producing power amplifier to transmit an equal amount of energy over a shorter period of time in order to stay coherent. Existing systems have not yet exploited these new LOs and examined what beneficial impacts they have on system performance. This project investigated techniques to decrease device SWaP and reduce receiver complexity. The project also created and tested new waveforms and experimented with new and novel signal processing techniques that took advantage of improved oscillator stability.

Summary of Accomplishments:

We built temperature-controlled crystal oscillator (TCXO) test boards and used them to test four representative TCXOs and a Sandia-developed OCMO. We worked with a collaborator to bin TCXOs to obtain best-in-class TCXO performance. We designed specialized waveforms and transmitted these waveforms over multiple RF channels and evaluated receiver complexity. We conducted multiple experiments for development of short-aperture signal processing algorithms with stable system clocks. We demonstrated stable clock and waveform performance with an over-the-air (OTA) test.

Significance:

As a result of this development and testing, we demonstrated a waveform with >100x reduction in receiver complexity. Our experimental tests demonstrated minimal error using short-aperture algorithms with stable system clocks. The project results provide techniques for improving the performance of RF systems as the stability of local oscillators improves. The novel waveforms that were developed could be applied in a variety of national security situations that require ideal cross correlation.

Moving Target Detection and Location in Terrain using Radar

158770
Year 3 of 3
Principal Investigator: D. L. Bickel

Project Purpose:

During the last decade, the requirement for detection of moving objects for intelligence, surveillance, and reconnaissance have grown dramatically. More recently, agencies such as National Geospatial-Intelligence Agency are incorporating various forms of motion intelligence information into their purview to help support this growing demand. Radar sensors, including joint surveillance and target attack radar system (JSTARS), have proven to be invaluable for detecting moving objects in battlefield and intelligence, surveillance, and reconnaissance (ISR) applications.

One of the currently unsolved problems in using radar systems for detecting moving objects is achieving satisfactory performance in complex environments that include steep terrain. For the radar system, the difficulty arises in the filtering of stationary clutter due to complications introduced by the terrain and radar geometry. The purpose of this project is to address this problem of detecting and locating moving targets in steep terrain via a combination of a new antenna concept, new radar sensor modes, and signal processing algorithms.

Summary of Accomplishments:

This project successfully designed, developed, built, and flew a novel antenna and radar system used to collect data against small, slow-moving targets in terrain. We processed the real radar data and demonstrated the ability to detect and locate these targets using this new approach. This approach has some advantages over other approaches, particularly for ConOps and flight geometries associated with smaller radar systems.

Significance:

Detection and location of small movers in terrain is a difficult and an important problem for ISR. The flexibility of this antenna and radar concept enables its consideration for ISR and other national security applications.

Electronic Battle Damage Assessment (eBDA)

158773
Year 3 of 3
Principal Investigator: J. T. Williams

Project Purpose:

Tactically, one of the greatest impediments to the application of high power microwave (HPM) weapons is the current inability to assess their effect on the intended target, battled damage assessment (BDA). The problem is further complicated since the effects achieved by such weapons can be temporary or permanent and are sometimes not repeatable given minor changes in the engagement scenario. Hence, the BDA tools for non-kinetic weapons, and even kinetic weapons targeting electronic systems, should be based upon on-site intelligence and electronic sensing.

An effective electronic BDA (eBDA) tool should be able to detect system changes based upon electromagnetic observables, assess the operational state of the target system given the detected system changes, and classify the success of the attack. Critical to developing such eBDA tools is the identification of tactically feasible electromagnetic (EM) observables that can be exploited by either active or passive electronic sensing systems. At close ranges, we have successfully identified many such observables in realistic environments. The intent of this project is to develop the techniques to measure state-related electromagnetic observables from relevant target systems at range. The outcome of this effort should be a technology readiness level TRL-5 prototype system that demonstrates effective eBDA principles and techniques.

This effort is extremely challenging and fundamental in nature. Many of the passive EM observables that can be used effectively for eBDA are low power level and clustered with other less-relevant emissions and background noise, making detection at range very challenging. In addition, the design of active EM signals that can be used to interrogate a specific target and produce measurable responses that can be related to its state is a relatively unexplored discipline. Yet, many of these issues can be resolved when proper measurement and signal processing techniques are brought to bear.

Summary of Accomplishments:

We have successfully demonstrated an ability to assess state-based information from measured unintended electromagnetic emissions for a number of relevant targets and target classes (e.g., computers, supervisory control and data acquisition (SCADA), communications networks). This includes developing and demonstrating both passive and active electronic battle damage techniques, many of which are effective at tactical ranges.

A list of key accomplishments:

- This project took advantage of the US Air Force Counter-Electronics High-Powered Microwave Advanced Missile Project (CHAMP) testing series, as a testbed to conduct realistic eBDA tests to discover the limits and challenges of detecting target state in a real world environment. The CHAMP testing allowed us to take significant amounts of relevant data that would have been impractical to acquire otherwise. This test data was obtained at minor cost to the project since the CHAMP program provided the test environment, relevant targets, the high power microwave (HPM) source and most of the logistics costs. As a result of these efforts, we were invited to conduct eBDA using a flight test of CHAMP. During the flight test, we successfully demonstrated the ability to conduct eBDA in a realistic engagement and resolved many important issues associated with obtaining data during a high peak power HPM attack.

- We demonstrated the ability to conduct eBDA at ranges up to 1 km.
- We identified that power supply emissions can be related to operational state.
- In collaboration with university researchers, we developed techniques for target localization in presence of scattering walls and ground that are particularly useful in multi-target environments.
- We developed time-domain based eBDA techniques that enhance weak signal detection and automation.
- We investigated active “harmonic radar” eBDA techniques.
- We developed a fieldable software radio based data acquisition system.
- We conducted eBDA at the Naval Surface Warfare Center-Dahlgren on relevant Navy targets.
- We acquired and instal led an HPM source and pulse power system (Stinger) for eBDA testing.

Significance:

We have successfully demonstrated the feasibility of eBDA and have developed a number of techniques to detect system changes based upon electromagnetic emissions and assessment of the operational state of the target system. We have established practical limits and expectations for the application of eBDA, and have positioned Sandia as a recognized leader in electronic battle damage assessment.

Refereed Communications:

J.T. Williams, L.D. Bacon, and M.R. Gramann, “Progress in Electronic Battle Damage Assessment,” presented (invited) at the *2014 Electric Fires Seminar*, Fort Sill, OK, 2014.

J.T. Williams, L.D. Bacon, and M.R. Gramann, “Electronic Battle Damage Assessment (eBDA),” presented (invited) at the *Emerging and Enabling Technology Conference*, Huntsville, AL, 2013.

Ablation Chemistry Effects on Boundary Layer Transition

158774
Year 3 of 3
Principal Investigator: D. W. Kuntz

Project Purpose:

Boundary layer transition (BLT) is the phenomenon that occurs within the boundary layer of flight vehicles when the flow changes from laminar to turbulent. As this process occurs, flow properties change significantly, most notably the aerodynamic heating rises drastically. Recent investigations have indicated that ablation chemistry effects resulting from the interaction of compounds introduced into the boundary layer as a result of ablation of the thermal protection system can have a significant effect on boundary layer transition. The purpose of this effort was to investigate this phenomenon and to specifically determine what effects ablation products have on transition.

Summary of Accomplishments:

Techniques have been developed for modeling the effects of heat shield ablation on the chemistry of the boundary layer surrounding a realistic hypersonic flight vehicle and, in turn, determining the effects of this chemistry on boundary layer transition. The results have indicated that ablation chemistry can have a significant effect on boundary layer transition. The techniques and computational tools developed during this effort have been demonstrated to facilitate the rapid analysis of boundary layer transition on realistic flight vehicles.

Significance:

The efforts involved in this research resulted in the advancement of state-of-the-art transition prediction techniques to a near-production level, increasing our ability to accurately predict boundary layer transition on future flight vehicle projects. This positions Sandia as one of the leaders in the nation to simulate the flow fields and transition behavior of hypersonic flight vehicles.

Inferring Organizational Structure from Behavior

158780
Year 3 of 3
Principal Investigator: T. L. Bauer

Project Purpose:

We will advance the state of the art in algorithms for detecting previously unknown networks by introducing the use of temporal correlations among behaviors, leveraging both information sources and metadata. We will validate the algorithms against two data sets. This will result in new algorithms and technology for applying them.

A lack of real-word data sets with both social network and behavioral information (as opposed to poll results, for example) has impeded the development of valid models for inferring social networks. However, newer data sets and recent research suggest that this problem might now be tractable. The rapid increase in crowd-sourced applications like Wikipedia is providing a rich set of data with both a record of behaviors and a set of direct interactions among individuals. Data sets with network ground truth are needed to develop and validate models.

This research will advance the state of the art by focusing on temporal correlations in behavior.

The ability to discover organizational structure from observable behavior would address multiple national security problems, such as technology surprise and nonproliferation. However, it is itself a basic scientific question. The core capability for doing this is most appropriately developed and validated in the context of scientific investigation before being transitioned to specific use.

We will focus on using implicit evidence, such as two people editing the same page, editing documents in the same topic, or participating in the diffusion of data in similar points. While none of these examples show direct connections among people, they do show that the people are “similar” in certain ways and may also be connected.

Summary of Accomplishments:

We implemented and tested an information theoretic based algorithm for inferring social networks based on behavior. The algorithm does not require content in order to infer relationships. Rather it is based on time stamps. Our results using the Wikipedia edit history as a baseline showed an approximately 20X improvement in precision at low levels of recall. We also implemented and tested a method for looking at content to infer points in time when an organization may be changing directions.

Significance:

In many data sets, one needs to infer things that they can’t directly observe. This algorithm shows that it may be possible to observe the external behavior of different entities, and to infer the internal relationships that are driving those behaviors. Also, it is often the case that one wants to analyze a data set, but does not know what the relevant features are, or perhaps even how to break a data set into features. We have shown that compression can be a reliable method for performing some analysis without breaking a data set into features. The results of this project may be beneficial to multiple national security missions where the development of analytical tools for helping analysts make sense of large bodies of data is essential.

Nonlinear Decision Theory Applied to Co-Hosting Analysis for National Security Space Payloads

158784
Year 3 of 3
Principal Investigator: S. M. Gentry

Project Purpose:

In constrained fiscal environments, national security space mission planners are often asked to perform multiple missions using a single joint space system (JSS). Theoretically, by using shared platforms to perform multiple tasks, joint systems have the potential to reduce technical duplication, to streamline operations, and ultimately, to reduce space mission cost. Practically, joint systems present both technical and organizational challenges that often impede the system's ability to achieve the envisioned cost savings or to realize the intended mission performance.

JSSs were first utilized in the 1970s when Defense Support Program satellites began hosting nuclear detection system payloads. Since this time, the national security space community has continued to develop JSSs for nuclear detection, for communications, and for operational support. While several of these JSSs have enjoyed considerable success, others have been mired by organizational, technical, and cost challenges. Despite this varied historic experience, there has not been a comprehensive study of JSSs that has identified specific impediments and enablers to their development. As a result, opportunities for future JSSs continue to be evaluated subjectively and through individual programmatic assessments. This project will use space systems architecting tools to inject both quantitative rigor and holistic systems thinking into this process. Specifically, we will study historic examples of JSSs, identify specific impediments and enablers to successful JSSs utilization, and create a methodology for systematically evaluating opportunities for future JSS development. The work is in collaboration with MIT.

To thoroughly evaluate opportunities for JSS development, mission planners must consider how the process of mission combination will affect a system's performance, operation, cost, and risk. Although technical analyses can illuminate performance impacts, traditional engineering tools cannot assess the operational, cost, and risk impacts of mission combination. Tackling the problem of JSS development requires a unique and innovative systems architecting approach that aligns well with the stated goals of the research.

Summary of Accomplishments:

We completed an exploration of the cost impact of acquiring complex government systems jointly. We reviewed recent evidence that suggests that joint programs experience greater cost growth than non-joint programs. We suggested an alternative approach for studying cost growth on government acquisition programs and we demonstrated the utility of this approach by applying it to study the cost of jointness on three past programs that developed environmental monitoring systems for low-earth orbit. Ultimately, we found that joint programs' costs grow when the collaborating government agencies take action to retain or regain their autonomy. We provided detailed qualitative and quantitative data in support of this conclusion and generalized its findings to other joint programs that were not explicitly studied. Finally, we presented a quantitative model that assesses the cost impacts of jointness and demonstrated how government agencies can more effectively architect joint programs in the future.

Significance:

This research showed the utility of nonlinear decision theory and an Object Process Network meta-language approach applied to national space problems; in this case, the assessment of joint development of space systems. The results show that consideration of technical organization autonomy has a strong impact to technical project success. The results provide a strong set of conclusions regarding how major cost growth in joint space system development could be avoided in the future.

Learning From Nature: Biomimetic Polarimetry for Imaging in Obscuring Environments

158785
Year 3 of 3
Principal Investigator: D. Scrymgeour

Project Purpose:

Imaging in obscure surroundings such as fog, smoke, dust, and under water is one of the most difficult environments encountered on earth. However, many key national security interests rely on communicating and seeing in these obscuring environments, such as helicopters landing blind due to obscuring dust or communicating/imaging through clouds and water. Even modest extensions in imaging ranges in these extreme turbid environments are a technological breakthrough and have wide-ranging impact on turbid-media signaling, imaging, and communications. T his project seeks to develop passive optimal polarization vision, utilizing both linear and circular polarization signatures, which has been shown to increase imaging distances three times compared to standard intensity imaging. Because the environmental variables (e.g., imaging wavelength, particle size density, size distribution, and index of refraction) are so diverse, specific optimization for imaging in critical conditions have not been performed. We will systematically develop polarimetry-imaging schemes specifically tailored for obscuring environments crucial to national security applications (clouds, dust, and oil plumes) through a combination of simulation and experimental techniques. This will allow the exploitation of polarimetry for tagging, tracking, and locating applications and to improve imaging in turbid media that is of interest to a broad application set including environmental monitoring, underwater communications, and rocket plume detection.

The stomatopod crustacean (mantis shrimp) has evolved an exquisite vision platform and has the capability to see in full polarization. Biologically evolved systems are often supremely adapted to their environment; solving complex problems that maximize visual information while minimizing metabolic energy consumption and signal processing requirements. These biologically evolved systems should be the inspiration for future imaging systems. Findings can be extended to both terrestrial and space based environmental imaging systems where turbidity is introduced by pollution, smoke, and clouds. This work is in collaboration with University of Arizona.

Summary of Accomplishments:

We have modeled the transport of polarized light through technically challenging scattering environments of fog and dust using a polarization tracking Mie and Rayleigh Monte Carlo simulation. Specifically, we have shown that there are different wavelengths in the infrared regime where the use of circular polarization may be utilized to increase imaging range in these scattering environments over traditional intensity imaging or linear polarization imaging. We have examined various types of foggy and dusty environments important in many national security applications. We have modeled both radiation fog, with particle sizes typically smaller than 10 microns, and advection fog, with larger particle sizes with diameters of 20-40 microns. The dust environments modeled were Sahara type dust for small particles (diameters less than 6 microns) and large particles (diameters greater 10 microns). Our models predict that circular polarization can increase imaging range in radiation fog both shortwave infrared (SWIR) and the mid-wave infrared (MWIR) regions and in advection fog using long-wave infrared (LWIR). Range was increased in small particle dust by imaging with MWIR circular polarization.

Simultaneously, we have performed experiments to confirm simulation results using easy to prepare and measure solutions of single size polystyrene spheres in water. A suitable experimental testbed was assembled and the polarization signatures from the polystyrene spheres in water were measured. Simulated results match well to the experimental data confirming the validity of the simulation models. Additionally, we collected data on signal range fog in Sandia's environmental testing facility. These results confirmed that circular polarization propagates farther than linear polarization.

Significance:

This work offers new insight into potential environments and wavebands of interest where circular polarization can be utilized to increase detection range and signal persistence. This work offers insight into solutions for imaging in traditionally difficult environments such as coastal settings with water interfaces and fog. Results could ultimately enable imaging systems with improved target identification and discrimination.

Refereed Communications:

J.D. van der Laan, D.A. Scrymgeour, S.A. Kemme, and E.L. Dereniak, "Increasing Detection Range and Minimizing Polarization Mixing with Circularly Polarized Light through Scattering Environments," in *Proceedings Polarization: Measurement, Analysis, and Remote Sensing XI*, p. 909908, 2014.

Optimal Adaptive Control Strategies for Hypersonic Vehicle Applications

161863
Year 3 of 3
Principal Investigator: J. M. Parish

Project Purpose:

The purpose of the project is to develop a reliable model-based control strategy for agile flight vehicles subject to large uncertainties and undesirable multibody dynamic behaviors. Unlike traditional control approaches, model-based nonlinear control methods are particularly well suited to construct tractable control designs for highly maneuverable vehicles subject to large aerodynamic uncertainties. In this method, nonlinear vehicle dynamics are assumed to be largely “canceled out” in an inner control loop. However, the unexpected presence of unmodeled dynamics has been shown to cause controllability issues, instabilities, and failures in both simulation and flight of actual vehicles. In general, this undesired behavior results from neglecting key nonlinearities in the rigid-body vehicle model typically employed in nonlinear control. There exists little literature in the community regarding multibody effects for this class of vehicle. Thus, control of these more comprehensive vehicle dynamical models remains a challenging, outstanding problem. This work develops a nonlinear control strategy for a complex, multibody dynamic model of a hypersonic glide vehicle. The approach of enhancing an existing nonlinear rigid body dynamic inversion controller with multibody dynamics is novel for control design for this class of vehicles. This broader view synthesizes existing control methods to improve the capabilities of advanced vehicle concepts. Furthermore, these developments will help guide development of future vehicle concepts by providing a more holistic modeling and control approach for assessing performance of candidate flight vehicle designs.

Summary of Accomplishments:

In this work, we reduced the uncertainty revolving around modeling multibody dynamics that induce inertial forces and moments unaccounted for in standard rigid-body models. A fairly comprehensive approach was taken to start from first principles and introduce reasonable assumptions as necessary to develop nonlinear multibody models of varying fidelities for a representative hypersonic vehicle. A significant validation effort was employed to compare these models against one other, to existing analytical models, and with ground and flight test data of real-world systems. To test these (and existing models), a flexible model-based simulation environment was developed and extensively tested. To streamline the construction of this simulation and accommodation of new modeling insights, a method for auto-generating the multibody governing equations was formed.

The ultimate goal of these modeling and simulation efforts was to design and test nonlinear model-based control laws that can mitigate destabilizing multibody induced forces and moments. In this work, we derived several potential control solutions to address this goal. A successful existing rigid-body control motivated the desire to supplement, rather than replace, the rigid-body portion of the existing control structure for the representative vehicle. The candidate control that best accommodated the original rigid-body control was chosen for further evaluation. Preliminary tests of this reduced-order model-based control solution in the full, nonlinear model simulation showed the desired weakening of the multibody induced dynamics while still retaining favorable vehicle performance when compared to an existing linear control strategy. Through this effort, we demonstrated the feasibility of using a complex, multibody model to augment an existing nonlinear controller to successfully reduce the effect of undesirable multibody dynamics.

Significance:

Realization of this multibody model-based control strategy could enable a more stable operating capability for hypersonic glide vehicles. For example, auto-generation of multibody dynamical equations has been applied to a booster controller as well as a new missile interceptor concept. Second, this modeling work has been used to independently verify enhancements to high-fidelity multibody simulations of a recent flight test vehicle. As the demands on the operating capability of this class of vehicles intensify, this research could provide beneficial analysis and control design capability.

Investigating Dynamic Hardware and Software Checking Techniques to Enhance Trusted Computing

164671
Year 3 of 3
Principal Investigator: C. Jenkins

Project Purpose:

Vision: Imagine a system in which a trusted authority (e.g., a proxy for accreditation authority, etc.) detects a loss in trust integrity in certain components of the system but needs to maintain certain critical service levels or functions, in spite of the untrusted nature of the compromised system. Further, imagine this system dynamically migrating or adapting to a low level of trust and associated functions while taking steps to reestablish higher trust levels.

As the field of determined and increasingly sophisticated adversaries multiplies, the trust level of deployed computing devices magnifies. Given the ubiquitous connectivity, substantial storage, and accessibility by a variety of users, and increased reliance on mobile platforms for access to critical services (banking, government, military, economic, critical infrastructure systems, etc.), the devices themselves are a point of vulnerability, especially commercial off-the-shelf (COTS) devices. The ability to check components of a system at both load time and runtime should mitigate the attack surface for compromising these types of devices.

This research investigates a new system-level software/hardware paradigm for designing secure computing systems — potentially utilizing security extensions of modern-day CPUs. The research looks at a new concept called "integrity levels." Based on the integrity level, the computing system may not process or send certain data until the desired level exists. Also, gracefully reducing functionality in a compromised system should allow critical and noncritical components to react in an effective manner. This research aims to discover general solutions that can be applied to various segments of interest.

Goal: This work intends to establish how to change integrity levels dynamically, versus assuming a static runtime security configuration. This research will identify features of current CPU technology needed to implement integrity levels as well as new features and/or capabilities for future systems.

Summary of Accomplishments:

There is a longstanding need to execute software in a trustworthy manner in a compromised system/ environment. We developed a new integrity-computing paradigm with the goal of creating more resilient computing environments. We sought to create a polymorphic computing environment to mitigate the effects of malware and advance persistent threats. While much work needs to be done to increase the technology readiness level, the components, prototype, and direction forward have been completed. We have identified potential use cases and utilized open source software to rapidly develop a prototype.

Previous work looks to detect and prevent attacks while providing avenues to recover. While our approach does not preclude those protections, we looked at different ways the computing environment could change to mitigate or thwart advanced attacks. To our knowledge, there is not a computing system in existence that attacks the problem in this novel manner.

Overall, we have only scratched the surface on a potential new way of designing computing environments.

Significance:
Cyber warfare is an emerging threat with no sign of decreasing in the future. Future generation systems need resiliency inherent within the system design. We have constructed a formal model to design resiliency into a computer environments. Our goal is to create a policy such that any malware inherently violates the policy. Furthermore, our work has potential reach outside of traditional computing devices and we look to understand how those application spaces could use our novel concept.

Refereed Communications:
C. Jenkins and L. Pierson, "Integrity Levels: A New Paradigm for Protecting Computing Systems," in *Proceedings of the International Conference on Trust, Security and Privacy in Computing and Communications (TrustCom-14)*, Beijing, China, 2014.

Mission Capability Analysis Environment for End-to-End Performance Assessment of Space Systems

164892
Year 3 of 3
Principal Investigator: D. P. Woodbury

Project Purpose:

By leveraging its strengths in remote sensing component technologies, Sandia has developed analysis capabilities to support high fidelity empirically based simulations and yield verified accurate end-to-end sensor performance estimates of electro-optical/infrared (EO/IR) systems. Current analysis capabilities, however, are limited to only designed and tested remote sensing assets. Current simulation code provides mission optimization tools for only specific systems based on experimentally determined parameters which are unknown for envisioned EO/IR designs. The combination of required mature sensor characterization inputs and lack of parameter optimization capabilities for a variety of systems prevents utilization of the existing code for rapid mission capability performance assessments of future EO/IR systems. The goal of this research is to develop a mission-based design and analysis environment that bridges the gap between accurate future mission needs and payload design requirements, without which there is a risk of making incorrect investing decisions in future space-based EO/IR systems and technologies.

The key innovations of the planned analysis environment are: 1) identifying the multidisciplinary set of first-principal physical constraints which couple the mission-critical design parameters of future EOIR space systems and 2) exposing this high-dimensional, nonlinear, mixed-discrete-and-continuous design space for improved parameter selection capabilities to support mission requirements. First-order EOIR system requirements can be based on a finite number of fundamental physical parameters, which provide the backbone of a system's performance characterization. This multidisciplinary set of variables can be partitioned into three sets of parameters which describe the desired mission scenario, the external conditions imposed on that scenario, and the payload design itself. Along with identifying these base sets of critical design parameters, we must also ascertain the physical constraints between these parameters and how parameter uncertainty evolves through these applied constraints. Finally, the performance of the system must be related to specific mission scenarios and detectability metrics must be identified in terms of quantifiable measures of mission success.

Summary of Accomplishments:

We identified a minimum set of twenty-two design parameters and nine associated metrics for first-order mission capability assessments. We developed the Target-based Operation Mission Capability Assessment Tools (TOMCAT) to quickly compare and evaluate sensor payload designs for the EO/IR mission areas. The TOMCAT architecture is a novel capability, which can be used to rapidly assess EO/IR pathfinder design concepts based on minimal initial knowledge. This rapid assessment and analysis capability provides the means to make strategic decisions regarding future EO/IR mission designs and component technologies.

We successfully integrated the capabilities of seven other internally developed modeling architectures into TOMCAT's unified simulation framework. This framework: 1) bridges the gap between literal mission needs and payload design requirements, 2) facilitates decisions by distinguishing between unneeded and transformational component technologies, 3) prevents the development of redundant sensors, and 4) enables the development of innovative systems necessary to fulfill mission area gaps. TOMCAT will be used in three additional upcoming projects.

Significance:

The development of a versatile EO/IR simulation environment could benefit organizations such as the Missile Defense Agency, Air Force Space Command, and the broader EO/IR community, enabling the ability to identify national security mission capability gaps as well as propose possible solutions. Furthermore, new mission areas can also be identified for deployed EO/IR assets. Based on trade studies and sensitivity analyses using component-based analyses, strategic decisions can be made regarding critical component technologies.

Precision Laser Annealing of Focal Plane Arrays

165545
Year 2 of 3
Principal Investigator: D. A. Bender

Project Purpose:

Detectors of optical signals in the visible or infrared (IR) often undergo thermal annealing in manufacturing to allow dopant activation, thermal oxidation, metal reflow, and chemical vapor deposition. Thermal annealing is typically done with equipment that heats the entire semiconductor wafer by using a flash lamp, hot plate, or furnace. Lasers are also employed with a cylindrical lens focusing a beam into a thin line that is swept across the wafer, homogenizing the surface. These techniques, however, are performed over the entire sensor and do not discriminate between adequately manufactured and defective regions. Ideally, processing techniques would precisely target only pixels or pixel clusters that are "hot" or noisy, while leaving functional pixels and surrounding electronics untouched.

Our idea is to perform laser annealing on detectors after they have been hybridized with readout electronics (ROIC). Targeted laser annealing on packaged focal plane arrays (FPAs) prior to mission use represents reinforcement to the state-of-the-art thermal annealing and laser procedures currently done during the manufacturing process. Laser annealing can be performed at any point after manufacturing and before mission commencement. If an FPA resides in flight storage or is exposed to damaging radiation for extended durations after manufacturing, laser annealing could be used to restore individual pixels or clusters that may have degraded with time or were substandard to begin with.

The time and cost associated with developing a technique to address handfuls of underperforming pixels is not economical for a volume-based commercial business. However, success in this project constitutes a method to reduce schedule delays by promoting engineering grade FPAs to science grade FPAs — a procedure with high commercial value. Additionally, missions relevant to national security sometimes require a few very high performance collection platforms. Making the effort to have the best possible collection capability motivates the development of laser annealing and results in a unique, innovative capability not found in the commercial marketplace.

Computer Network Deception

165547
Year 2 of 3
Principal Investigator: V. Urias

Project Purpose:

The modern approach to computer network defense has led to an assumption that our networks will likely be compromised. This assertion stems from the idea that the existing defense tools (intrusion prevention systems, intrusion defense systems, firewalls, antivirus, along with 15+ years of research into honeypots, honeynets, etc.) are challenged in defending against today's threats. Enterprises are consistently compromised by multiple classes of adversaries, despite significant amounts of money and effort. Research needs to focus on revolutionary, and not evolutionary, defenses that will affect a broader class of threats and threat vectors.

Threat is outpacing the capacity to defend. The asymmetric ability of an adversary to gain unauthorized access to machines and data has forced net-defense to adopt a reactive security posture. This project is developing novel approaches to threat intelligence through a variety of novel tools, systems (networks), monitoring, and emerging technology to create and improve the cyber posture. The project is exploring a variety of tools such as virtualization, software defined networking, and hypervisor introspection to aid in creating an immersive environment for adversaries to stay and explore.

Graphene Survivability

165551
Year 2 of 2
Principal Investigator: S. W. Howell

Project Purpose:

The purpose of this project is to understand mechanisms that influence graphene survivability in various environments. The isolation of graphene monolayers in 2004 has spurred an explosion of international graphene research interest due to its exotic Dirac quantum mechanics-based electronic properties. Although intrinsically a high mobility semi-metal (~200,000 cm^2/Vs when defect-free, versus ~1500 for Si and ~8500 for GaAs), graphene's physical strength, adaptability to planar processing, micron-scale room temperature ballistic electronic transport behavior, and potential for real-time bandgap manipulation (via chemically doping or application of internal/external electric fields) makes it a promising candidate for advancing and possibly replacing silicon technology in the nanoscale regime, as well as the creation of disruptive carbon-based electronic applications. The promise of graphene, as a high-performance electronic material, has recently attracted great interest. Currently, a large amount of research has concentrated on understanding the electronic and material properties of graphene in controlled environments. However, little is known about graphene survivability in less than ideal environments. To address this lack of understanding, we will develop differentiating and synergistic approaches to: 1) characterize graphene device performance after exposure to various environments and 2) understand the root causes of graphene device failure in those environments using standard failure analysis techniques. The linkage to a complete suite of coordinated Sandia characterization/modeling efforts is another differentiating factor of our effort that assures project impact and leadership within the competitive and rapidly moving graphene research community.

Summary of Accomplishments:

We successfully tested graphene devices in less than ideal environments. Furthermore, we examined self-heating and resulting failure of graphene devices made with: 1) epitaxial graphene atop SiC, 2) transferred graphene atop SiC, and 3) transferred graphene on top of a SiO_2/Si stack. By imaging the temperature distribution with infrared thermography for each of the devices and comparing it to the strain and carrier concentration profiles obtained via Raman imaging, we find that the enhanced coupling to the substrate in epitaxial graphene devices actually reduces the amount of power that a graphene device can dissipate before failing.

Significance:

The results of this project may have an impact on national security mission. There has been widespread international speculation regarding the potential robustness of graphene devices. This LDRD not only quantified the robustness of the devices but also generated new scientific insight regarding graphene device robustness in harsh environments.

Combination Bearing/Flexure Joint for Large Coarse Motions and Fine Jitter Control

165552
Year 2 of 2
Principal Investigator: P. S. Barney

Project Purpose:

High-precision pointing systems are required for space applications in order to stabilize sensors to meet stringent requirements for jitter (uncompensated, high-frequency motions). Minimizing the jitter is especially difficult for payloads that are flown on multi-mission spacecraft because those vehicles are not optimized to mitigate the base disturbances into the payload. The jitter requirements for new systems only get more demanding as higher-density focal planes are coupled to telescopes with increasing optical power. The joints of these high-precision payloads are typically supported by high-quality bearings that are strong enough to ensure survival of the launch loads, yet as smooth as possible to minimize drag during moves. Even the best bearings have nonlinear friction characteristics, which adversely affect the control system performance. A combination of a bearing and a flexure is envisioned that will allow: 1) large motions using the bearings across the field-of-regard (FoR) to maximize area coverage by the payload sensors, and 2) for linear and repeatable small motions even during direction reversal thereby decreasing jitter. This combination of two technologies will allow systems to exceed the performance of existing systems, which will increase the capabilities and mission space.

This project will develop a new design that incorporates a bearing, a flexure, as well as a braking mechanism. The most challenging aspect in the development of such a device is to balance the flexible linear portion of the system with the large FoR nonlinear portion while allowing for a robust controller. The active braking system could be the key to success; this will need to be balanced against the true cost of added complexity. A testbed will be used to identify performance and operational limits. This project will result in technology readiness level that is mature enough to allow the hybrid design to be baselined for future, customer-funded development.

Summary of Accomplishments:

Current trends in the imaging community require lower jitter than is currently possible using conventional bearings due to nonlinearity in the bearing. This project attempted to address that issue by developing a hybrid bearing capable of large motions while allowing for linear motions at small motions thereby reducing jitter. Within the course of this project, we were able to design and manufacture a flexible bearing with properties suitable for a precision-pointing system to have a more linear character, thereby reducing jitter. Using the new flex bearing in series with a conventional bearing, we developed, analyzed, and tested the precision-pointing capabilities of a system with a single axis testbed.

Using the single axis testbed, we were able to more fully understand, tune, and model the classical bearing for precision pointing. Techniques were used to minimize the nonlinear aspects of the classical bearings and tools were developed to characterize them for higher fidelity simulation. The interaction with the flex bearing and the classical bearing were modeled for the testbed, which allowed for a higher quality controller design. The designed controller was implemented on the testbed, which showed reasonable increase in performance.

As part of the testbed development, new sensors and actuators were identified that allow for a simpler, higher resolution and more robust system. The identification and testing of the new sensors is currently being incorporated into new designs as well as knowledge captured to reduce traditional bearing issues.

The flex bearing as designed and tested has a feature that allows significant variation in stiffness as a function of hub temperature. This change in stiffness manifests itself as a tunable modal frequency.

Significance:

This project has provided an enabling technology to the field of very precise pointing applications and has addressed a contributing factor that limits our ability to detect dim and closely spaced targets. By utilizing techniques developed here, jitter can be reduced which allows for a better ensquared energy and ability to detect dimmer targets as well as allowing for better background frame differences and better detections. A technical advance has been applied for in the area of the tunable modal frequency aspect of the flexure bearing. This work is on the leading edge of capability for precision-pointing systems.

Wound Ballistics Modeling for Blast Loading, Blunt Force Impact, and Projectile Penetration

165554
Year 2 of 3
Principal Investigator: P. A. Taylor

Project Purpose:

Light body armor development for the warfighter is based on trial-and-error testing of prototype designs against ballistic projectiles. Torso armor testing against blast is nonexistent but necessary to protect the heart and lungs. In tests against ballistic projectiles, protective apparel is placed over ballistic clay and the projectiles are fired into the armor/clay target. The clay represents the human torso and its behind-armor deflection is the principal metric to assess armor protection. Although this approach provides relative merit assessment of protection, it does not examine the behind-armor blunt trauma to crucial torso organs. We plan to study and develop a modeling and simulation (M&S) capability for wound injury scenarios to the head, neck, and torso of the warfighter. We will use this toolset to investigate the consequences of, and mitigation against, blast exposure, blunt force impact, and ballistic projectile penetration leading to damage of critical organs comprising the central nervous, cardiovascular, and respiratory systems. We will leverage Sandia codes and our M&S expertise on traumatic brain injury to develop virtual anatomical models of the head, neck, and torso and the simulation methodology to capture the physics of wound mechanics. Specifically, we will investigate virtual wound injuries to the head, neck, and torso with, and without, protective armor to demonstrate the advantages of performing injury simulations for the development of body armor. The planned toolset constitutes a significant advance over current methods by providing a virtual simulation capability to investigate wound injury and optimize armor design without the need for extensive field testing.

Ground Moving Target Extraction, Tracking, and Image Fusion

165555
Year 2 of 3
Principal Investigator: T. J. Ma

Project Purpose:

Real-time dim target detection and tracking with a remote sensor is a very difficult problem. Setting a lower detection threshold may detect the target but can also introduce a higher false alarm rate. Less target pixels are detected, making it very difficult to obtain characteristics such as shape and texture information to extract the target. Filtering out false detections becomes a difficult task. Traditional velocity matched filter (VMF) techniques are known to be effective in enhancing target signal-to-noise-ratio (SNR), but the VMF algorithm carries huge computational complexity which makes real-time application less feasible. Traditional VMF techniques also require the number of targets to be known in advance. This a priori information is usually not available in real-time unsupervised application. The purpose of this R&D project is to develop a dim-target detection and tracking capability that operates in a constrained environment. We have developed a constrained velocity matched filter (CVMF) algorithm that uses geographical maps as constraints to improve detection of dim targets. This approach can be combined with a detection-and-track approach that counters the drawbacks of the traditional VMF. Additionally, we have developed a dynamic constrained velocity matched filter (DCVMF), which uses state and covariance estimates from a Kalman filter to dynamically constrain the number of matched filters. Moreover, we have developed a new detection and tracking classification technique using a convolutional neural network. We plan to investigate a new concept of fused-before-detect approach by applying image fusion prior to detection and tracking. If images were fused prior to detection processing, it is possible that the input image can be enhanced so that the detector can potentially detect more useful information as a result of the fused image instead of an image gathered by a single sensor.

Radio Frequency Environment Characterization through Novel Machine Learning Techniques

165563
Year 2 of 2
Principal Investigator: S. M. Patel

Project Purpose:

There are multiple scenarios that require an unaffiliated wireless radio frequency (RF) communicator to enter an environment and establish communication with a group of affiliated RF devices with no a priori knowledge of their wireless communication protocol. This poses a difficult problem for the unaffiliated communication device because it has to learn how to establish a link based on observations of other communicators in the environment. This requires it to understand the various RF signal information, such as center frequency, modulation, and signaling rate. It also needs to understand protocol behavior, such as link establishment (handshaking and authentication), and digital packet data structures, such as specific identification of error correction codes, cyclic redundancy checks, and synchronization patterns. This project seeks to identify methods for autonomously detecting and characterizing this information between two or many affiliated communicators based purely on observed information. This project is topical in the area of dynamic spectrum access and cognitive radio research.

Machine-learning algorithms have been studied for many years and can be considered an established science. However, the use of machine learning algorithms in certain application areas requires a qualitative and quantitative analysis of the available data and an understanding of how the data is relevant, which is an art. This project is performing a study of various machine-learning techniques to characterize a digital wireless communication link based on observations of the RF environment. Using techniques such as Bayesian and neural networks, we are developing a probabilistic model of a protocol and its digital data format, which will enable the unaffiliated communication device to establish communication. Machine learning techniques have been rigorously employed in the analysis of financial markets for the creation of predictive inference models. The novelty of this project is to perform similar research for sensor optimization.

Summary of Accomplishments:

We discovered and implemented several techniques to model a RF digital communication protocol based on traffic message observations. We discovered new techniques for understanding and parameterizing the observables of an RF communication system, and associating those observables with specific outcomes. We discovered new techniques for determining the message exchange protocol, and through statistical analysis, we can determine causality between observed RF messages.

Significance:

This project developed novel techniques for the analysis of RF communication data that are broadly applicable to several national security mission areas. The techniques can be used to analyze data from telemetry, seismic, acoustic, and biometric sensors. The techniques can also be used to determine causality in temporal event data.

A Thermo-Optic Propagation Capability for Reducing Design-Cycle Time, Improving Performance Margins, and Lowering Realization Costs

165571
Year 2 of 2
Principal Investigator: K. Schrader

Project Purpose:

Due to the increasing complexity of space-borne optical systems, on-orbit performance requirements must be verified by analysis with validation against a subset of ground-based testing. These systems experience dynamic thermal loads by virtue of their orbital geometries, where varying sun illumination angles and earth eclipse subject them to extreme heat and cold. Since thermal loads degrade performance of an optical system by misaligning, distorting, and altering the optical properties of components, detailed thermo-optical analyses are required to complete the requirements verification.

Current methods of thermo-optic analysis are extremely laborious and predominantly compartmentalized according to discipline: structural, thermal and fluid mechanics, and optical propagation analysis. The method of integrating data for final optical analysis involves mapping into a form compatible with the chosen tools. This mapping is not a true multiphysics implementation and yields only an approximate solution at best. It is susceptible to error and cannot account for effects of field angle and compounded errors of upstream components. The S&T short fall in thermo-optical modeling is primarily due to multidisciplinary complexities. A true multiphysics solution requires integral collaboration at the optical modeling level.

This project intends to create a true multiphysics, thermo-optical propagation capability by creating a custom module within the Zemax optical analysis tool. This module will directly read output files of structural and thermal analyses and compute the nonlinear optical propagation through components under thermal load. This capability has never been demonstrated within a validated, commercially available, optical analysis product. If successful, the resulting tool will provide a new understanding of thermal effects on broad field of view optical imaging systems, and the compounded effects of thermal disturbances on complex, multielement systems.

Summary of Accomplishments:

We developed and demonstrated a new theoretical construct for optical ray tracing in a finite-element volume. The new construct resolves the coordinate transformations from physical Cartesian coordinates to normalized finite-element coordinates and provides the gradient ray-trace formula using the intrinsic finite-element methods for computing gradients and surface normals. The method was implemented in the MATLAB environment, and compared to closed-form gradient-index methods, with impressive results.

We also developed a software architecture to implement the method in the Zemax commercial ray-trace code, using the user-defined surface (UDS) application programming interface (API). The software architecture provides hooks to insert custom analyses and verification methods into the Zemax environment, allowing the user to rapidly assess optical performance, coordinate frame alignment, and correlation of various optical performance metrics to the finite element (FE) data.

Laboratory experiments were performed on two different precision optical window components of BK7 and fused silica material, to collect verification and validation (V&V) data for the developed models. Imaging thermography and thermocouple data were used to assess accuracy and tune the FE thermal models. Interferograms of surface deformations and measurements of optical thickness were collected for comparison to the ray-trace predictions of the newly developed software.

Significance:

The new method and software enables direct import of finite-element models into a ray-trace program, where rays can be traced and analyzed “on-the-fly” with no pre-processing requirements. This capability rapidly accelerates the system-level thermo-optic analysis cycle, allowing the process to be implemented earlier in the optical system design cycle with improved optimization prior to production.

It also enables higher-order analyses of coupled-physics optics problems, such as thermo-dynamics effects in high-energy laser cavities, self-focusing effects of high-power, short-pulse lasers, and optical laser ablation of materials.

Refereed Communications:

K.N. Schrader, S.R. Subia, J.W. Myre, and K.L. Summers, “Ray Tracing in a Finite Element Domain using Nodal Basis Functions,” *Applied Optics*, vol. 53, pp. F10-F20, August 2014.

Self-Powered Thin Electronic Systems

165572
Year 2 of 2
Principal Investigator: B. Jokiel, Jr.

Project Purpose:

The purpose of the project was to develop a new method for designing and building thin electronic systems that are wearable and self-powered. Technical challenges included compatibility of materials including substrates, adhesives, inks, and other electronic assembly materials while maintaining biocompatibility. Transferring and integrating the electronic trace designs with other graphics in a multilayer design also was initially challenging. The solution was to uniquely repurpose and merge a variety of electronic design, graphics design, printing, and electronics assembly techniques to develop a complete methodology to design, build, and assemble small electronic systems that are self-powered. All of the materials, printing processes, printers, electronic components, and substrates were commercial off the shelf. A multi-pass printing method was used to print each layer of the circuit and deposit the materials for the electrical traces and interconnects. Electronic components were added using common manual pick and place machines. Laser cutting was used to singulate the devices from the build substrate, leaving the circuitry, electronic components, adhesive film, and the top level design graphics intact.

Summary of Accomplishments:

Commercially available printing processes and equipment were investigated for print quality and compatibility with a wide variety of print media including plastic, paper, and other coated substrates. Interconnect strategies and materials were also examined for ease of use, durability, and compatibility with the printing process and materials. The project was successful in creating a complete strategy to build self-powered, wearable, multilayer electronic devices using off the shelf graphics software, printers, electronic components, and conventional pick and place techniques. Techniques developed were applied to three different applications. The technique was used to produce a set of wearable devices that were applied to and successfully tested on humans. Device lifetime was demonstrated up to 12 hours with an average of six hours. It was speculated that higher lifetimes are achievable with further process improvements and material substitutions and additions, but were not attempted. Single layer, multilayer conductor devices, and applications to larger-area devices were investigated and demonstrated. The processes developed comprise a system to rapid prototype a low number of thin, flexible electronic systems, and provides an integration backbone for future, new, or different component technologies.

Significance:

The results enable an agile capability that can build low numbers of customized electronic systems without long lead or expensive thin printed circuit boards (PCB) fabrication. It also allows design to update, adapt, and change designs and easily reprint them. Systems built with the process are wearable and may be suitable for use in applications where flexible electronic devices are preferred or required. The capability is relevant to a large array of national security mission space where inexpensive devices are needed quickly.

Large Motion High Cycle High Speed Optical Fibers for Space-Based Applications

165574
Year 2 of 2
Principal Investigator: P. G. Stromberg

Project Purpose:

Future remote sensing applications will require higher resolution and, therefore, higher data rates (up to perhaps 100 gigabits per second) while achieving lower mass and cost. A current limitation to the design space is high-speed high bandwidth data does not cross movable gimbals because of cabling issues. This requires the detectors to be off gimbal. The ability to get data across the gimbal would open up efficiencies in designs where the detectors and the electronics can be placed anywhere on the system. Fiber optic cables provide lightweight, high speed high bandwidth connections. Current options are limited to 20,000 cycles as opposed to the 1,000,000 cycles needed for future space based applications. To extend this to the million+ regime requires a thorough understanding of the failure mechanisms and the materials, proper selection of materials (e.g., glass and jacket material), allowable geometry changes to the cable, radiation hardness, etc.

We will use advanced characterization and modeling tools to answer the fundamental question: are there surface or interfacial cyclic fatigue mechanisms in optical fibers? Cyclic fatigue of fibers could jeopardize fiber reliability in remote sensing environments, either limiting design options (i.e., limiting to designs which enforce zero movement of the fibers) or reduced reliability/life in applications that require the fibers to move with a gimbaled payload. Emphasis is placed on fundamental understanding of the micromechanical origins of strength degradation in cyclic fatigue. One possibility is that fatigue strength is controlled by nm-sized surface pits formed by moisture reacting with the glass surface. Such pits could sharpen in cyclic fatigue due to effects of wedged debris or asperity contact. Another possibility is that the elastically mismatched core-clad interface delaminates during cyclic loading to cause fracture. Fundamental understanding of the degradation mechanisms and quantification of their effects will enable us to develop a model that can be used to specify safe design limits for optical fibers.

Summary of Accomplishments:

Over the course of the project, we built a baseline of material properties to evaluate and model the Nufern GR-140/100 rad fiber. Initially, we worked on the material properties with careful evaluation of modulus, and strength of the glass fiber, and the two coatings that are on the outside of the flight grade fiber. We also tested and measured the strength and transmission of the fibers before and after radiation exposure to determine suitability for the transmission of data in the space environment. Extreme care was necessary as the humidity has a significant impact on the strength of the glass fiber. Multiple-day soaks were required to stabilize results, at times greatly complicating the testing.

Testing required that we design new fixtures to enable the radiation exposure, light transmission before and after, and accommodate the automatic strength tester.

We also modeled and validated the stress and deflection in the fiber. Validation included use of image-edge detection to establish the curvature comparison from actual parts to the model.

We also surpassed current testing of the cyclical properties of the material and reached 90k cycles.

Significance:

Current interest in the distributed computing format supported by the fiber interface could support future generations of higher resolution and fast framing FPA's, potentially enabling national security missions. With successful implementation of the fiber across gimbal, FPA's and distributed computing electronics can be co-located with sensors helping to achieve lower SWaP and new design options.

Chemical Stability and Reliability of Petroleum-Based Products

165579
Year 2 of 2
Principal Investigator: R. D. Rasberry

Project Purpose:

Petroleum-based products are the economic cornerstone of modern society and remain essential to US economic security, stability, and growth. The purpose of this project is to examine the reliability of commonly used petroleum-based materials (e.g. fuels, road materials, electrical insulators, adhesives, etc.) and how environmental changes may affect performance and utility. This work explores the potential for synergistic effects between environmental variables and chemical additives. In this topical area, product enhancement has had unanticipated secondary effects, leading to costly alterations to industrial practices and infrastructure. For example, petroleum additives that have unintended deleterious effects are developed as efforts to improve processing and performance (methyl t-butyl ether or tetraethyl lead increased gasoline octane number but ultimately had negative environmental impacts). The work herein represents an evolutionary departure in additive research as it is aimed to anticipate deleterious additives. Ultimately, an exploration of unintended consequences to S&T will allow for the development of detection and mitigation technologies, which will ensure petroleum product supply continuity and, thus, continued domestic economic prosperity and security.

Summary of Accomplishments:

We investigated domestic petroleum-based supply chain threats for energy surety. Our goal was to determine petroleum vulnerabilities to possible chemical modification and our approach was to experimentally validate potential vulnerabilities. A few of the key R&D accomplishments include fuel soluble metal salts which induce hydroperoxides/gum formation, low molecular weight organogelators (LMOGs) which gel fuel at low concentrations and mild conditions, and bacteria/fungi growth at fuel/water interfaces which causes oxidation problems leading to sludge, loss of product quality, and deterioration of storage tanks and pipes.

Significance:

All of these experimentally validated approaches could potentially improve energy assurance of US petrochemical supply chains, benefitting DOE and DHS.

Enabling Technologies for the Development of Very Small, Low-Cost Interceptors

165580
Year 2 of 2
Principal Investigator: N. R. Harl

Project Purpose:

To counter emerging threats, a demand has surfaced for small, low-cost ballistic missile defense (BMD) interceptors that can be used in much larger numbers than current interceptors. The small size and relative affordability of such weapons would allow for more rounds to be used, providing improved defense against large missile raids. Unfortunately, the investigation of small, low-cost interceptor paradigms has received little attention, because the Missile Defense Agency is focusing on traditional kill vehicles lofted by large boosters.

One of the primary challenges for the development of small interceptors is that for the interceptor booster to be small and low-cost, the kill vehicle must be very small. A kill vehicle of less than 5 kg could utilize a much smaller booster than current BMD interceptors. This kill vehicle size limits the technologies that can be used, and leads to limited end game divert capabilities. Through a novel and proprietary combination of new and old technologies, potential exists for the creation of new miniaturized seekers and steering systems for very small, lightweight interceptors. However, these technologies have never been applied to BMD interceptor applications.

This project will investigate and model technologies necessary for the development of small, low-cost interceptors. Specifically, novel miniaturized seeker and steering system concepts will be analyzed. Since the development of these miniaturized technologies is a challenging problem with notable risk, several options will be analyzed and compared. The result of these efforts will be a conceptual interceptor design that is dramatically smaller than traditional BMD interceptors.

To analyze the efficacy of the miniaturized technologies, a high fidelity, model-based, simulation environment will be developed. The environment will be specifically designed and configured to support performance assessment of terminal, seeker-based, homing-guidance-systems and their end-use implementation. A challenge in developing this environment will be making it useful both with broader simulation environments, such as Sandia's VEGA, and higher fidelity hardware-in-the-loop (HWIL) environments.

Summary of Accomplishments:

Two novel miniaturized seeker designs were developed in the first year of this effort that combine the advantages of strapdown and gimbaled seekers. In particular, the designs offer a wide field of view to allow for star sightings to be performed, and high-resolution accuracy around a specific object in the field of view. These capabilities could potentially provide large benefits to current interceptor seeker paradigms.

To test the seekder designs as well as a thrust vane model that was created, a high-fidelity 6-DOF simulation environment in Simulink was developed. The environment was especially designed to support performance assessment of terminal, seeker-based, homing guidance systems and their end use implementations. This environment proved advantageous for testing the designs, and can be leveraged in future Sandia projects involving homing guidance applications.

Finally, a Hardware-in-the-Loop simulation environment was developed that allows testing of seeker-based homing systems with realistic target scenes and flight-like seeker hardware. The Hardware-in-the-Loop design combines the scene generation capabilities of Sandia's VEGA software, a commercial off-the-shelf (COTS) machine vision camera, and the image processing capabilities of Simulink's Image Processing Toolbox. Similar simulation environments within the aerospace industry require a significant amount of funding for development, so the fact that such an environment was created at Sandia at reasonable cost is a notable achievement.

Significance:

The technologies that were designed and tested during this project can be enabling factors in the development of small, low-cost interceptors. Small interceptors can be crucial assets in missile defense against raids, where large stockpiles of interceptors are necessary to counter a large number of incoming threats. The small size also allows the interceptors to be tasked/launched quickly against threats.

This work produced a detailed design of a gimbaled seeker that can perform star sighting while also tracking/resolving a target. This type of seeker can be advantageous for current interceptor designs.

The creation of the hardware-in-the-loop simulation environment with reasonable cost is a notable achievement, as many large aerospace companies spend millions of dollars to achieve similar simulation capabilities.

Turbocharging Quantum Tomography

165581
Year 2 of 2
Principal Investigator: R. J. Blume-Kohout

Project Purpose:

Quantum information processors (QIPs) promise a revolution in computing, communication, and sensing. To achieve these goals, every quantum hardware component (e.g., qubits that store quantum information, and logic gates that transform them) must perform to extraordinarily high precision. Methods for characterizing, diagnosing, and verifying the behaviors of quantum devices are known collectively as quantum tomography.

Standard tomographic methods are very resource intensive, thanks to the peculiar nature of quantum systems. Describing an N-qubit device requires exponentially many parameters, none of which can be measured directly. So, to characterize a device, an experimenter must measure many different observables, repeat many times to gather statistics, and finally transform the data into an estimate via some estimator. Accuracy, reliability, and efficiency all depend on the observables measured and the estimator used. Today, most tomographic experiments still use naive and inefficient protocols, due to a lack of efficient, sophisticated methods that have been rigorously tested and validated.

We will develop and benchmark new tomographic protocols that achieve higher accuracy and greater reliability, with more efficient use of scarce resources. Our results will pave the way for a comprehensive suite of tomographic "best practices" to characterize and validate quantum device technologies across many laboratories.

Quantum hardware is sufficiently advanced that many research groups desperately need methods for reliable, accurate tomography. Our tomographic capability will enable the design and evaluation of devices with higher accuracy, higher confidence, and fewer resources. This capability is critical for addressing measurement bottlenecks that stem from limited time and equipment. It will benefit a wide array of quantum information technologies developed at Sandia, while the underlying capability development will establish a leadership position in a critical area of quantum information science.

Summary of Accomplishments:

By far the most important accomplishment of this project was the invention, development, and implementation of gate set tomography (GST). GST is a method for tomographic characterization of quantum logic gates on as-built qubits. Unlike all previous methods, it is: 1) completely robust to calibration errors, 2) hyper-accurate, characterizing gates to within 1 part-per-million using as few as 5 million observations, and 3) capable of fully characterizing every parameter of the gates.

GST was conceived and a breakthrough led to the algorithm for linear GST (LGST). LGST provides unconditional robustness to calibration errors, using only closed-form mathematics (linear algebra) instead of iterative, failure-prone optimization algorithms. LGST was first implemented in Sandia's trapped-ion qubit, and worked perfectly. While highly robust, LGST's accuracy is comparable to previous methods.

GST was extended to analyze long sequences of quantum gates (e.g., many repetitions of the same gate). These long sequences amplify errors. Long-sequence data was analyzed for Sandia's trapped-ion qubit, and

University of Wisconsin's silicon quantum dot qubit. For the first time, GST was able to diagnose severe non-Markovian noise in the Wisconsin qubit.

Further algorithms development led to two algorithms for reconstructing the gates from the results of these hypersensitive sequences: extended LGST (eLGST) and least squares GST (LSGST). These algorithms were implemented to analyze data in experimental collaborations with University of California Santa Barbara's XMon qubit. The results showed that GST is capable of extreme accuracy, and demonstrated non-Markovian noise at a significant (but previously undetected) level.

We developed algorithms to select long sequences with guaranteed hypersensitivity, and a comprehensive self-consistency check was developed that provides extensive debugging information to the experimenter, about all forms of noise including non-Markovian errors.

Significance:

GST provides revolutionary and unprecedented capabilities for verifying, diagnosing, and debugging the operation of quantum logic devices (e.g., qubits). These are the foundation on which quantum information processing may be built and, therefore, GST's role is critical to development of quantum information processors (a priority for maintaining US information technology acuity and leadership). GST is rapidly becoming the gold standard for quantum device characterization. Its robustness, accuracy, and sensitivity to all forms of noise make it the very first characterization protocol that can achieve the performance required for the development of useful, stable quantum information processing hardware.

Refereed Communications:

R. Blume-Kohout, "Gate Set Tomography: Calibration-Free Full Characterization of Quantum Devices using Error-Amplifying Circuits," presented (invited) at *New Horizons in Statistical Decision Theory*, Oberwolfach, Germany, 2014.

L.A. Rozema, D.H. Mahler, R. Blume-Kohout, and A.M. Steinberg, "On the Optimal Choice of Spin-Squeezed States for Detecting and Characterizing a Quantum Process," to be published in *Physical Review X*.

R. Blume-Kohout, "Quantum Gate Set Tomography," presented (invited) at *APS March Meeting*, Denver, CO, 2014.

Nonlinear Response Materials for Radiation Detection

165701
Year 2 of 3
Principal Investigator: D. R. Wheeler

Project Purpose:

The specific detection of special nuclear material is vital in a variety of national security scenarios. Special nuclear materials have distinct radiation signatures. The special nuclear materials emit neutrons and gamma rays. Indication of the proximity of nuclear materials could be achieved with two independent sensors, provided that the sensors do not have cross sensitivity and have either very nonlinear response or a threshold-based response. Typical neutron and gamma sensors rely on data processing to address background radiation. We envision opportunities that, through materials design and implementation, can function as sensors that obviate the need for continuous background radiation measurements. We will create autonomous materials with intrinsic behaviors to give nonlinear responses to radiation.

We are striving to develop new materials that are especially sensitive to neutrons and/or gamma rays to serve in novel sensor architectures. We will develop novel microelectronic architectures using existing materials so that we can enable the utilization of new materials in an optimal fashion. The payoff for new autonomous materials that function to discriminate background from targets is immense. Despite the payoff, the risk of failing to develop materials and methods to utilize them has driven the sensor community to lower risk approaches and the reliance on data processing to address materials shortcomings.

Development of a Rapid Field Response Sensor for Characterizing Nuclear Detonation (NUDET) Debris

170798
Year 2 of 3
Principal Investigator: S. Mitra

Project Purpose:

Rapid in situ analytical techniques are desirable for the isotopic analyses of special nuclear material. Techniques that use destructive analysis are time-consuming and require sample dissolution. For nondestructive analysis, proof-of-principal studies are performed to demonstrate the utility of employing low energy neutrons from a portable pulsed neutron generator for rapid isotopic analysis of nuclear material. The key challenge is isolating the signature gamma rays from the prompt fission and beta-delayed gamma rays that are also produced during the neutron interrogation. To address the challenge, a commercial digital multichannel analyzer has been specially customized to enable time-resolved gamma-ray spectral data to be acquired in multiple user-defined time bins within each of the ON/OFF gate periods of the neutron generator. In particular, time-sequenced data acquisition, operating synchronously with the pulsing of a neutron generator, partitions the characteristic elemental prompt gamma rays according to the type of the reaction; inelastic neutron scattering reactions during the ON state and thermal neutron capture reactions during the OFF state of the generator. Preliminary results on new signatures from depleted uranium as well as modeling and benchmarking of the concept have been obtained.

Real-Time Case-Based Reasoning using Large High-Dimensional Data

170800
Year 2 of 3
Principal Investigator: J. Woodbridge

Project Purpose:

Case-based reasoning (CBR) systems are an effective tool for improving decision making in many domains. CBR systems aid in decision processes by comparing current cases to past well-known cases. Current CBR systems often focus on low-dimensional data or small archives of historical data. However, richer high-dimensional datasets are essential in understanding many measured phenomena. Large archives of historical cases are necessary to account for variations in how a phenomenon is revealed. For example, a seismogram can be used as conclusive evidence that the source of activity was a potential nuclear test and not an earthquake, but only after properly accounting for other important factors, such as the source to receiver path through the earth. It is necessary to analyze large archives of both types of events recorded for a variety of paths to conclusively make the distinction. Unfortunately, large high-dimensional archives are not currently feasible for CBR systems due to the complexities of search in high-dimensional spaces.

This project investigates a new paradigm in high-dimensional search. The proposed technique learns the structure of a dataset in high-dimensional space to construct an inverted index for the high-dimensional space. The index is applicable to any measure of similarity with any configuration across multiple domains. Several core theoretical advancements must be made in this area over a two-year timeframe. The results of this project may potentially be applied to a specific domain for the implementation of a specialized CBR system. Potential domains include any program that requires analysis of high dimensional data (such as time series, images and feature vectors). Example potential applications include nuclear explosion monitoring, cybersecurity (such as network behavior analysis), and satellite monitoring.

Integration of a Neutron Sensor with Commercial CMOS

170803
Year 2 of 3
Principal Investigator: W. C. Rice

Project Purpose:

Commercial microelectronics are subject to constant cosmic irradiation. These radiation fields routinely cause device interrupts known as single event upsets (SEUs) in the internal structure of the complementary metal-oxide semiconductor (CMOS). SEUs can range in severity from individual memory bit flips to more catastrophic single event function interrupts (SEFIs) which can lead to destruction of the electronic device. The effects of the SEUs can often be resolved or mitigated by error correction codes (ECCs), which restore the device operation by, for example, rewriting the memory to correct the false bit, or cycling the power to remove a lockup condition. However, unless a precaution is taken, a latency can occur in time between the SEU and its correction by ECCs. This can happen for example, when the device is operating in stand-by mode. Latencies lead to increased device damage. Therefore, it is extremely useful to be able to detect incoming radiation as soon as it occurs.

Existing microelectronics are being explored to determine the fundamental properties of device physics leading to SEUs in memories. Tests to study the response to SEUs under a variety of radiation types and energies have been designed. Based on initial results obtained from experiments performed in Sandia's Ion Beam Laboratory, research has progressed on the underlying physics determining CMOS behavior in these radiation environments. Several radiation mitigation strategies have emerged. The mitigation strategies will be assessed for their effectiveness in reducing the risks to systems operated by these electronics.

Liquid Metal Embrittled Structures for Fragmenting Warheads

170806
Year 2 of 3
Principal Investigator: J. J. Rudolphi

Project Purpose:

The purpose of this project is to investigate novel materials to assess their application in fragmenting structures. Specifically, the goal of the project is to quantify the behavior of these novel materials when exposed to rapid material failure during explosive fragmentation and assess the technology's viability to be incorporated into fragmenting devices. Typically, fragmenting devices are macroscopically weakened to create fragments of a specified shape and size. Furthermore, the ductility of the fragmenting material must be considered to determine the statistical spread of fragment sizes. This project considers a quasi-metallurgical technique that creates weakened regions of variable ductility through the incorporation of special agents into the fragmenting materials' microstructure. This specific method has not been used before to control fragment size and size distribution. By creating a practical method of material modification that allows a wider and more controllable range of particle sizes to be accessed, fragmenting devices could be engineered that create a wider and more variable range of effects.

Currently, there is a great interest in devices that have a more predictable and controllable fragment size and size distribution. This project could provide the warhead designer with another tool to control these important features.

Speech Detection with MEMS Zero Power Acoustic Sensor

173043
Year 1 of 2
Principal Investigator: B. Griffin

Project Purpose:

We propose a microelectromechanical system (MEMS) zero power acoustic sensor capable of responding to frequencies of speech. Eliminating standby power is critical to extending the lifetime and reducing the size of these devices. Ideally, such a device would remain in standby consuming zero power until an event triggers power-up of the entire device for data logging, processing, or transmission. In reality, processing the wake-up event often requires significant power consumption, particularly for complex event signatures, which limits device lifetime and size.

The challenges of creating a wake-up sensor are generating a large enough signal, consuming minimal power, having sensitivity in the audio band (20Hz–20kHz) while in a small form factor, and rejecting undesired acoustic signatures. MEMS represent an opportunity for small form factor sensors. We will address the challenge of speech detection using resonant, piezoelectric MEMS technology.

The envisioned sensor operates based on piezoelectric transduction of mechanical strain due to pressure waves. The pressure perturbation of an acoustic wave causes deflection of a membrane creating strain in the piezoelectric material. Under strain, the piezoelectric film generates an electrical signal. This eliminates the need for a constant voltage supply. Since the sensor structure can be engineered to respond to frequencies of speech, complex profiles can be programmed into the sensor and processed passively in the mechanical domain.

Enabling Nanoink Materials for Direct Write and Additive Manufacturing

173045
Year 1 of 2
Principal Investigator: A. Cook

Project Purpose:

Advancements in electronics printing and integration techniques are changing how engineers use additive manufacturing for the deployment of conductive circuitry. Materials development can further the operational design space afforded by additive manufacturing. Commercially available feedstocks for electronics printing notably lag behind the process improvements of the deposition tools. Tailored nanoparticle ink formulations that can accommodate numerous metals with select deposition arrangements will advance the printed electronics and additive manufacturing state of the art. To affect this, a fundamental understanding of multicomponent nanoparticle ink dispersions and the processing conditions is required to induce phase separation. The main challenge of this project is creating enabling materials compatible with direct write and additive manufacturing technologies. The definitive mechanisms associated with previously observed phase separations are unknown. Variations in elemental density, thermodynamic energies, laser absorption and reflectivity of nanoparticles layers, and atomistic variance will be explored to determine governing forces.

The development of single-solution, multimetal nanoinks with controlled deposition and processed states that can incorporate dielectric elements, and conductive oxide inks compatible with aerosol jet deposition processes represent a necessary research effort due to the lack of fundamental understanding in this research field. It is critical that a fundamental understanding of how to control the mixing of complex nanoparticles (i.e., conducting, semiconducting, and dielectric, or insulating components) that have an inherent tendency to phase separate be overcome in the liquid ink-phase; however, this must be reversed during the sintering process. A central understanding of precursor properties, surface wetting, templating, mixing energy, and cooling behavior is required and will be studied in detail. There are no efforts presently reported that are exploring this approach. This research on multicomponent ink systems, such as silver-copper, or gold-copper, have enabling potential but carry risks associated with unknown nanoparticle interactions and their governing forces. Once established, Sandia mission and customers could be enabled to generate tailored nanoink materials with specific properties.

Automated Blind Signal Characterization

173047
Year 1 of 2
Principal Investigator: J. R. Templin

Project Purpose:

Blind signal characterization (BSC) is the practice of detecting, classifying, and identifying radio frequency (RF) transmissions. This technique is valuable to various efforts at Sandia. For field-deployable systems, there is a need to make the process more efficient and real-time such that BSC can be accomplished with greatly reduced computing resources. Doing so requires a great optimization/improvement to the current state of the art in BSC, and could ultimately be implemented on workstation-class computers and as a post-processing step.

This research seeks to explore the feasibility of developing embedded, autonomous BSC solutions. This involves the process of doing computation complexity analysis of existing algorithms, optimization of algorithms for embedded and real-time execution, and the development and demonstration of a prototype embedded BSC system. For the algorithms whose computational complexity is beyond the capability of real-time, embedded systems, alternatives will be explored and created.

Microscale, Low Power RF Power Detector using IC-Based Calorimeters

173048
Year 1 of 2
Principal Investigator: K. Wojciechowski

Project Purpose:

We plan to develop a novel microscale radio frequency (RF) signal power detector (RFPD) with broad applicability to Sandia's missions. State-of-the-art (SOA) RF signal power detection methods require integrated circuits (ICs) that must operate at the RF frequency of interest (often 100's of Mega-Hertz to 10's of Giga-Hertz) with very low noise levels. As a result, these RF ICs use very high levels of supply/battery power (100's of milliwatts). Our solution relies on the ability to create devices on the microscale that are highly sensitive to applied RF power. Their main advantage is that the thermally based detection mechanism is independent of the input RF frequency. Hence, these devices do not require power hungry high frequency circuitry to perform RF signal/power detection and use very little battery/supply power (sub-microwatts). Such microstructures result in ultra-small, low supply, power detectors that can sense very small RF signals. In addition, arrays of these novel detectors monitoring different RF frequencies can be integrated in a small area. Their low power consumption and potential to have many RF channels enable new capabilities such as: long term continuous monitoring of a wide range of the RF signals (FM radio, cell phone, commercial, and military RF/radar bands) while using 10's-100's of microwatts of supply/battery power on a single IC. Current SOA single IC RFPDs require duty cycling (are off most of the time) to enable low power consumption and often can only continuously monitor a single frequency. The planned detector is expected to have an input bandwidth of up to 20GHz, be 10-100X smaller, have a sensitivity of -88 dBm, and achieve a 1000X reduction in power when compared to SOA. SOA detectors have sensitivities of -100 dBm and RF input bandwidths approaching 10 GHz. Currently, we have demonstrated devices that are up to ~700X lower power than SOA with -82 dBm sensitivity.

Carrier Lifetime Mapping for Infrared Detectors

173050
Year 1 of 2
Principal Investigator: G. Soehnel

Project Purpose:

Material defects are a common problem among infrared detectors. These defects create high rates of carrier recombination, which in turn, produces pixels in focal plane arrays (FPAs) with high dark currents and other undesirable characteristics. Defects can range from individual pixels to clusters hundreds of pixels or more in size. One method of characterizing a detector or semiconductor sample is to perform carrier lifetime mapping. Locations with a decreased lifetime indicate material defects. This capability exists in very few places, particularly for infrared materials. We will modify an existing detector spot scanning station to perform a photo-luminescent decay measurement. A pulsed laser will excite the sample, and the decay of photons in time created by radiative carrier recombination will be recorded. The ability to perform this measurement would give us an important tool that can characterize materials with a passive noncontact measurement.

Time resolving the physics of defect-dependent carrier recombination requires the use of impulse excitation and sufficient signal-to-noise to resolve differences in the Shockley-Read-Hall (SRH) lifetime. This happens at relatively low carrier densities, so collecting and sensing enough emitted photons leaving the sample will be challenging. We intend to improve on the current state of the art in two key areas: working distance and spatial resolution. The current spot scanning system has a custom lens that allows for a working distance of ~50mm. This will allow for the sample under test to be housed inside a Dewar with all the optics and moving/scanning parts outside. The lens is also capable of delivering spot illumination on the order of 5 microns in diameter compared to ~500 microns for current state-of-the-art systems. We may modify the optical design to maximize signal collection and employ a variety of data analysis techniques.

High Speed Remote Sensing of Optical Signatures

173051
Year 1 of 2
Principal Investigator: D. A. Bender

Project Purpose:

Remote sensing of optical signatures for intelligence, surveillance, and reconnaissance (ISR) is of great importance to national security. While remote sensing is not new, recent advances in high-speed imaging are creating opportunities for new capabilities and missions and are the basis for this project. Light contains information in its spatial, spectral, and temporal content, much of which is currently not being measured and interpreted. This project aims to expand the field of optically measuring and characterizing certain high frequency signals. Doing so will help us identify activities of a nefarious nature.

This project will seek to deepen our understanding of high frequency signals present in light through experimental characterizations as well as modeling. We will use high frame rate focal plane arrays (FPAs) that are Sandia assets and also commercially made FPAs to determine what we can measure, at what distance, and how best to analyze the measurement. FPA sensor technology has advanced to the point where high 2D resolution and fast frame rates are possible simultaneously. This will allow us to spatially resolve multiple sources of light while at the same time extracting the high frequency content present, thus pinpointing signals of a malevolent origin in a cluttered environment. We will also model the optical sources and develop computer algorithms to build a tool for evaluating new capabilities and missions beyond what we are able to experimentally characterize. All of these things will lead to new knowledge about what kind of information could be extracted from optical signals, and how the signals could be measured and analyzed. Valuable information will be gained that can help identify and execute new remote sensing missions.

Reversible Electrical Interconnect

173052
Year 1 of 2
Principal Investigator: S. S. Mani

Project Purpose:

This project addresses an opportunity for yield enhancement of large area focal plane arrays. Currently, the photo detectors undergo limited to no testing prior to being mated or hybridized to the read out integrated circuit (ROIC). Large area device fabrication is resource intensive; hence, yield enhancement is desirable. In the previous year, we explored and prioritized different temporary interconnect material options that would enable characterization of large area detectors prior to permanent bonding. The reversible interconnect candidates are conductive polymers, anisotropic conductive films, and additive manufacturing using silver filled epoxies. These materials were selected for their good electrical conduction, reversible bonding, and potential for streamlined microsystem processing. A conductive polymer, specifically polyaniline, is the least mature of the three candidates. Progress included large feature definition using a lift-off process. The next steps are to perform the hybridization step, test for electrical connectivity, and create a cleaning process to prove the reversible nature of the polymer. A more mature option is the anisotropic conductive film. These films are commercially procured from BTech Corp. In this case, we have demonstrated electrical connectivity on large features, and bonding reversibility using heat. Bonding process parameters are currently being optimized to improve the electrical performance. The most encouraging option is the additive manufacturing approach with silver nanoparticle filled epoxy. Here, we demonstrated both electrical conductivity on large features and removal of printed bumps through solvent cleaning. Bonding is still to be performed. In all cases, large features were used to get a preliminary response. We plan to reduce the feature size to demonstrate performance on the scale needed for photodetector characterization and optimize processing parameters for further prioritization and evaluation of the interconnect materials.

Large-Scale Tracking of Unresolved Targets

173053
Year 1 of 1
Principal Investigator: R. H. Byrne

Project Purpose:

The technical question that we are trying to answer is: "What is the best approach for tracking large numbers of unresolved low signal-to-noise (SNR) targets?" and "What system parameters have the greatest impact on system performance?" Recent advances in computing have enabled the application of multiprocessor GPU's (graphics processor units) for processing large blocks of data in parallel. We plan to create and demonstrate the most promising algorithms in GPU hardware. An integral part of the research is an optimization of parameters that drive system performance and design when the goal is to track and classify large numbers of targets in unresolved image data.

Current approaches have not addressed this problem for several reasons. First, the application of GPU technology to tracking applications is relatively new (e.g., the first general purpose GPU's became available ~2006). Second, most tracking applications operate on either point source data or higher resolution data, but not on resolutions in between these bounds. For this effort, we will focus on the intersection of these traditional approaches. This makes the project unique, and also opens up a wide range of potential strategies.

This effort will have four main goals. The first is to identify the phenomenology associated with a range of pixel resolutions (e.g., sub-pixel targets to several pixels per target), which will lead to improved detection and classification algorithms. The second is to create scalable tracking algorithms that can track hundreds to thousands of targets simultaneously (with reasonable computing power). The third is to evaluate the most appropriate high performance computing (HPC) architectures for tracking large numbers of targets simultaneously. The last is to develop an optimization methodology of key parameters that drive detection/tracking/classification system design for different applications. The parameter space that we plan to cover includes the following: target phenomenology, background phenomenology, tracking algorithm, probability of detection/false alarm rate, revisit time/frame rate, and GPU architecture.

Summary of Accomplishments:

We analyzed the performance of six tracking algorithms, two of which were developed by Sandia, for large scale tracking applications (e.g., tracking vehicles in an urban environment). The algorithms are: probabilistic multi-hypothesis tracker (PMHT), random sample consensus (RANSAC), Markov chain Monte Carlo data association (MCMCDA), tracklet inference from factor graphs, a proximity tracker, and a traditional Kalman filter based algorithm. Sandia made extensions to an existing RANSAC algorithm and designed the proximity tracker algorithm. While the PMHT theoretically scales well to large numbers of targets, implementation concerns (e.g., sensitivity to initial conditions and convergence issues) led us to dismiss this algorithm as a viable approach. The algorithms were tested on simulated traffic data, an Air Force Research Laboratory (AFRL) publicly available imagery dataset of a video flyover of Wright Patterson Air Force Base, and low-resolution night traffic video of Albuquerque, NM, taken from a nearby mountain. While each algorithm had strengths and weaknesses, a common challenge was broken tracks and the difficulty maintaining a single track over long periods.

In order to quantify the detection and classification challenges posed by vehicle traffic in an urban environment, the Digital Imaging and Remote Sensing Image Generation (DIRSIG) model was employed to generate simulated scenes with a Peterbilt 359 semi-truck and an Audi A3 car. The DIRSIG simulations were evaluated under varying sun position, imaging platform position, and target azimuth rotation configurations. These results provided insight into the design of detection and classification algorithms.

Significance:

The results of this effort are relevant to the DOE national security mission "strategic partnerships to address broad national security requirements." This project also aligns with the NNSA goal to "expand and apply our science and technology capabilities to deal with broader national security challenges." An improved capability to detect, classify, and track large numbers of targets could benefit other DHS mission goals.

Exploration of JAS Architecture for Multi-Mission Applications

173054
Year 1 of 1
Principal Investigator: C. W. Graham

Project Purpose:

The purpose of this project is to evaluate the applicability of the Joint Architecture Standard (JAS) hardware to future computationally intensive space and airborne applications in synthetic aperture radar (SAR), overhead persistent infrared (OPIR), advanced radio frequency (RF), tagging tracking and locating (TTL), and software defined radio (SDR). Another related goal is to investigate alternative single event upset (SEU) mitigation strategies in the event of the obsolescence of the Xilinx SEU immune reconfigurable field-programmable gate array (FPGA) Single Event Immune Reconfigurable FPGA (SIRF) that is central to the JAS reconfigurable sensor interface retropharyngeal (RP) node. We will investigate commercial FPGA replacements utilizing triple modular redundancy (TMR), the status of currently available automated TMR tools, and other SEU mitigation approaches such as dual modular redundancy and time triple modular redundancy. JAS was originally developed with a specific set of space payloads in mind, but detailed analysis of challenges such as processing high data rate sensors, bottlenecks resulting from network latency when dividing large problems across multiple nodes, and hardware scalability had not been performed prior to this project. We will evaluate the JAS architecture against both the current and next-generation data processing requirements of a diverse set of mission spaces.

Summary of Accomplishments:

Our investigations into multiple application spaces revealed key limitations in the current state of the JAS hardware in processor performance, memory capacity and bandwidth, interfaces, serial rapid IO (SRIO) network architecture, and form factor. We used the results of these investigations to develop a standards-based set of architecture enhancements that would serve to make JAS more viable for future missions. Examples of these enhancements include adding a SRIO networking switch to significantly improve the scalability of JAS systems and making JAS compatible with commercial standards such as Open VPX which would allow for rapid prototyping with commercially available hardware and better intellectual property (IP) reuse. We identified possible Xilinx Virtex-6 and Virtex-7 commercial FPGA replacements for the Virtex-5 SIRF and analyzed their digital logic resources, memory, digital signal processing (DSP) blocks, input/output capacity, and IP features versus those of the SIRF. We evaluated the performance of automated TMR tools from Xilinx, Brigham Young University, Los Alamos National Laboratory, and Synopsys using several designs currently implemented on JAS hardware. We also investigated and documented other SEU mitigation strategies currently in use in industry. The results of these studies provide potential paths forward in the event of the obsolescence of the Xilinx SIRF.

Significance:

The recommended architecture enhancements that resulted from this research could be used by future programs to make JAS hardware or subsequent node-based architectures more reusable, robust, and scalable to meet the needs of a broad set of future national security missions. Developing a standards-based reusable architecture will significantly reduce the required nonrecurring engineering needed to execute future programs. The research also identified potential ways to improve hardware performance by utilizing leading-edge technologies that have evolved since JAS was first designed.

Persistent Space Situational Awareness

173055
Year 1 of 2
Principal Investigator: D. D. Cox

Project Purpose:

Space situational awareness (SSA) is critical to US national security. The SSA community has specifically identified the geosynchronous orbit (GEO) regime as an area in need of further assessment and innovative solutions. We believe persistent SSA of GEO resident space objects (RSO) can be accomplished with the right combination of sensors and sensor placement addressing the gaps of the current Space Surveillance Network. This project leverages existing sensor and astrodynamic modeling and simulation tools and knowledge of advanced technologies developed during Sandia's rich history to assess space, and potentially ground-based solutions, for enhancing space situational awareness in the GEO regime by determining effective combinations of sensors and architectures for key SSA functional needs.

Co-Design of Sensors and Analysis Methods for Optical Remote Sensing of Spectral-Temporal Signals

173056
Year 1 of 3
Principal Investigator: M. W. Smith

Project Purpose:

We intend to create a new process for co-designing remote sensing instruments and the accompanying data analysis methods for application to spectral-temporal signals. Events, or signal sources, are in fact generally the items of primary interest. The collection and analysis of signals are means to the end goal of retrieving information about the signal sources. Our philosophy is that sensors and analysis methods should be designed together from the beginning to produce a system that efficiently delivers high value information. The co-design process should incorporate field measurements and phenomenology models to identify important features in the signals. This project will develop a new co-design process by targeting events that produce transient spectral-temporal optical signals, specifically lightning and small chemical explosions. Lightning is a ubiquitous background signal in optical remote sensing, and there is wide application for characterizing munitions from optical signatures.

Our co-design approach stands in contrast to the practice of designing sensors based on simple signal-to-noise ratio (SNR) and related metrics. The end result of the prevailing practice can be a system that collects enormous volumes of data in multiple channels with high inter-channel correlation, expending more resources than necessary while perhaps still failing to capture key information. Our team will apply a combination of phenomenology models, sensor models, observations, and data visualization and analysis to: 1) predict key spectral-temporal features of the optical signals produce by small explosions and lightning, 2) measure real signals, 3) analyze the signals in the spectral-temporal domain, 4) identify key features, and 5) create a conceptual design for a sensor that is optimized to characterize small explosions and lightning. Co-design of a sensor and analysis algorithms is a new paradigm that, we believe, should be prototyped using ubiquitous signals.

Onboard Jitter Mitigation using Image Feedback

173057
Year 1 of 1
Principal Investigator: G. I. Magee

Project Purpose:

The purpose of this project is to understand the feasibility of reducing jitter by processing image data onboard in order to improve jitter performance.

Minimizing jitter is important in many applications. In imaging systems, jitter is a limiting factor in resolving sensor data. Traditional techniques for mitigating jitter include using gyros or rate sensors to provide motion feedback to a control loop. These techniques are limited in their ability to reduce jitter by the resolution and error of the rate sensors as well as the accuracy of system models relating those measurements to pointing motion. Using image data collected by the system in real time allows further reduction in jitter.

Using image data to mitigate jitter is attractive because the corrections provided are based on end-to-end measurements rather than local measurements, such as those provided by rate sensors. This project studied the feasibility of reducing jitter by processing image data and feeding back corrections to the pointing control algorithms. This technique has not been previously utilized in space systems due to the long latency of flight-to-ground communications and severely limited onboard processing resources. Key parameters to understand include the control bandwidth needed to implement this form of jitter mitigation onboard and an estimate of the achievable performance improvement.

The image processing needed to provide a measure of jitter is nontrivial. In an already resource-constrained system, it is challenging to free up the resources needed. Consequently, advanced, leading-edge algorithm development is required to maximize resource utilization. To make these algorithms usable, they must be robust against potential failure modes including highly dynamic scene composition and featureless scene composition.

The potential benefit of increased jitter mitigation is tremendous. Onboard jitter mitigation utilizes full-system, end-to-end measurements and corrections, where other jitter mitigation techniques use measurements local to the sensor performing the measurement.

Summary of Accomplishments:

We analyzed the feasibility of improving jitter performance using onboard image data processing. Two algorithms were studied, a centroid method and a one-bit transform method. The centroid method calculates the centroid of fiducials and then calculates the motion of the centroid between frames. The one-bit transform method uses a multi-bandpass filter to reduce each pixel to a single bit and then calculates the motion of each bit between frames. We also analyzed the control simulator for an existing project to understand the modifications necessary to inject a simulated data stream, use the test algorithms to calculate the motion, and feed corrections into the control algorithms.

We learned about the limitations of using onboard jitter mitigation from a sensor configuration standpoint, and about the limitations imposed by the computational complexity of the problem. Onboard image processing is most effective when the data frame rate is high and the scene composition is varied. The class of techniques studied would be most effective in systems designed to aid the onboard processing. Example system changes could include adding a fast-framing sensor specifically for jitter mitigation or modifying the onboard data-processing pipeline to allow the highest frame-rate data to be used for jitter mitigation.

We clarified areas where further research could be beneficial. These include analyzing the potential of re-registering image frames onboard and quantifying the cost/benefit trade-offs for using image processing for jitter mitigation in place of traditional approaches.

Significance:

The information learned in this project improves our understanding of the requirements and benefits of onboard jitter mitigation and prepares us to apply the techniques studied to other projects. This knowledge allows us to make the design decisions necessary to successfully employ onboard image processing for jitter mitigation. Using these techniques enables our systems to improve their jitter performance and advances the frontiers of pointing control. We are also better positioned to explore additional research avenues and know where to focus future efforts.

Advanced Beamsplitter Fabrication Techniques for Enabling a Novel Compact Multispectral Diffraction-Limited Imaging System

173058
Year 1 of 2
Principal Investigator: T. D. Henson

Project Purpose:

A novel design for an extremely compact gimbaled telescope system that operates with diffraction-limited performance over visible and infrared wavelengths has been developed. This space-based design provides increased performance relative to previous designs while simultaneously reducing the overall size, weight, and power requirements. The design requires a beamsplitter that passes visible wavelengths and reflects infrared wavelengths, the opposite of what dichroic coatings traditionally do. Current technology for reflecting infrared utilizes beamsplitter coatings that consist of both metallic and dielectric layers. The metal layers in these coatings reduce the transmittance, negatively impacting the radiometric sensitivity of the system. An all-dielectric design will improve the transmittance but will require a very large number of layers to produce high reflectivity in the infrared, thereby making fabrication difficult.

Additional requirements are that the beamsplitter must be very thin (a diameter-to-thickness ratio of 20) and must have a precise wedge angle to control aberrations in the system. These increase susceptibility to deformation due to coating, mounting, and thermal stresses and damage due to the launch acoustic and vibration environment.

This project seeks to prove the capability of designing and fabricating a thin, all-dielectric beamsplitter that transmits visible light while reflecting infrared light. Novel coating techniques will be utilized to minimize stresses and improve adhesion. Advanced modeling techniques will be utilized to design and characterize a beamsplitter mount that protects the beamsplitter over expected environments while minimizing mount and thermal induced stresses. Optical models of surface deformations due to coating, mount, and thermal stresses will be created to determine the potential impact to system performance.

Deployable, Ground-Based, Discrete Zoom Telescope

173059
Year 1 of 3
Principal Investigator: E. G. Winrow

Project Purpose:

Many optical system missions require both a wide field and high resolution views for both scanning and characterization activities. The high cost of large-aperture optics and high- performance detectors often requires a system to be either one or the other. We plan to create a hybrid zoom system capable of both mission areas, utilizing a single large aperture optic and a single detector, with reconfigurable smaller optics in the train. A ground-based system is planned to prove out concept, manufacturability, and cost. Technologies and methods devised will be instrumental in enabling future air and space optical systems.

Major technical challenges will be to devise an achievable optical design with few moving components and a stable, lightweight, robust structure that holds the optics in multiple precise locations without excessive complexity or cost.

The desire to create an affordable, lightweight, zoom telescope has been approached by several methods from deformable mirrors to complicated optical correctors. Most of these concepts are never realized in actual hardware and remain either exercises in optical design or structural design only. Our team of engineers will bring a more practical approach to the problem through truly integrated optical and structural design.

The envisioned system will achieve zoom capability over a wide field of view in the visible-to-infrared wavelength band through a combination of high-precision movements of the components and novel optical design forms. The optical design will be tailored to reduce the number and magnitude of moving parts. Phase diversity techniques will enable precise imaging with affordable optical fabrication and alignment/motion tolerances. Advancements in optical alignment techniques, tooling, and adhesive bonding will enable precise optical alignments without the need for ultra-precise and expensive hardware. Relying on each of these advancements holds risk, and bringing all together into an elegant, unified system is both high-risk and high-reward.

Broadband Digital AESA Radar Prototype for Multi-Mission ISR Applications

173060
Year 1 of 3
Principal Investigator: H. Loui

Project Purpose:

The purpose of the project is to develop a broadband active-electronic-scanned-array (AESA) radar prototype for broad mission intelligence, surveillance, and reconnaissance (ISR) applications to counter anti-access/area-denial (A2/AD) strategies that may actively jam, spoof, or interfere with our frontline electromagnetic sensors. Currently, the lack of practical, compact, low-loss, broadband, high-resolution, analog phase shifters (APSs) and true-time-delay (TTD) devices at radio frequencies (RF) limits bandwidth, reduces efficiency, and constrains electronic beam steering of existing electromagnetic sensors. These difficulties ultimately result in complex mission-specific radars that require significant time and exorbitant costs to develop, build, maintain, and upgrade.

Our approach to broadband AESA-based radar avoids the aforementioned difficulties by not utilizing any analog RF APS and TTD devices for beam steering. An initial proof-of-principle experiment at Sandia has demonstrated multi-GHz of instantaneous electronically steerable bandwidth. Though impressive, this feat was produced using expensive, heavy, and bulky general-purpose bench-top equipment. Hence, a miniaturized prototype must be created to demonstrate feasibility in practical applications, a task carrying tremendous risk. If successful, mission-agile radars using broadband AESAs will enable rapid mode reconfiguration and in-the-field enhancements. Multichannel, multiple phase-center, and multibeam capabilities would allow adaptive nulling of jammers, multiple-target tracking while scanning, rapid target identification, and broadband secure communications.

Motion Estimation and Compensation for Focusing Maritime Targets

173061
Year 1 of 2
Principal Investigator: D. W. Harmony

Project Purpose:

An unmet need in maritime surveillance is the ability to create high-resolution synthetic aperture radar (SAR) images of moving surface vessels for ship and boat identification. Although Sandia's SAR systems are exceptional in producing well-focused images of stationary objects, they cannot presently compensate for unknown object motion to create high-resolution ship images. The planned solution will develop algorithms that combine the unique capabilities of Sandia radars with a dual axis monopulse antenna to automatically resolve and compensate ship motion yielding high resolution focused images in real time. Current ship focusing methods work under too many restrictive assumptions to reliably provide useful information over a broad set of conditions involving vessel size, speed, and sea state. This research will lead to a substantial advance in radar imaging of moving targets.

Developing a System for Testing Computational Social Models using Amazon Mechanical Turk

173062
Year 1 of 2
Principal Investigator: K. Lakkaraju

Project Purpose:

The US faces persistent, distributed threats from malevolent individuals, groups, and organizations around the world. Computational social models (CSMs) help anticipate the dynamics and behaviors of these actors by modeling the behavior and interactions of individuals, groups, and organizations. The Behavioral Influence Assessment tool being developed at Sandia is one example of a CSM. For strategic planners to trust the results of CSMs, they must have confidence in the validity of the models. Establishing validity before model use will enhance confidence and reduce the risk of error.

The major problem with validation is designing an appropriate controlled test of the model, similar to the testing of physical models. Lab experiments can do this, but are limited to small numbers of subjects, with low subject diversity and are often in a contrived environment. Natural studies attempt to test models by gathering large-scale observational data (e.g., social media); however, this loses the controlled aspect.

Our new approach will run large-scale, controlled online experiments on diverse populations. Using Amazon Mechanical Turk, a crowd-sourcing tool, we will draw large populations into controlled experiments in a manner that was not possible just a few years ago. If successful, the methods developed here will revolutionize our ability to test social theories by allowing large-scale, temporally extended, controlled experiments of diverse populations.

This project will be cutting edge in developing an entirely new means of systematically and rigorously testing and validating CSMs. By testing these theories, we can develop better CSMs, potentially enabling us to anticipate events such as terrorist attacks, cyber incidents, and social disruptions.

There is high risk as we are utilizing an online platform to do large-scale experiments and we do not know, yet, how to design, execute and interpret the results of these new types of experiments.

Holistic Portfolio Optimization using Directed Mutations

173063
Year 1 of 2
Principal Investigator: M. A. Smith

Project Purpose:

The purpose of this project is to develop much better algorithms for helping military decision makers design optimal portfolios of systems over time where both the system technologies and the counts of systems are decision variables. Important examples of such portfolios are: 1) fleets of vehicles, aircraft, or ships, 2) grids of electric power source technologies, and 3) networks of information processing and communications devices. The problem is particularly hard due to the nonconvexity of the decision space, which is defined by binary technology choices and integer system counts.

Current approaches to this problem involve separate optimization steps, first optimizing individual system technology choices over multiple objectives and then optimizing the integer number of these systems in the portfolio over time. This two-step approach simplifies the problem at the risk of ignoring important decision variable interactions. Solving the problem in one step has proven computationally intractable because of the large scale combined with having a nonlinear multi-objective trade space.

Our holistic solution to the problem is to search the design space more rapidly by using large, yet coordinated steps. In particular, coordinated steps in system counts will be generated using gradient information from the performance measures. These steps will be included as mutations in an iterative genetic algorithm (GA) to evolve a Pareto optimal trade space of portfolios to help inform military decision makers.

Directed mutations based on gradients have been used in GAs for single-objective continuous optimization, but their use in multi-objective integer optimization is new. To make this approach work, we have to devise, run, and analyze new algorithms for using gradient information to suggest intelligent portfolio design changes. This makes the project a high risk for production work, although it has the potential for high value to many military customers. Success in this effort would open up new approaches to the field of operations research more generally.

Imaging LIDAR and Raman Imaging LIDAR through Fog and Dust for Maritime Surveillance

173064
Year 1 of 3
Principal Investigator: S. A. Kemme

Project Purpose:

This project supports Airborne Intelligence, Surveillance, and Reconnaissance for tactical situational awareness in challenging environments with modified imaging LIDAR (light detection and ranging). LIDAR produces an irradiance-based scene with high, 3D, spatial resolution — differentiating reflecting surfaces and surface textures not just for target detection, but also target recognition.

LIDAR is generally prevented from working through all weather, as the traditional source wavelengths are scattered and/or absorbed by fog, clouds, and dust. However, we at Sandia and other researchers have identified and quantified improved optical propagating wavelength regimes, taking advantage of the Christiansen effect, and polarization strategies that should open this otherwise opaque operating window for LIDAR.

We will explore the feasibility of a water Raman imaging LIDAR for maritime surface surveillance and detection of objects very close to the water surface, such as mines and divers, which present serious challenges to current surveillance technology. We envision an imaging LIDAR that uses Raman scattered light from water (the hydroxyl stretch at 3400 cm^{-1}) where absence or significant reduction of signal would be indicative of the presence of an object near the surface — that is, a negative image is formed by the object.

As far as we know, forming a negative LIDAR image using Raman scattering from the water layer near the surface is a new concept with significant potential for detection of objects at or near the water surface. The spatial resolution for such a LIDAR would be smaller than the size of the search object to provide sufficient signal contrast between the object and the sea.

We will demonstrate modified imaging LIDAR's utility and ability to produce images in environments that have been challenging for traditional LIDAR (fog, dust) systems as well as environments that are challenging for RADAR/SAR (target identification, water interfaces, foliage penetration) systems.

Modeling and Experimental Validation of Jet Vane Forces for a New Type of Missile Defense Kill Vehicle Steering System

173065
Year 1 of 2
Principal Investigator: L. A. Jones

Project Purpose:

Current exo-atmospheric and high endo-atmospheric missile defense interceptors are too large and expensive to be deployed in the numbers required to address the increasing numbers of threat missiles. To create smaller and less expensive interceptors that could be deployed in larger numbers, the size and mass of the interceptors' kill vehicle must be reduced, thus allowing the use of smaller boosters to achieve the same fly-out speeds. The miniaturization of current US kill vehicles is largely limited by the complex cruciform steering system used to achieve hit-to-kill. A cruciform steering system uses four throttle-able thrusters that occupy about one-half of the mass and volume of current kill vehicles. A novel steering system that is much smaller and simpler is planned. It consists of a single, continuously thrusting solid rocket motor for end game steering that uses miniaturized jet vanes in the exhaust of the rocket motor to point the rocket thrust.

We will model and experimentally test the lateral forces that can be generated by a new miniaturized jet vane system operating in the flow of a small solid rocket motor. Vane heating and erosion will also be investigated. By the end of this project, we will have the validated data needed to design a complete jet vane system for steering a new type of smaller, simpler missile defense kill vehicle. This new approach to kill vehicle steering will enable the development of much smaller missile defense interceptors that can be deployed in numbers appropriate for the increasing threat.

Adaptive Waveform and Signal Processing Techniques that Mitigate Adversarial Anti-Access/Area Denial (A2/AD) Technology

173066
Year 1 of 3
Principal Investigator: R. C. Ormesher

Project Purpose:

The global proliferation of electronic warfare (EW) technologies and electronic attack (EA) devices has strengthened adversarial anti-access/area denial (A2/AD) capabilities. These threats pose a significant risk to our national security missions that rely on intelligence, surveillance, and reconnaissance (ISR) systems. The objective of this project is to develop techniques that can mitigate select adversarial A2/AD technologies and maintain mission performance. Mitigation will primarily focus on developing waveforms and signal processing techniques for electronic counter-countermeasures (ECCM). Challenges associated with mitigating A2/AD conditions include understanding the effects of advanced jamming techniques, synthetic signal generation and high jammer-to-signal ratios.

This project will develop and analyze new waveforms and techniques that preserve ISR system performance in A2/AD environments.

Dynamic Analytical Capability to better Understand and Anticipate Extremist Shifts within Populations under Authoritarian Regimes

173067
Year 1 of 3
Principal Investigator: M. L. Bernard

Project Purpose:

The US' inability to adequately assess geopolitical and sociocultural dynamics of extremist groups has led to failures in understanding, anticipating, and effectively responding to shifts in their movements and allegiances. Recent attacks within the US highlight the need to more precisely understand and anticipate changes in societal attitudes and behaviors due to radicalization. This is particularly important, as new terrorist cells have begun in Southeast Asia and Somalia. A significant concern is their stated intent and effort to plan and conduct terrorist attacks against the US.

We intend to create a generalizable data- and theory-supported capability to better understand and anticipate (with quantifiable uncertainty): 1) how the dynamics of allegiance formations between various groups and society are impacted by active conflict and by third-party interventions and 2) how/why extremist allegiances co-evolve over time due to changing geopolitical, sociocultural, and military conditions.

We seek to develop a standalone computational assessment tool for evaluating dynamic military, geopolitical, and socioeconomic interaction effects of extremist groups. Using engineering and social science validation techniques, this effort will produce a capability to quantifiably assess current events and choice options ("what-if" queries) concerning geopolitical inter-group/regional dynamics within a distribution of likely rest-of-the-world reactions to investigate underlying attitudinal and behavioral (extremist) shifts across time. The resulting structure will be designed to be broadly applicable across different ethnic, political, and social groups and will focus on specific extremist group behaviors in response to military, social, economic, and political intercessions.

Imaging Mass Spectrometry for Biometric and Forensic Detection

173069
Year 1 of 3
Principal Investigator: J. M. Hochrein

Project Purpose:

There is significant need to unambiguously determine a person's identity and prior locations they have been. Traditional biometric approaches including fingerprinting, hair analysis, DNA, and retina/ iris scanning, typically target one characteristic and often require previous knowledge of the individual. We will use imaging mass spectrometry to identify new biometric signatures addressing several characteristics simultaneously and generating a fingerprint map. High-resolution mass spectrometry combined with imaging is a highly versatile tool applicable to many analytes such as small molecules, semi-volatile, and nonvolatile species including biomolecules. This technique has been demonstrated on explosive residues, drugs of abuse, inks, and many other organics. In most cases, complex matrices have not been investigated and specific markers remain to be characterized that would be of interest to identify not only a specific person or group of people but also provide information on their activities or working environment.

The key innovation of this project will be the identification and characterization of new biological and environmental signatures that result from fingerprints. The ultimate goal will be the identification of an individual based on chemical and biological signatures from their fingerprint and the generation of a high-resolution image based on the intensity and distribution of those markers. Environmental signatures in combination with specific biological markers may indicate habits, places of work, places of travel, and presence of other personal indicators making identification possible. For instance, isotope ratios are often indicative of specific regions and can be used for identification of areas of travel or habitation. In addition, we will investigate various surface materials that can be used to enhance detection limits and gain temporal information about each of the chemical and biological markers. This will greatly increase the amount of available forensic information associated to a particular individual, potentially impacting efforts of national security and DHS.

Quantifying the Uncertainty of Risk Assessment for High Consequence Flight Tests

173070
Year 1 of 3
Principal Investigator: T. M. Jordan-Culler

Project Purpose:

High consequence flight tests require review and approval of the risks associated with any flight program involving Sandia personnel or assets. The Range Commanders Council 321-10 Standard has provided guidelines to quantify uncertainty in probabilistic risk assessments. The large number of models and approximations for debris, trajectories, motor and component malfunctions, and population/asset demographics used in flight risk assessment has considerable uncertainty. DoD continues to fly increasingly more complex flight tests, which will be better designed when informed about uncertainties.

This project will investigate novel techniques of incorporating uncertainty into the current Sandia range safety probabilistic assessment tool, PREDICT, without significantly increasing computer run time. Analysts who run probabilistic risk assessments for national ranges do not have the expertise to be able to develop uncertainty quantification; as a multiprogram national security laboratory, Sandia has such expertise.

Risk assessment software must include the ability to reevaluate the risk based on the latest day of launch information related to wind, atmosphere, and demographics in a near real-time mode such that high consequence launch decisions can be made quickly. This project will incorporate uncertainty determination into the risk assessment methodology, such that the near real-time requirement is still achieved. Novel techniques will be employed — such as local and global reliability methods to estimate aleatory uncertainty, and interval optimization to estimate epistemic uncertainty. A major focus will be to generate interval bounds on risk values per unit area (worst case scenarios) as well as second-order probability ("probabilities of probabilities") for distributions of outcomes from PREDICT.

Unknown is whether interval representations or probabilistic representations will be the best method to incorporate uncertainty quantification into flight risk assessments. Simply bounding inputs doesn't necessarily reduce risk area. Identification of models or approximations, which contribute the greatest uncertainty to risk assessment, will allow analysts to focus on improving approximations.

Assessing the Security Impact of Moving Target Defense (MTD) Approaches

173071
Year 1 of 3
Principal Investigator: B. P. Van Leeuwen

Project Purpose:

While moving target defense (dynamic defense) approaches promise to increase complexity and cost for attackers by continually changing the operating cyber environments, their security impact to the overall network is largely unexamined. Dynamic reconfiguration of computing elements and their connectivity must take into consideration the stability and security impact to the overall networked system. While an attacker may encounter unpredictability in a moving target defense (MTD) environment, system and network administrators must also assure the stability and overall security of such a continuing and changing environment. Current MTD techniques assume that the effect of change is contained, localized, and does not have any adverse impact to system-wide operation and security.

Recently MTD approaches extend to IPv6 networks and use software-defined-networking (SDN) to dynamically change the underlying network along with end-point configurations. A major challenge is how to determine the effectiveness and security impact of MTDs. Currently, there are no such tools and techniques to assess MTD at scale. We plan to develop a large-scale IPv4/IPv6, SDN-based analysis platform for the assessment of MTD. We will also seek to develop a more realistic and quantifiable set of evaluation metrics for the assessment.

This research is advancing a cyber analysis platform modeling technology and providing a novel capability for the development and assessment of MTD for cyber network defense.

The operational and security impact of MTD to real-world enterprise network environments are largely untested. This research seeks to answer these important questions by developing a large-scale analysis platform with capable data analytics and a set of quantifiable metrics for security assessment. Critical features of the analysis platform will be the capability to deploy IPv4/IPv6 networking components and to deploy SDN technologies at large scale. Our research will advance Sandia to the forefront of cyber-analysis-platform technology with capabilities for large-scale assessments of MTD.

Application of Advanced Network Topologies to Reliable Space-Based Computing Clusters

173072
Year 1 of 1
Principal Investigator: A. J. Hill

Project Purpose:

The purpose of this project was to explore fault tolerance analysis techniques applied to next-generation satellite payload designs for space-based processing systems. This project developed a modeling toolbox for system design engineers to utilize for payload design and expand for future mission requirements. Next-generation space-based system design will take advantage of node-based architectures and require a network analysis toolbox to support sophisticated design requirements. There are many design questions when implementing node-based architectures. What is the best network topology to use for the specific mission? What is the best node configuration within a topology that optimizes a given set of performance criteria? How does the network handle a node failure and what does the transient network response look like between time of failure and resolution? This project identified and developed a foundational modeling and simulation environment package complete with Serial RapidIO and SpaceWire network models and documentation to lay the foundation for future system designers to begin to answer these tough questions. With this modeling and simulation environment, we can begin to explore concepts such as optimal topology and node configuration selection, automated corrective actions to failures during mission operations, and hardware validation of the models. This toolbox is scalable and flexible to future growth allowing for new model designs to be developed, more stringent real world model requirements to be implemented and verified, and demonstrated conformance to the standards represented within these network models.

Summary of Accomplishments:

We demonstrated a modeling and simulation environment to support future space-based processing systems built on the design principles of network connected node-based architectures. This environment lays a foundation of future growth potential for system architects and engineers to optimize future designs for satellite payload processing systems. This tool can be utilized for optimal network topology selection and node configuration against fault tolerance metrics and other performance requirements to meet mission specifications, study real-time, in-mission fault and recovery dynamics, and reduce development cost by validating designs before hardware is built.

Significance:

The modeling and simulation environment identified and developed in this project allows system designers to make confident design choices that will lower cost, provide fault tolerance to component failure, and reduce development time for future space-based processing systems. The results of this project may provide a foundation for optimal design choices for future satellite payload designs.

Optical Detection of Ultratrace Molecules

173073
Year 1 of 2
Principal Investigator: C. F. LaCasse, IV

Project Purpose:

The intent of this project is to create a new optical remote sensing technique for measuring ultra-trace concentrations of gas phase particles of interest. Various techniques for remote sensing of gas phase species already exist. However, with existing techniques the length of the optical absorption path is generally limited to a single pass from an illumination source out to a scattering agent (either a solid surface or atmospheric aerosols) and then to a receiver. The finite length of the absorption path is one parameter that constrains the minimum detectable quantity of a given absorbing species. The goal of this project is to create a new active remote sensing technique that will use a multipass effect to dramatically increase the effective length of the absorption path and reduce the minimum detectable quantity of various gas phase particles of interest.

This work is inspired by a technique known as intra-cavity laser absorption spectroscopy (ICLAS), which is a method for measuring extremely faint optical absorptions by placing a sample of gas inside of a laser resonator cavity. While extremely sensitive, ICLAS as currently practiced is strictly an in situ measurement technique. The planned creative approach consists of employing the basic mechanisms of spectrally selective extinction, light amplification, and optical feedback, but replacing the traditional laser resonator cavity with a different gain and feedback loop to allow open path measurements. The technique is innovative since, while the ICLAS was originally developed in the 1970s, after 40 years no analogous remote sensing technique has been attempted. We call the new approach extended cavity laser absorption spectroscopy (ECLAS). This approach is new and unproven, but it has the potential to establish a new remote sensing modality with unprecedented sensitivity to ultra-trace concentrations of gas phase particles of interest.

Technology Improvements for the Design and Analysis for Hypersonic Scramjets for Prompt Strike Applications

173074
Year 1 of 2
Principal Investigator: J. Fulton

Project Purpose:

In the arena of prompt global strike, there is currently a lack of understanding of the comparative benefits and losses between an unpowered boost-glide system and one propelled by hypersonic engines such as ramjets or scramjets. Before comparison studies can be performed, a capability must be developed to quickly simulate the operation and analyze the performance of hypersonic propulsion systems in a multitude of configurations and scenarios. The need to resort to simulations to predict the performance of a hypersonic propulsion system is due to the fact that, unlike conventional low-speed jet engines, hypersonic engines must be highly integrated with the vehicle's airframe and the airflow therein exhibits highly coupled, complex behavior that is nearly impossible to isolate or simplify enough to perform less intensive analyses.

It is very difficult to bring together accuracy and speed during computer simulation of hypersonic engines due to the complexity of the flow within, and so one of the goals of this project is to develop a robust, multi-fidelity hypersonic engine simulation tool that can operate at a number of locations along the speed vs. fidelity spectrum. This is being accomplished by bringing together two well-established codes: the low-fidelity SRGULL code created at NASA Langley, and high-fidelity REACTMB solver developed at North Carolina State University. In addition, a multi-fidelity capability will be developed. Once this integration has been done, analyses will be performed to compare the performance of propelled weapons with boost-glide. This could potentially provide ways to significantly increase the capabilities of prompt strike weapons.

Plasmonic-Based Optical Modulators and Switches

173490
Year 1 of 3
Principal Investigator: W. F. Seng

Project Purpose:

Traditional interconnect wiring at the chip level is too slow and not able to carry the massive amounts of information required by "Big Data." Optical fibers and photonic circuits can handle the data, but their components are currently too large to be integrated at the chip level to merge with electronics. Surface plasmon-based circuitry is the key way to integrate electronics with photonics at the nanoscale for chip level application, achieving a circuit that can carry both electrical current and optical signals.

Current photonic sensors, switches, and mixers are constrained both in frequency response and overall size, weight, and power requirements. A new approach is needed to address the need demanded by exploding bandwidth usage. Exploring nanoscale device structures, offering the possibility to achieve sub-wavelength mode volumes, will result in previously unattainable light-matter interactions. Therefore, such efforts offer truly unique opportunities for switching/modulation and wave-mixing applications, and devices operating based on this approach are anticipated to greatly surpass the performance of the current state of the art in speed, size, loss, and efficiency. These devices could ultimately have direct application in optical networking and in creation of chemical and biological sensors that will fuel future growth in health and energy industries. The work is in collaboration with UCLA.

Simulation of Optical Phenomena in the Upper Atmosphere

173491
Year 1 of 3
Principal Investigator: W. C. Sailor

Project Purpose:

The purpose of this project is to develop a detailed simulation code for the production of auroral light. This type of code would be valuable for comparison against our standard codes. This type of code would also be valuable to the external scientific community's understanding of the factors that influence measured auroral spectra. The aurora is mainly caused by high-energy electrons originating from the sun and entering Earth's atmosphere in regions centered around the geomagnetic poles. The electrons collide with atmospheric particles, which are excited to higher energy levels. These excited particles emit rapidly varying light in a curatin-like volume as they return to lower energy levels, thereby creating the aurora. The major visual aspects of auroral displays are dependent on the spatial and energy distribution of the incident electrons. We found no software that solves the electron transport problem other than Monte Carlo simulations. The best that we have found is an approximation of the electron transport problem that is solved by a code that was intended for a related problem. We plan to develop a deterministic simulation of electron transport in the upper atmosphere to advance the state of the art in this area. After the software is written, it will be tested against auroral measurements to assess how well it performs. Once the testing phase is complete, we will use the software code for predictive simulation purposes.

Ephemeral Connectivity and Locality for Large-Scale Emulytics

174373
Year 1 of 1
Principal Investigator: V. Urias

Project Purpose:

Sandia has shown the ability to build remarkably large and complex emulation environments that are representative of real world networks with reasonable fidelity. However, modern networks are increasingly dynamic, end points no longer stay stationary on the network, and are often continuously moving from one segment to another. Ephemeral connectivity is also not limited to computing resources; peripherals such as USB (universal serial bus) devices, CDs, and printers often move from endpoint to endpoint. Network defenders have few resources to test the effectiveness of tools in a dynamic environment and what few tools do exist cannot emulate many of the operational scenarios that introduce the most risk. Risks such as compute resources may move from a well-controlled company network to public WiFi and back again.

No tools exist to emulate an infected USB device or malware laden CD-ROM being passed from one employee to another, or a company laptop connecting to a public network in a controlled, instrumented, or repeatable fashion. The purpose of this project is to create a system whereby virtual machines can come and go on a network and emulated peripherals can be attached at will to endpoints. The ability to create and manage such a system would provide excellent resource for understanding layered security and testing existing defense tools by emulating the highly dynamic networks currently in operation. A system where events can be scripted and repeated would also allow for a training environment where a control team can craft events by hand and then expose wholly new teams to the events in exactly the same manner, decreasing testing and training costs.

Summary of Accomplishments:

We successfully developed a system to dramatically increase the realism and volatility of test scenarios, and researched and developed the following features:

- Simulated network disconnects
- Moved endpoints between segments
- Altered core routing infrastructures physical topology
- Dynamically instantiated and destroyed entire network segments
- Dynamically extended network
- Attached and detached removable storage devices
- Dynamically mapped USB devices to endpoints
- Recorded physical topology activity and replay actions

Significance:

Sandia and the nation's government, military, economic, and critical infrastructure rely on our information technology infrastructures. Consequently, an improved ability to test advanced defensive tools in a more realistic computer network will benefit the government, military, and economic security of our nation and help to ensure the continued reliability of our critical infrastructure. An advanced and adaptive testbed framework could enable an organization to model their network and model real world events representative of how they actually occur within an enterprise.

Novel Materials and Devices for Solid State Neutron Detection

176117
Year 1 of 3
Principal Investigator: D. R. Wheeler

Project Purpose:

Until recently, thermal neutron detection has been primarily limited to physically large devices. Miniaturization would allow broader use in nuclear medicine, nonproliferation, etc. Recent research shows promise in creating smaller neutron detectors through the combination of high-neutron-cross-section converter materials and solid state devices. Yet, it remains difficult to measure low neutron fluxes by solid state means given a lack of designs capable of capturing all conversion products. Gadolinium-based (Gd) semiconductor heterojunctions have detected electrons produced by Gd-neutron reactions but only at high neutron fluxes. One of the main limitations to this type of approach is the inability to capture all the conversion electrons due to device thickness limitations, the broad energy range of the electrons and geometric configuration. In this project, we will utilize different converter materials and different semiconductors to attempt to capture a greater percentage of the conversion electrons, both low and higher energy varieties. In particular, we will study detector size scaling and the effect of band bending in heterojunction devices in improving response. We also intend to explore novel geometrical implementations of the converter to increase sensitivity. The advancement of sensitive, miniature neutron detectors will have benefits in energy production, nonproliferation and medicine.

Rocket Engine Test System for Development of Novel Propulsion Technologies

176311
Year 1 of 3
Principal Investigator: W. Saul

Project Purpose:

A novel small-scale rocket engine testing capability is needed for development of new propulsion systems — specifically green propellants that eliminate toxicity of current systems. By leveraging Sandia's unique background in propulsion systems engineering with cutting-edge instrumentation and imaging techniques being developed at New Mexico Tech (NMT), the result will be a testbed for propulsion initiatives developed at both institutions. The initial goal is development of a test capability including an instrumented rocket engine test stand for liquid propellant engines (control and delivery systems have been completed). The test capability will have both hot- and cold-flow testing of rocket engines with a thrust range of 10-200 pounds, thus allowing for sufficient, but manageable, propellant flow rates and enthalpies for Sandia and NMT research interests. This test capability will utilize a blow-down fuel and oxidizer system with high-pressure nitrogen push gas eliminating the need for expensive pumps. The test stand will have the capability to measure thrust produced and allow for significant optical access of the exhaust plume and nozzle exit. This will provide both a unique test capability for NMT and Sandia and as well as important research results in alternative green propulsion technologies, necessary for the development and advancement of safer and more economical propulsion systems.

Following test and diagnostic development, the primary focus of the research will explore performance and limitations of novel green liquid propellants. This research will include development and implementation of unique experimental diagnostic techniques. Schlieren image velocimetry will be used for measuring the nozzle exhaust plume velocity flow-field and optical thermography will quantify exhaust plume temperature and combustion product species distributions. Plume shape and signature characterization would have high-consequence impact on system targeting. Long-term goals include improving combustion and propulsion capabilities for exploration of novel nontoxic propellant combinations.

Towards Global Persistent Surveillance

177966
Year 1 of 2
Principal Investigator: M. E. Buckman

Project Purpose:

Global persistent surveillance is viewed to be a critical enabler for US national security. Some existing sensor systems achieve global persistence in one or more sensing modalities (seismic, low-resolution optical, etc.) but trade away other performance attributes, such as sensitivity, resolution or accuracy, for their large area coverage. In contrast, some persistent sensor systems provide exquisite performance over relatively small areas, and thus depend on multiple sensors and appropriate tasking to gain access to high priority areas. This tradeoff is partially due to fundamental limitations (physics, phenomenology, deployment constraints, etc.) while part is driven by technology/cost constraints. Recent advances in semiconductor and focal plane array (FPA) technologies suggest that very large-scale persistent space-based sensors may be technically realizable within the next decade, possibly at significantly lower cost. However, other system considerations, such as communications, processing, command/control, and satellite bus/launch costs must be addressed to develop viable global persistent sensing systems.

This project will design large-scale persistent sensor architecture for space and analyze its performance, limitations, and potential applicability to emerging mission needs. A viable architectural design requires quantifying the interdependencies between advanced FPAs and other key sensor elements including optics, bandwidth, and processing, and their relationships to space deployment considerations such as orbit regime, space/weight/power, altitude, and number of assets. Exemplar sensors/architectures will be designed and modeled to evaluate performance and reveal related system-level implications in order to determine the levels of persistence vs. other performance attributes that could be realized in practice. The most promising sensor architectures will be analyzed for relevance to national security needs, and a first-order estimate of cost drivers and areas for potential savings will be developed. If successful, this project could lead to a state-of-the art persistent architecture, resulting in a technical advance that could enable a paradigm shift in national security remote sensing.

Multi-Resolution Image Fusion

178851
Year 1 of 2
Principal Investigator: E. A. Shields

Project Purpose:

Ground sample distance and field-of-view of remote sensing electro-optical infrared (EO/IR) systems are inversely proportional to the distance between the sensor and the target of interest. At higher altitudes, sensing is often less resolved but more persistent because of an increase in field of view. At lower altitudes, sensing is more resolved but less persistent because of a decrease in field of view.

Persistent systems can more easily track targets, however, detecting and identifying them is more difficult. What may be readily identifiable by a low-altitude system may appear as a point object to the high-altitude system.

For these reasons, a single imaging system cannot both effectively identify and track a moving target. This project will study how information from two or more systems with different resolutions can be fused to maintain custody of an identified target for an extended period of time.

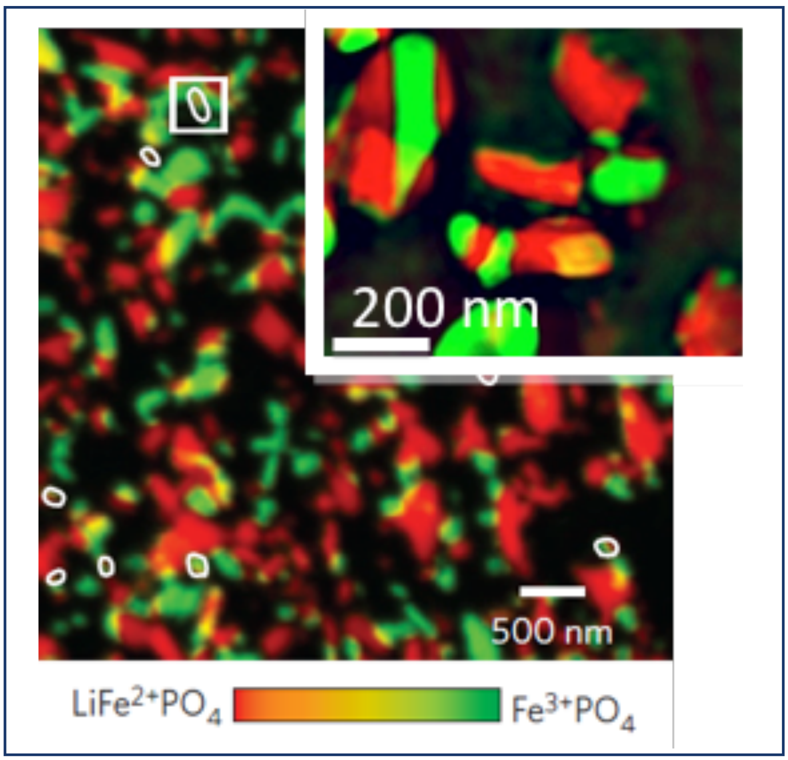
Numerous techniques will be advanced to solve this problem. First, imagery from multiple systems will be appropriately fused. Multi-modal image registration techniques (i.e., techniques for registering images from different systems) will be studied to determine how to best combine the imagery. Image fusion techniques may also prove useful for providing a single, fused image to present to the analyst. Super-resolution techniques will be employed as appropriate to improve the resolution of more persistent systems.

Software for tracking identified targets via high-persistence/low-resolution imagery will be developed. Information from previous detections of the target will be used to maintain confidence that target custody has not been lost. This information may include, among other things, previous locations and headings, multi-spectral data, suspected destinations, and known traffic paths. A metric for target identification confidence will be created and presented to the analyst.

The techniques developed are innovative in their use of multi-resolution data. Information from different systems will be fused to provide a unique tracking and identification capability to the user community.

ENERGY, CLIMATE, AND INFRASTRUCTURE SECURITY

This Investment Area (IA) is focused on research and development that creates options for four areas: Energy Security, Climate Security, Infrastructure Security, and Enabling Capabilities. The IA encourages research and development, building directly on the results of fundamental research to provide real solutions to the most pressing challenges in our mission. The ECIS IA LDRDs are investments to develop and create products and capabilities to incubate solutions for future program needs. The challenges include reducing our dependence on foreign oil through R&D focused on renewable energy alternatives; increasing the use of low carbon power generation; advancing credible carbon management strategies; assuring water safety, security, and sustainability; increasing security and resiliency of the electrical grid and energy infrastructure; and, providing the foundation for a global climate treaty.



The development of novel in situ characterization methods and electrochemical analysis capabilities that apply to commercial-scale electrodes can be used to better understand battery degradation. Shown here is a map of the lithium content of each particle in a LiFePO4 electrode charged at high rate – from Li, et al., *Nature Materials*, (2014). Inset shows ultra-high resolution x-ray ptychography. (Project 158810)

ENERGY, CLIMATE, AND INFRASTRUCTURE SECURITY

Designing Greenhouse Gas Monitoring Systems and Reducing their Uncertainties

158809
Year 3 of 3
Principal Investigator: R. Bambha

Project Purpose:

A global climate treaty will likely be based on greenhouse gas (GHG) inventories supplied by participating countries. The inventory-based approach, which assigns emissions on the basis of economic and socioeconomic factors, is fraught with unacceptably large uncertainties in anthropogenic emissions. A "top-down" approach, based on atmospheric measurements, will be critical for compliance verification on countrywide or regional scales. Furthermore, US compliance with a climate treaty will require implementation of effective policies at city, state, and regional levels. To evaluate policy effectiveness, state and municipal decision makers will need estimates of GHG emissions based on emissions sectors, such as transportation, power generation, and biomass burning. Existing attribution methods are inadequate for either treaty verification or policy evaluation, largely because they focus nearly exclusively on measurements of the most abundant GHG, CO_2, which has an enormous variable natural background. Inversion of CO_2 concentration measurements to source locations provides no information on source types, and current measurement databases used for these inversions lack the necessary spatial and temporal coverage.

We will design a new measurement and analysis system for GHG source attribution suitable for treaty verification and regional or municipal policy evaluation. Our approach uses measurements of gases and particulates co-emitted with anthropogenic and biogenic GHGs, which serve as tracers of specific sources and can provide powerful information on source type and strength. This information is valuable for evaluating policy decisions and narrowing uncertainties on inversions for treaty verification, but the multi-dimensional nature of the associated inversion renders it intractable without co-design of the models and measurements to systematically constrain the problem. We will leverage Sandia's unique GHG mobile laboratory to characterize sources and provide an attribution testbed. Sandia's numerical simulation and analysis capabilities will be tightly coupled to support experiment design, characterize uncertainties, design sensor networks, and infer sources.

Summary of Accomplishments:

In this project, we have developed atmospheric measurement capabilities and a suite of atmospheric modeling and analysis tools that are well suited for verifying emissions of GHGs on an urban-through-regional scale. We developed a regional greenhouse gas source inference system that integrates atmospheric dispersion simulation and Bayesian inference and uncertainty quantification algorithms. We have, for the first time, applied the community multiscale air quality (CMAQ) model to simulate atmospheric CO_2 at relatively high spatial and temporal resolution with the goal of leveraging emissions verification efforts for both air quality and climate. The use of CMAQ allows for the examination of regional-scale transport and distribution of CO_2 along with air pollutants traditionally studied using CMAQ, many of which could help attribute GHGs from different sources.

We have developed a bias-enhanced Bayesian inference approach that can remedy problems of transport model errors in atmospheric CO_2 inversions. We have tested the approach using data and model outputs from the TransCom3 global CO_2 inversion comparison project. A separate prototyping study employed polynomial chaos expansion to accelerate the evaluation of a regional transport model and enable efficient Markov Chain Monte Carlo sampling of the posterior for Bayesian inference. Another prototype approach we developed uses deterministic inversion of a convection-diffusion-reaction system in the presence of uncertainty.

We have established an atmospheric measurement site in Livermore, California and are collecting continuous measurements of CO_2, CH_4 and other species that are typically co-emitted with these GHGs. Automatic calibrations using traceable standards are performed routinely for the gas-phase measurements. We are also collecting standard meteorological data at the Livermore site as well as planetary boundary height measurements using a ceilometer. The location of the measurement site is well suited to sample air transported between the San Francisco Bay area and the California Central Valley.

Significance:

In addition to addressing needs for GHG treaty verification, the methods developed are suitable for monitoring geological CO_2 sequestration, emissions following large-scale disasters, or battlefield plumes. Our approach leverages Sandia's expertise in systems design, advanced computing, uncertainty quantification, data assimilation, atmospheric sciences, Bayesian experimental design, and field measurements and has advanced S&T capabilities in these areas. This effort will position Sandia for a leading role in the future multiagency greenhouse gas information system (GHGIS) with potential sponsorship from DOE BER, NASA, NOAA, and state and local agencies. DOE, DoD, DOT, EPA, and FEMA are potential customers for other monitoring applications.

Refereed Communications:

Z. Liu, R.P. Bambha, J.P. Pinto, T. Zeng, J. Boylan, M. Huang, H. Lei, C. Zhao, S. Liu, J. Mao, C.R. Schwalm, X. Shi, Y. Wei, and H.A. Michelsen, "Toward Verifying Fossil Fuel CO_2 Emissions with the CMAQ Model: Motivation, Model Description and Initial Simulation," *Journal of the Air and Waste Management Association*, vol. 64, pp. 419-435, April 2014.

H.A. Michelsen, R.P. Bambha, Z. Liu, P.E. Schrader, B. LaFranchi, K. Sargsyan, C. Safta, H. Najm, E. Roesler, M.A. Taylor, M.D. Ivey, F. Helsel, and A. Halloran, "Black Carbon, Methane, and Carbon Dioxide: Measurement, Modeling, and Source Attribution," presented (invited) at meeting with California Governor's Climate Action Team, Sacramento, CA, 2014.

The Science of Battery Degradation

158810
Year 3 of 3
Principal Investigator: J. P. Sullivan

Project Purpose:

DOE has identified the transformation of our nation's energy systems towards clean energy technologies as its first mission statement goal. Electrical energy storage in the form of batteries is a key component of this vision. However, current large-scale battery technologies need substantial improvements in capacity and lifetime in order to meet performance and reliability goals. Although there has been considerable work to develop new battery materials, research to understand the limits of battery lifetime has lagged. The objective of this project is to develop new approaches that go far beyond traditional electrochemical methods for the identification, at the atomic level, of the leading mechanism(s) that give rise to battery degradation. Our approach combines new experimental characterization tools with atomistic modeling to achieve unique insight. Specifically, we will develop in situ characterization methods that are based on transmission electron microscopy (TEM), scanning transmission x-ray microscopy (STXM), and high-sensitivity optical spectroscopies, and apply these approaches to realistic full-scale lithium-ion battery electrodes and isolated battery particles. We will also develop new electrochemical approaches, including quantitative nanoscale electrochemistry and electrochemical entropy measurements as a function of cycling. Modeling methods include ab initio modeling of electrolyte decomposition at electrode surfaces and modeling of the structure of multi-component oxide cathodes that then feeds into interpretation of x-ray absorption spectra. These methods and models will be used to evaluate leading proposed mechanisms of degradation, including electrolyte decomposition, which leads to solid-electrolyte interphase formation and growth, and mechanical fracture, cracking, and delamination within the solid electrodes. Importantly, we will monitor changes in commercially relevant electrodes as they are cycled to the point of significant degradation. At the conclusion of this project, we expect to have a suite of experimental and theoretical tools that can be applied to a broad spectrum of commercial-scale battery electrodes for the purpose of identifying degradation mechanisms.

Summary of Accomplishments:

We developed several innovative and unique approaches for the understanding of degradation mechanisms during the course of this project: 1) using electron and x-ray microscopy techniques, we invented a technique based on ultramicrotoming to section commercial scale battery electrodes for sampling deep inside the battery, 2) we developed a new approach to understand how lithium transports through battery cathodes using scanning transmission x-ray microscopy (STXM), 3) we created two new in situ liquid cell capabilities for real-time electron and x-ray microscopy, 4) we developed a new optical cell for in situ Raman spectroscopy and applied this technique for the study of redox flow cells, 5) we invented an approach for performing ab initio simulation of electrochemical reactions under potential control and applied this to study electrolyte degradation, and 6) we developed an electrochemical entropy technique combined with x-ray based structural measurements for understanding origins of battery degradation. These approaches led to a number of scientific discoveries. Using STXM, we learned that lithium iron phosphate battery cathodes display unexpected behavior during lithiation wherein lithium transport is controlled by nucleation of a lithiated phase, leading to high heterogeneity in lithium content at each particle and a surprising invariance of local current density with the overall electrode charging current. We discovered, using in situ transmission electron microscopy, that there is a size limit to lithiation of silicon anode particles above which particle fracture controls electrode degradation. From electrochemical entropy measurements, we discovered that entropy changes little with degradation but the origin of degradation in cathodes is kinetic in nature (i.e., lower rate cycling recovers lost capacity). Finally, our modeling of electrode-electrolyte interfaces revealed that electrolyte degradation may occur by either a single or double electron transfer process depending on thickness of the solid-electrolyte-interphase layer, and this can be predicted.

Significance:

This project advances DOE's objectives in clean energy and energy self-sufficiency by eliminating obstacles to the deployment of large-scale battery-based energy storage systems. We developed new approaches for understanding degradation that can be applied to all battery systems — including liquid-based batteries — for vehicles and the electric grid. Noteworthy publications from this project are advancing the science for predicting reliability of energy storage systems — a new area of importance for energy security.

Refereed Communications:

K. Zavadil, Y. Liu, K. Jungjohann, P. Kotula, and N. Hahn, "Quantitative Electrochemical TEM to Study Alloying for Advanced Battery Anodes," presented at the *TMS 2014 Meeting*, San Diego, CA, 2014.

K. Leung, "Towards Predicting Voltage Dependences of Electrode/Electrolyte Interfacial Processes in Lithium Ion Batteries," presented at *Ohio State University Materials Week*, Columbus, OH, 2014.

K. Leung, "Towards Predicting Voltage Dependences of Electrode/Electrolyte Interfacial Processes in Lithium Ion Batteries," presented at the *Thermec Meeting 2014*, Las Vegas, NV, 2013.

K. Leung, "Towards Predicting Voltage Dependences of Electrode/Electrolyte Interfacial Processes in Lithium Ion Batteries," presented at the *Materials Research Society Spring Meeting*, San Francisco, CA, 2014.

K. Leung, "Towards Predicting Voltage Dependences of Electrode/Electrolyte Interfacial Processes in Lithium Ion Batteries," presented at the *American Chemical Society Spring Meeting*, Dallas, TX, 2014.

M.S. Leite, D. Ruzmetov, Z. Li, L.A. Bendersky, N.C. Bartelt, A. Kolmakov, and A.A. Talin, "New Insights from In Situ Electron Microscopy into Capacity Loss Mechanism in Li-ion Batters with Al Anodes," to be published in the *Journal of Materials Chemistry A*.

Y. Li, F. El Gabaly, T.R. Ferguson, R.B. Smith, N.C. Bartelt, J.D. Sugar, K.R. Fenton, D.A. Cogswell, A.L.D. Kilcoyne, T. Tyliszczak, M.Z. Bazant, and W.C. Chueh, "Current-Induced Transition from Particle-by-Particle to Concurrent Intercalation in Phase-Separating Battery Electrodes," *Nature Materials*, vol. 13, pp. 1149-1156, September 2014.

J.M. de la Hoz, K. Leung, and P.B. Balbuena, "Reduction Mechanisms of Ethylene Carbonate on Si Anodes of Lithium-Ion Batteries: Effects of Degree of Lithiation and Nature of Exposed Surface," *ACS Applied Materials and Interfaces*, vol. 5, p. 13457, 2013.

K. Leung, "Ab Initio Molecular Dynamics Simulations of Electrolyte Electrochemical Reactions on Battery Electrode Surface," presented at the *ACS Meeting*, San Francisco, CA, 2014.

N. Hudak, M. Rodriguez, J. Griego, L. Davis, and G. Nagasubramanian, "Ex Situ XRD Characterization of Cycled Metal Oxide Electrodes for Lithium-Ion Batteries," presented at the *Denver X-Ray Conference*, Big Sky, MT, 2014.

Opportunities for Waste and Energy

159302
Year 3 of 3
Principal Investigator: J. Westbrook

Project Purpose:

Increasing concern regarding the cost, security, and environmental impacts of fossil fuel energy use is driving research and investment towards developing the most strategic methods of converting biomass resources into energy. Analyses to date have examined theoretical limitations of biomass-to-energy through resource availability assessments, but have not thoroughly challenged competing tradeoffs of conversion into liquid fuel versus electricity.

Existing studies have focused on energy crops and cellulosic residues for biomass-to-energy inputs; however, the conversion of these biomass resources is often less energetically efficient compared to fossil energy sources. Waste streams are beginning to be recognized as valuable biomass to energy resources. Municipal solid waste (MSW) is a low-cost waste resource with a well-defined supply infrastructure and does not compete for land area or food supply, making it a potentially attractive, renewable feedstock. This project will create the waste biomass to energy pathway model (WBEM) using a system dynamics approach to analyze the impact of converting MSW biomass to either bioelectricity or liquid fuel. The WBEM will incorporate macroscale feedback from supply chain costs, energy sector impacts, and greenhouse gas (GHG) production within the competing pathways of MSW to: 1) landfill, 2) transportation fuel, and 3) electricity in two states with distinct electric mixes: California and Wisconsin.

Current DOE biomass-to-energy strategies focus on liquid fuel and electricity pathways separately, rather than their direct competition. Regional diversities in energy supplies, costs, and biomass resources suggest considering these pathways in competition. MSW-to-energy modeling remains in its infancy, providing Sandia an opportunity to lead within this field. The system dynamics methodology allows a quantitative exploration of tradeoffs between these pathways by considering dynamics and feedback across them over time. This capability will guide understanding of how waste-to-energy technologies could more strategically advance bioenergy in the US and provide a flexible framework able to apply to waste streams beyond MSW.

Summary of Accomplishments:

This project enabled the development of novel analyses of the impacts of waste biomass to energy for the nation's transportation and electricity energy sectors. This included the characterization of competing bioenergy pathways to better understand and quantify biomass to energy implications. In this process, the team developed new capabilities in the characterization of MSW biomass and landfill gas as reliable bioenergy feedstocks.

The main analysis findings for the California state case study are as follows. Waste biomass to landfill represents the least favorable use of biomass over time from an environmental perspective. The conversion of waste biomass to energy is costly; however, it may be cost-competitive with other renewables under certain circumstances. The thermochemical conversion of paper and organic MSW to ethanol represents the waste to energy pathway with the greatest displacement of GHGs per dollar invested compared to all other MSW pathways considered. In addition to the MSW to energy case study findings, the detailed modeling of the transportation network represented by the transport of MSW from cities to landfills crated an opportunity to develop novel routing algorithms using distance matrices.

Significance:

The waste biomass to energy pathway model creates a dynamic quantitative modeling capability that directly examines waste and biomass to energy questions the state of California and the greater US are currently attempting to address with policies. Robust, quantitative modeling analysis results can potentially inform these policy decisions, enabling policy makers and analysts to craft policies with the quantitative analysis they need to defend them in this national security area.

Theoretical Foundations for Measuring the Groundwater Age Distribution

161864
Year 3 of 3
Principal Investigator: W. P. Gardner

Project Purpose:

Groundwater flow rates have important implications for groundwater resources, contaminant migration, and the isolation of hazardous wastes; however, flow rates and residence times inferred from individual environmental tracers have significant uncertainties. This project will explore the theoretical foundations for measuring the groundwater residence time distribution in complex 3D aquifer systems using a broad suite of environmental tracers and incorporating this information in numerical models of groundwater flow. "Apparent" groundwater ages derived from tracer concentrations have been compared to modeled groundwater mean age, dramatically reducing parameter estimation uncertainty. However, a groundwater sample is a collection of particles with a complex residence time distribution; thus, comparison of a single modeled and tracer inferred age is fraught with uncertainty. There is a need to simulate both the residence time distribution and the concentrations of multiple environmental tracers and assess methods of interpreting the residence time information from tracers and the formal reduction in uncertainty of subsurface parameter estimates using tracer information.

Current work in this area suffers from two limitations: 1) most efforts have been tied to a particular field location, limiting universal application and 2) actual concentrations of tracers are not simulated due to the computational expense, thus incorporating inherent error by comparing a single fluid residence time. In this project, methods to constrain the residence time distribution from the concentration of multiple tracers will be derived, and tracer information will be incorporated into formal parameter estimation and uncertainty analysis routines using synthetic data sets. Finally, these methods will be used with an existing data set from a regional flow system. By focusing first on theoretical, numerical experimentation with the extensive numerical power at Sandia, this project can resolve fundamental questions of how to best utilize tracer information, the data worth of different tracers, and the computational requirements. These fundamental insights can then be applied to field data in any setting.

Summary of Accomplishments:

As a result of this work, we significantly improved the tool chest for isotope hydrologists to model, interpret, and apply natural tracer data. We performed the first massively parallel simulations of multiple environmental tracers in heterogeneous domains. We showed that cutting edge groundwater flow and transport codes are capable of simulating the concentration of multiple groundwater age tracers in 3D heterogeneous domains. We used this new technique to investigate the systematics of tracer transport and groundwater age in these domains and to gain insight into the estimation of groundwater age from tracer concentrations. We showed a large uncertainty and discrepancy between actual groundwater age and the tracer-derived age. We then investigated the use of tracer concentrations in reducing the uncertainty in subsurface parameter estimation problems. We show that environmental tracer concentrations can provide large reductions in parameter uncertainty even though the tracer age and groundwater age do not agree.

Significance:

Many problems in the national interest deal with groundwater flow and transport including energy production, energy storage, and nuclear waste disposal. The principal problem to be overcome in groundwater flow problems is the large uncertainty in subsurface parameters that control flow and transport. As a result of this study, we have provided building blocks to drastically reduce this uncertainty and to provide improved predictions of groundwater flow and transport in all these areas.

Refereed Communications:

W.P. Gardner, G.E. Hammond, and P.G. Lichtner, "High Performance Simulation of Environmental Tracers in Heterogeneous Domains," *Groundwater*," Epub ahead of print, December 2013.

Chloride-Insertion Electrodes for Rechargeable Aluminum Batteries

161866
Year 3 of 3
Principal Investigator: N. Hudak

Project Purpose:

Demand for rechargeable battery systems continues to increase with the emergence of electric vehicles and the introduction of stationary energy storage to the electrical grid. Rechargeable batteries based on aluminum are attractive alternatives to those based on conventional chemistries (e.g., lithium and zinc) because of the high theoretical energy density and low cost of aluminum. An emerging type of rechargeable aluminum battery is based on room-temperature ionic liquids containing aluminum chloride. Aluminum metal has been extensively studied in such solutions, forming the basis for the negative electrode in a rechargeable aluminum battery. We are conducting an exploratory study of candidate materials for the positive electrode, which have been far less explored. We focus on the demonstration and evaluation of conducting polymers as reversible anion-insertion electrodes in room-temperature ionic liquids. This represents a significant advance, as there has been limited investigation of positive electrode materials for nonaqueous, room-temperature aluminum batteries. These materials are quantitatively evaluated using performance metrics that are relevant to rechargeable batteries for electric vehicles and/or stationary storage. This work addresses issues of energy reliability and security because of the need for new battery chemistries that are based on inexpensive, domestically produced materials. The research addresses one of the major obstacles preventing further development of aluminum batteries: quantification of the charge-storage capacity and cycling performance of positive electrode materials. Conjugated polymers are especially interesting for this purpose because they are inexpensive, electronically conductive, and easily synthesized by chemical polymerization or electropolymerization.

Summary of Accomplishments:

The electrochemical synthesis and characterization of conducting polymer films on glassy carbon electrodes with chloroaluminate ionic liquid (CIL) electrolyte was performed to investigate cycling mechanisms and fundamental electrochemical performance of the materials. Fourier transform infrared (FTIR) spectroscopy, mass measurements with a laboratory balance, and elemental analysis were used to prove that polypyrrole films synthesized in this way were doped with chloroaluminate anions from the electrolyte solution. The doping level was measured as approximately four monomer units per anion dopant molecule. Cyclic voltammetry showed faradaic and non-faradaic electrochemical activity in both polypyrrole and polythiophene, with the electrochemical activity of polythiophene concentrated at higher potentials. Galvanostatic cycling of both types of polymer films was highly stable, showing negligible losses in capacity after 50-400 cycles. The high coulombic efficiencies approaching 100% showed that anion doping of the polymers in CIL electrolytes is highly reversible and appropriate for a rechargeable battery. Electrochemical quartz-crystal microbalance was used during electrochemical polymerization to estimate the amount of deposited mass on the electrode, and these values were used to estimate gravimetric capacities. The resultant estimates of 30-100 mAh/g (specific to polymer mass) were on par with theoretically predicted values. Prototypes of the aluminum battery cells were assembled by preparing composite electrodes containing polypyrrole or polythiophene powder with polymer binder and conductive additive. These electrodes were combined with CIL-soaked separator and aluminum metal anode in a sandwich configuration in sealed cells. Although the galvanostatic cycling of these cells was not as stable as that of the electropolymerized films, they retained a significant amount of capacity with high coulombic efficiency after 100 cycles. The observed electrochemical performance was used to estimate the gravimetric energy density relative to the active cell components. The energy density of the polythiophene-CIL-aluminum cell chemistry was estimated as 44 Wh/kg, and that of the polypyrrole-CIL-aluminum cell was 46 Wh/kg.

Significance:

In terms of basic science, this work presented new discoveries in the electrochemistry of conducting polymers and ionic liquids. Regarding energy security, the development of the smart grid, incorporation of renewable energy sources, and widespread adoption of electric vehicles require advances in energy storage using materials that are inexpensive and domestically available. This project proved that an aluminum-based battery operating at room temperature can exhibit excellent performance and competitive energy density. As battery components based vanadium, lead, lithium, and cobalt become more expensive and limited in supply, the prototype batteries demonstrated in this project may have significant cost and safety advantages.

Refereed Communications:

N.S. Hudak, "Chloroaluminate-Doped Conducting Polymers as Positive Electrodes in Rechargeable Aluminum Batteries," *The Journal of Physical Chemistry C*, vol. 118, pp. 5203-5215, February 2014.

Hybrid-Renewable Processes for Biofuels Production: Concentrated Solar Pyrolysis of Biomass Residues

161868
Year 3 of 3
Principal Investigator: A. George

Project Purpose:

This project seeks to improve the efficiency and reduce the cost of biorefining by developing a greater understanding of solar-biomass processing. The viability of thermochemically derived biofuels can be greatly enhanced by reducing the process parasitic energy loads. Gasification processes are globally endothermic, requiring 20-45% of the feedstock to be consumed allothermally. Additionally, in air-blown gasification, high CO_2 and N_2 dilute the product syngas. Integrating renewable power into biofuels production is one method by which these efficiency drains can be eliminated. There are a variety of such potentially viable "hybrid-renewable" approaches — one is to integrate concentrated solar power (CSP) to power biomass-to-liquid fuels (BTL) processes, both during pyrolysis and/or gasification operations as well as downstream. Barriers to CSP integration into BTL processes are predominantly the lack of fundamental kinetic and mass transport data to enable appropriate systems analysis and reactor design.

Combined CSP-for-BTL is a nascent field. It has, therefore, only been sporadically addressed from a fundamental science and a process-systems engineering perspective; many important questions need to be answered to enable uptake of this technology. This project will develop a reactor scheme by which high-quality fundamental data on the conversion of biomass-to-liquid fuels, via CSP will be obtained.

The viability of the planned process has yet to be established. Establishing viability would enable a significant contribution to the US' renewable energy targets. Our approach would be the first time fundamental process data has been obtained that attempts to decouple reactor configuration from the behavior of biomass particles undergoing solar irradiation, in terms of kinetics, yields and product quality. The feedstock will be lignin, a copious residue derived from bioprocessing of lignocellulose. Using this waste for fuel will significantly enhance bioprocessing economics. The process will be modeled from a process systems engineering perspective.

Summary of Accomplishments:

A novel design for the reactor has been created that can allow biomass particles to be suspended in a flow of inert gas (or gasification environment) and be irradiated with a simulated solar flux. Pyrolysis conditions were investigated and a comparison between solar and non-solar biomass pyrolysis was conducted in terms of product distributions and pyrolysis oil quality. We demonstrated that the fuel characteristics of oil produced from solar sources was different to that produced from other heating mechanisms, for an equivalent nominal temperature. This is important because we showed that we can use renewable sources of energy to produce renewable fuel. A novel method was also developed to analyze pyrolysis products, in particular heavier molecules, which are more challenging to upgrade to fuels, and an investigation into the aging of gasification tars was made. This has impact, as understanding the inherent instability of bio-oils produced will enable the development of strategies to mitigate this instability. Finally, this project led to the discovery that genetically modified biomass exhibits different pyrolysis behavior to the plant in its native form, which can lead to strategies to improve bio-oil quality via in planta biomass modifications.

Significance:

This work is deeply rooted in the nation's mission to enable energy security, by furthering research into new approaches for producing environmentally neutral biofuels.

Refereed Communications:

A. George, T.J. Morgan, and R. Kandiyoti, "Pyrolytic Reactions of Lignin within Naturally Occurring Plant Matrices: Challenges in Biomass Pyrolysis Modeling due to Synergistic Effects," *Energy Fuels*, vol. 28, pp. 6918-6927, September 2014.

Integration of SD and PRA to Create a Time-Dependent Prediction of the Risk Profile of a Nuclear Power Plant

162299
Year 3 of 3
Principal Investigator: M. R. Denman

Project Purpose:

Probabilistic risk assessment (PRA) is the primary tool used to risk-inform nuclear power regulatory and licensing activities. Risk-informed regulations are intended to reduce inherent conservatism in regulatory metrics that are built into the regulatory framework by quantifying both the total risk profile and the change in the profile caused by an event or action.

PRAs are currently representations of the average risk posed to the public at the time when the analysis was conducted. Changes to the plant, either physical or managerial, are only characterized during revisions to the entire PRA. Thus, slowly evolving changes to public risk are often not calculated until these changes are large enough to warrant a revision of the PRA. This may introduce non-conservative approximations to the PRA — the consequences of which are not always obvious.

Dynamical analysis (DA) has been used to understand unintended time-dependent feedbacks in industrial/organizational settings. We will use DA models to simulate reliability changes in structures, systems, and components that can adjust basic event probabilities at a fault tree's base. Dynamic system models will adjust the trees to explicitly incorporate aging effects and/or examine changes in system reliability. These tools can dramatically expand the applications of risk-informed decision making by adjusting risk metrics for evolving conditions.

A primary outcome will be to identify plausible behavior modes for systems undergoing maintenance and aging, along with dynamic events (e.g., startup, shutdown) that might benefit from reliability-dynamics analysis, utilizing three different dynamic models:

- Functional — How does the system interact?
- Aging and Maintenance — How does time affect performance?
- Operational — How to develop risk-informed Severe-Accident-Management-Guidelines?

The project will build aging, maintenance, and operational models linking them to the quasi-static fault tree-produced reliably equations. This involves treating aging and component uncertainty as external inputs, parameter changes, or state changes. Ultimately, PRA-DA coupling will remove non-conservative approximations and improve stakeholder confidence.

Summary of Accomplishments:

Dynamic systems (DS) PRA provides powerful tools for evaluating evolving risks to nuclear power plants and may be especially powerful in evaluating the risk of nuclear facilities during accident management. Existing research at Sandia on probabilistic accident management have benefited from the techniques developed in this project to dynamically quantify changing probabilities in both the long (e.g., plant life extensions) and short (e.g., accident mitigation) time frames.

This project demonstrated the need of examining plant aging in existing light-water reactors (LWRs) by showing limited change in high pressure injection system failure probabilities upon demand, and by showing orders of magnitude change in the conditional failure probability once the system has been demanded. This project also highlighted the importance of dynamic modeling of safety relief valve performance in a generic small modular reactors response to a beyond design basis accident.

Significance:

Part of DOE's mission is to address energy and nuclear challenges and informative PRA is fundamental to ensuring the safety of nuclear power plants. This project was primarily aimed at improving nuclear power plant safety by creating time-dependent PRA models, thus removing the inherently non-conservative time-averaging approximation. This methodology for coupling DS models with fault and event trees can be employed for any high-consequence system with a dynamic risk, especially systems which currently use fault and event trees to model risks (e.g., stockpile assurance, transportation reliably, and hydrogen production and distribution safety).

Heavy-Duty Vehicle and Infrastructure Futures

164667
Year 3 of 3
Principal Investigator: A. C. Askin

Project Purpose:

The purpose of this project is to create a capability for evaluating heavy-duty vehicle fleet alternative fuel and efficiency technology evolution in order to identify the drivers toward reduced petroleum consumption and emissions to help solve energy security and environmental issues.

In the US, heavy-duty vehicle (HDV) fleets comprise a significant fraction of total fossil fuel consumption, which has profound implications for national security, environmental sustainability, and economic stability. Therefore, directing the future development of this sector toward reducing petroleum consumption while meeting the needs of fleet operators is critical to mitigating future consequences. New alternative fuel and power system technologies in varying stages of development and commercialization comprise a broad portfolio of options for new vehicle design and current vehicle modifications. The breadth of this portfolio necessitates a tool to evaluate the interdependency of the technical, economic, and stakeholder factors driving the evolution of HDV resource consumption and emissions generation. A heavy-duty vehicle pathways model was constructed to address questions about the economic feasibility of technological advances and to assess their potential for positive impact.

Although some modeling efforts have begun to illuminate the complexities of transforming the HDV sector, a comprehensive, parametric model accounting for the breadth of vehicle inventory, the impact of potentially transformational technologies and the necessary infrastructure development remains missing. This project constructed a capability for evaluating the HDV fleet evolution based on supply-demand interactions, fuel and infrastructure availability, technology readiness, and primary energy sourcing. The model provides the ability to assess technology development portfolios and identify critical decision points for sector transformation. The model enables identification and understanding of the principal mechanisms driving the trajectory of HDV industry sectors with regard to resource consumption and environmental sustainability.

Summary of Accomplishments:

The heavy-duty vehicle model segments the fleet by vehicle size, location of operation, vehicle type, fleet size, refueling location type, and powertrain. These dimensions were selected because of their relevance to the applicability or desirability of alternative fuels or energy efficiency technologies. Structuring the model in this way allows for consideration of a broad array of alternative fuel or technology options.

Parameterizing uncertain model quantities enables the investigation of the impacts of modeling assumptions. Previous models in the field generally focus on small sets of specific scenarios, which can miss compounding effects and do not enable assessment of the relationships between inputs and outputs.

Applying the model to evaluate the future of natural gas heavy-duty vehicles and SuperTruck vehicles indicates that diesel will remain the dominant powertrain until 2050 under a wide array of assumptions. Therefore, focusing on technologies that incrementally improve the efficiency of diesel vehicles, and either mandating adoption or making them very financially attractive, can lead to more significant petroleum and emissions reductions than encouraging a shift to natural gas.

Significance:

This heavy-duty vehicle model provides a unique capability for assessing the future of the heavy-duty vehicle sector and its impact on energy security and sustainability. It provides a platform for assessing the potential for impact of new alternative fuel and power system technologies.

Nanoscale Piezoelectric Effect Induced Surface Electrochemical Catalysis in Aqueous Environment

165464
Year 3 of 3
Principal Investigator: H. L. Schwarz

Project Purpose:

We plan to advance the knowledge of the piezoelectric induced surface catalysis in ferroelectric nanostructures. Ferroelectrics are "smart" functional materials whose physical properties are sensitive to changes in external conditions like electric field, pressure, and temperature. Although ferroelectrics are widely used in sensors and microelectromechanical systems (MEMS), activating and catalyzing surface electrochemical reactions via the surface charges generated by piezoelectricity or pyroelectricity is poorly understood. We anticipate that advancing the scientific understanding of the reactivity of nanoscale ferroelectrics in fluidic environments will open a broad range of new applications for ferroelectric material-based surface catalysis and aqueous sensing, establishing a differentiating leading edge capability relevant for addressing future national security mission needs.

As an initial demonstration, we plan to investigate industrially scalable electrospun ferroelectric nanofibers as a novel membrane component for mitigating membrane biofouling in water treatment (a major obstacle that decreases membrane life and prompts excessive back-washing). Embedded ferroelectric nanofibers in filtration membranes have the potential to electrochemically decompose organic matter in situ on the membrane surfaces, and thereby mitigate membrane biofouling.

We will investigate reactivity of mechanically excited ferroelectric nanofibers in fluidic environments to identify the microscopic mechanism of effective piezoelectric effect and electrochemical reaction coupling. Electrospun nanofibers will be used because they have particularly large reactive surface areas. Nanofiber geometry can also potentially enhance the piezoelectric responses due to intensified piezoelectricity ascribed to the flexoelectric effect on the nanoscale, and observations that nanofibers possess high sensitivity to small forces. With fabrication and materials engineering through electrospinning and sol-gel techniques, systematic studies of electrospun ferroelectric nanofibers will offer optimum size and material selection as an excellent platform to study nanoscale piezoelectricity induced electrochemical reactivity on ferroelectric surface in solutions.

Summary of Accomplishments:

We exploited the use of mechanical energy to enable direct chemical reactions on the ferroelectric surface by the piezoelectric effect. We successfully developed an electrospinning and sol-gel process combined with proper heat treatment to synthesize highly crystalline ferroelectric $BaTiO_3$ nanofiber as the study platform. We proved that transient local electrostatic potentials on ferroelectric surface evoked by external mechanical excitation through the piezoelectric effect can activate redox reactions in solution, and that metal particles were reduced in predefined domain locations. Conversion of mechanical — via electrical — to chemical energy is realized. The $BaTiO_3$ nanofibers do not require poling because heterogeneous chemical reactions occur on the randomly distributed charged surfaces. Therefore, this approach offers great convenience of using this technology.

Significance:

Polarization-enabled surface chemistry directly impacts soft-matter manipulation at liquid-solid interfaces. Piezoelectric-effect induced chemical reactions in fluidics provides a new interface for adsorption, catalysis, and electrochemistry. This could lead to revolutionary use of ferroelectric materials via interfacial engineering by its piezoelectric properties, which includes wide fields of applications in degradation of organics (biofouling self-cleaning), molecular sensing, catalysis, and surface wettability, etc. At places where light is unavailable, this technology can be complementary to the photochemical catalysis. Finally, nanofiber-based ferroelectric materials can be developed as new generations of energy harvesting components. This research is potentially relevant to DOE programs in smart sensing, environmental cleanup, water safety, and renewable energy.

Advanced SMRs using S-CO_2 Power Conversion with Dry Cooling

165619
Year 2 of 3
Principal Investigator: B. Middleton

Project Purpose:

Small modular reactors (SMRs) continue to be proposed around the world to meet ever-increasing energy demands, particularly in areas where large-scale transmission is not feasible. DOE recently announced a program of nearly $1 billion aimed at the licensing of light-water-cooled SMRs, demonstrating the high priority placed on the use of SMR technology.

Light-water SMRs are promising in the near term, however, current designs require a large nearby water source for evaporative cooling, and ultimately suffer from the same waste issues and shutdown heat removal concerns as their larger predecessors. Any power production plant built in regions where sufficient water is not available will suffer from the same problem. This includes fossil fuels and solar plants. This project identifies two ways in which a supercritical- CO_2 (S-CO_2) working fluid is uniquely capable of addressing these problems: as the secondary side of a light-water or liquid-metal reactor system, or as the primary coolant in a direct-cycle nuclear turbine. The use of S-CO_2 for power conversion will help to alleviate these concerns.

Recent modeling studies have shown that the S-CO_2 power cycle is strongly compatible with dry-air cooling. Because the cycle is optimized to reject heat at temperatures above 88 °F, its efficiency with increasingly high ambient temperatures does not degrade significantly unlike steam plants. This allows siting of plants in remote desert areas without penalty.

Turbomachinery size and capital cost both strongly favor S-CO_2 power systems over steam. In addition, CO_2 near its critical point experiences sharp changes in density with small temperature changes, affecting large natural circulation flows and establishing decay heat removal for safe shutdown during accidents.

This project seeks to develop an accurate dynamic model of the natural circulation of S-CO_2 near the critical point. Assessment of dimensionless numbers that characterize the flow and heat transfer capabilities of S-CO_2 near the critical point will also be investigated.

Active Suppression of Drilling System Vibrations for Deep Drilling

165620
Year 2 of 3
Principal Investigator: D. W. Raymond

Project Purpose:

A high-reliability drilling system is needed for construction of a deep borehole disposal system reaching depths of 5 km in continental crystalline basement rock. A reference design has been developed that demonstrates viability of the engineered system that can be realized with currently available drilling technology. Drill string vibrations are one potential cause of trouble relative to deep-hole drilling, as they increase the technical risks and final costs of well construction. They are a constant issue in all drilling operations and cause increases in drilling trouble and damaged components, and decreases in the rate of penetration, and bit and tool life.

While the drilling industry routinely attempts to deal with these dysfunctions using fixed-rate damping tools, the consequences are exacerbated when drilling deep wells due to increased drill string flexibility and greater times to replace worn or damaged components. Additionally, the mechanism of self-excitation depends upon the rock formation being drilled, which changes continually in heterogeneous rock. Vibrations are particularly problematic in high strength rock where the risk of tool failure increases dramatically. Drill string stabilization is imperative for improved reliability and drilling performance.

Advanced development is needed to create an autonomous and adaptive solution for the range of conditions encountered during drilling. Conventional drilling systems do not use autonomous and adaptive techniques — it is non-trivial, as drill string property variations must be adjusted remotely. The planned development possesses high potential and has applicability throughout commercial drilling sectors to make deep drilling more efficient and less costly in terms of minimizing damaged equipment. Current science and technology has not solved this problem due to: 1) telemetry limitations during drilling operations making field observation of the problem challenging, 2) difficulty with laboratory simulation of the problem due to geometric limitations in the laboratory, and 3) the challenge of developing controls/tools with autonomous features.

Climate-Induced Spillover and Implications for US Security

165630
Year 2 of 3
Principal Investigator: V. C. Tidwell

Project Purpose:

Developing nations incur a greater risk to climate change than the developed world due to poorly managed human/natural resources, unreliable infrastructure, and brittle governing/economic institutions. These vulnerabilities often give rise to a climate-induced "domino effect" of reduced natural resource production — leading to economic hardship followed by desperate emigration, social unrest, and humanitarian crises. The impact is not limited to a single nation or region but "spills over" to adjoining areas with even broader impact on global markets and security. While the US will be forced to deal with the brunt of the spillover impacts, current planning by the DHS, DOS, and DoD fails to adequately address the spillover issue, because of the lack of technical capacity, let alone quantify the risks and preparedness options.

Toward this problem, we will develop a model of climate-induced spillover. We will create and demonstrate a differentiating analysis tool set, incorporating appropriate technical and socio-economic factors of energy, water, climate, and infrastructure resiliency. The unique aspect of this work is the integration of social, economic, infrastructure, and resource dynamics/constraints to provide a comprehensive risk assessment of climate change on human welfare and security. This model will be used to perform uncertainty quantification using the climate forecasts of the United Nation's Assessment Report 5. We will quantify the risk (intensity and frequency) of "spillover" emanating from developing nations that affects US interests (or homeland security). Specifically: 1) identify regions at highest risk, 2) quantify the emergent risks, 3) characterize resilient solution options, and 4) provide usable and defensible information to policy makers. The resulting model and analysis will be unique in its application of a risk-based assessment framework for determining what preemptive adaptive measures are most necessary, when and where.

Natural Gas Value-Chain and Network Assessments

165631
Year 2 of 3
Principal Investigator: P. H. Kobos

Project Purpose:

Due to the abundance of shale gas and cheap extraction techniques, there is a boom of natural gas (NG) supply in the US, with a corresponding drop in prices. This has spurred increased use of NG in electric power generation, industrial and commercial uses, as well as other uses. With its intrinsic thermal efficiency and low carbon-hydrogen ratio, there are also engineering and environmental benefits to using NG. However, growing the market share of NG is dependent on consumers, producers, and infrastructure stakeholders having confidence that low prices will continue in the future. Future price shocks, either upwards or downwards, resulting from unforeseen economic, technological, or regulatory events could be disruptive and diminish new applications of NG. If the US economy becomes more dependent on NG, it also becomes more vulnerable to its price or supply volatility. This project is developing capabilities to identify the propagation pathways of NG price or supply shocks through the economy. By doing so, we can highlight the risks, vulnerabilities, and mitigation strategies across the NG value chain. Hence, we could begin to assess the feasibility of using NG heavily in all economic sectors and/or of becoming a net NG exporter.

This project has three primary components, focused on the supply, infrastructure, and demand dynamics of NG. The supply-side investigation captures the multitude of economic, technological, and geoscience factors that impact production. The infrastructure component builds upon a model of all major North American gas pipelines to understand the infrastructure expansion necessary to support increased demand and serves as a basis for the third task. The demand side is developing a novel agent-based model (third task) that can represent both equilibrium and disequilibrium dynamics to capture shock propagation through the system. This will focus on the interplay and competition between different demand types and new technologies, such as liquefied natural gas exports.

Novel Metal-Organic Frameworks for Efficient Stationary Energy Sources via Oxy-Fuel Combustion

165632
Year 2 of 3
Principal Investigator: T. M. Nenoff

Project Purpose:

Oxy-fuel combustion is a well-known approach to improve the heat transfer associated with stationary energy processes. However, its overall penetration into industrial and power markets is constrained by the high cost of existing air separation technologies for generating oxygen. Cryogenic air separation is the most widely used technology for generating large flows of oxygen but is a complex and expensive technology. Pressure swing adsorption (PSA) is a competing technology that uses separations materials such as activated carbon, zeolites and polymer membranes. Current PSA technology is expensive and limited to moderate purity O_2 applications because of limitations of existing separations materials. Metal-organic frameworks (MOFs) are cutting edge materials for gas separations at ambient pressure and room temperature, potentially revolutionizing the PSA process and providing dramatic process efficiency improvements through oxy-fuel combustion. This project will produce fundamental knowledge on novel MOFs for gas separations that will be leveraged to applied studies and/or commercialization of new oxyfuel processes. Our energy analysis of MOF air separation processes coupled to oxy-fuel combustion will demonstrate greater than 5% efficiency improvement, with decreased overall carbon emissions. Our project is both an innovative approach for developing novel high selectivity MOFs for O_2 purification and is cutting edge for: 1) optimized MOF synthesis, 2) testing of preferred O_2 sorption from multicomponent streams, 3) combined molecular dynamic (MD) simulations and crystallography of gas siting in pores for structure-property relationship studies, 4) combustions testing, and 5) systems analysis to aid in real-world implementation.

Sandia's Twistact Technology: The Key to Proliferation of Wind Power

165633
Year 2 of 3
Principal Investigator: J. P. Koplow

Project Purpose:

DOE's report, "20% Wind Energy by 2030," estimates that wind power could supply 20% of all US electricity without requiring development grid energy storage technologies. But, wind power only becomes competitive with coal-generated electricity when scaled up to multi-megawatt (MW) turbines. Unfortunately, the traditional gear-box-plus-induction-generator wind turbine architecture does not scale up well. The extremely high shaft torque of slowly rotating multi-MW wind turbines results in frequent gear-box failure. Direct-drive generators are, therefore, required — specifically high-pole-count synchronous generator technology. The choice must then be made between a permanent magnet and electrically excited rotor. The problem with electrically excited synchronous generator technology is the requirement for high-current slip rings (also known as "brushes"), which have a short operating lifetime. Materials costs have always been the main stumbling block for permanent magnet synchronous generator (PMSG) technology. And recently, worldwide demand for rare earth magnet materials overtook production, resulting in a 500% to 1,000% price increase during the last year. This has created a crisis in the wind power industry. Sandia's Twistact technology is a fundamentally new architecture for high current slip rings that eliminates the sliding contact and electrical arcing inherent to existing slip-ring technology, and thus eliminate the maintenance problem.

The primary purpose of developing Sandia's Twistact technology is to eliminate the need for rare earth magnets in multi-MW wind turbines, which is the last major hurdle to proliferation of cost effective ($0.04/kW-hr) wind power. A central goal of this project is to demonstrate that Twistact technology can support an operating current of 1,000 A with a series resistance of no more than 1.0 milliohm. During this past year, we demonstrated 2,000-amp operation at an electrical resistance of 0.65 milliohms. We are now focused on accelerated lifetime testing and have achieved 20 million rotation cycles to date.

Work will continue to focus on the metallurgical belt/sheave intersection that governs belt longevity and current handling capacity. We will also continue to examine high rpm operation for such applications as electric vehicles and homopolar motors/generators.

Calibration, Validation, and Uncertainty Quantification for Turbulence Simulations of Gas Turbine Engines

165635
Year 2 of 3
Principal Investigator: J. A. Templeton

Project Purpose:

Large eddy simulation (LES) has the potential to reduce pollutant emissions and increase the fuel efficiency of gas turbine engines through model-based investigations of engine design space. High-fidelity LES simulations have greatly enhanced our understanding of turbulent combustion. Engineering calculations, by contrast, use low-order numerical methods necessitated by the coarse, unstructured grids needed in complex geometries. High-fidelity LES often produces excellent agreement with experiments while engineering LES of the same case does not yield sufficiently accurate data for engine design. Such results lead to key questions regarding the applicability of LES models to the engineering process: in what situations will they work and why? Is the true solution even within the space spanned by existing models? How will uncertainties in model parameters impact the results? This work will answer these questions using validation and uncertainty quantification (UQ) to connect science-quality LES with desktop calculations design engineers can then use to improve gas turbine engine performance.

Our solution builds on the Advanced Strategic Computing Program's validation and UQ expertise while developing innovations to handle challenging chaotic flows from engine simulations. Novel UQ approaches will be created to account for the fluctuating turbulent structures. These UQ strategies will enable the calibration and validation problems to be posed in a statistical sense relative to high-fidelity solutions leveraged from existing and on-going scientific calculations. Higher-risk work will utilize more complex functional forms that add more physical information but require the detail present in the well-resolved LES for proper calibration. This will determine if existing LES models are capable of the necessary fidelity at acceptable costs. Finally, models will be considered to be probabilistic rather than deterministic to measure model-induced uncertainty and to demonstrate whether they retain sufficient accuracy when validation data is lacking. These approaches will greatly enhance design engineers' ability to utilize high-performance computing to improve engine performance and efficiency.

Developing Next-Generation Graphene-Based Catalysts

165636
Year 2 of 3
Principal Investigator: T. N. Lambert

Project Purpose:

We are developing next-generation catalysts based on nanoscale 3D networks of graphene, ceramics, and graphene-ceramic hybrids in order to establish a leading role for Sandia in nanoscale-based catalysis. High electrocatalytic (EC) activity, selectivity, and stability for the oxygen reduction reaction/oxygen evolution reaction (ORR/OER) is critical for successful transition of next-generation fuel cells and rechargeable metal/air batteries into today's renewable energy technologies. Platinum's (Pt) high cost and overall rarity preclude it from use in larger-scale widespread commercial applications. Pt-based catalysts in fuel cells also suffer from crossover and fuel poisoning issues, which severely lowers the EC activity and performance. Replacing Pt with less costly ceramics, graphene and/or graphene-ceramic materials is in support of the critical materials supply issues. Electrocatalysts based on nanoscale 3D networks of EC carbon represent a promising approach to developing cost-effective electrocatalysts that operate at higher current densities and cell voltages, with significantly greater EC stability in metal-air batteries and fuel cells. Practical EC applications of graphene are still severely limited by the lack of fundamental understanding on the origin of its EC properties, and its 2D morphology, as the fabrication of practical 3D electrodes for ORR/OER is currently not established. A way to assemble these graphene-based materials into larger macroscopic 3D EC form factors is also needed. We aim to demonstrate that such 3D structures can be prepared in a meaningful way and that they can be utilized to improve electrochemical devices. Additionally, we have discovered that 3D porous ceramics can have exceptional activity for bifunctional oxygen electrochemistry and that these catalysts can be prepared without binder materials, thereby improving their activity and overall utility.

Coating Strategies for High Energy Lithium-Ion

165637
Year 2 of 3
Principal Investigator: C. Orendorff

Project Purpose:

Many reliability and safety issues for lithium-ion batteries result from interfacial phenomena at the positive and negative electrodes. A prominent example is the solid electrolyte interphase (SEI) layer that forms on the graphite anode. This SEI layer is known to effect performance and capacity of lithium-ion batteries. Interfacial reactivity between the electrolyte and the cathode is also known to initiate electrolyte combustion during thermal runaway events that compromise battery safety.

Ultrathin coatings on the electrodes can very sensitively influence interfacial phenomena. These ultrathin coatings can profoundly alter the interaction between the electrode and the electrolyte. This project is focused on developing atomic layer deposition (ALD) and molecular layer deposition (MLD) coatings for electrode surfaces. These ALD and MLD coatings can dramatically improve lithium-ion cell reliability and safety.

ALD and MLD are thin film deposition techniques based on sequential, self-limiting surface reactions. ALD and MLD can deposit ultrathin and conformal films on high aspect ratio and porous substrates such as composite particulate electrodes in lithium-ion batteries. Recent results have revealed that ultrathin coatings of Al_2O_3 ALD have a dramatic effect on the capacity stability of electrodes for lithium ion batteries such as graphite anodes and $LiCoO_2$ cathodes.

Few other materials have been tested to determine their effectiveness and may show even better improvements in capacity stability or may display much higher reliability and safer performance. This project will explore new ALD and MLD based coatings such as AlF_3 and metal oxide-carbon composites. These alternative coatings may offer improved ionic and electrical conductivity, mechanical stability, and cell performance over Al_2O_3 ALD coatings. These new ALD and MLD coatings have the potential to significantly improve lithium ion reliability and safety.

This work is in collaboration with the University of Colorado at Boulder.

Synthesis of Heterometallic Manganese oxo Clusters as Small Molecule Models of the Oxygen-Evolving Complex of Photosystem II

165638
Year 2 of 2
Principal Investigator: T. J. Boyle

Project Purpose:

This research will synthesize manganese complexes supported by a multi-nucleating ligand framework as models of the oxygen evolving complex (OEC) of Photosystem II, which is an enzyme found in plants that catalyzes the oxidation of water to molecular oxygen. These model complexes will be studied to better understand the role of the calcium ion in catalysis and the mechanism of oxygen-oxygen double bond formation. Previous approaches have relied on self-assembly of the manganese oxo clusters, which have limited the control of cluster nuclearity and geometry. This project is in collaboration with California Institute of Technology (Caltech).

Summary of Accomplishments:

This project developed a synthetic methodology for the synthesis of heterometallic manganese oxido clusters related to the structure of the oxygen-evolving complex of Photosystem II. Heterometallic tetranuclear clusters containing different redox-inactive metals were isolated in several different oxidation states. Electrochemical studies of these complexes demonstrated a linear dependence of the reduction potentials of these clusters on the Lewis acidity of the redox-inactive metal, with potentials shifted over a range of more than 1 V. These results point to a role of Ca^{2+} in the oxygen-evolving complex (OEC) for tuning the potential of the cluster for water oxidation. These studies also suggest that redox-inactive ions can be incorporated into heterogeneous metal oxide systems to change their electrochemical potentials with the goal of improving their catalytic activity.

Significance:

Applied research that potentially follows from this fundamental study will allow for transformative robust catalysts that enhance the solar conversion of O_2 to energy. This will have the effects of reducing our dependence on foreign oil, decreasing the carbon footprint, and assuring improved sustainable energy sources. Overall, the security of the nation will be enhanced based on a reduction in dependence on foreign sources.

Refereed Communications:

E.Y. Tsui, J.S. Kanady, and T. Agapie, “Synthetic Cluster Models of Biological and Heterogeneous Manganese Catalysts for O_2 Evolution,” *Inorganic Chemistry*, vol. 52, pp. 13833-13848, December 2013.

Enabling Novel Nuclear Reactors with Advanced Life-Time Modeling and Simulation

165644
Year 2 of 2
Principal Investigator: W. J. Martin

Project Purpose:

To enable long-life advanced nuclear reactors, especially novel small modular reactors (SMRs) well beyond the scope of current and near-term DOE studies, a study is needed into the true lifetime of the reactor system. A full-scale investigation of the lifetime of the reactor core, materials, and secondary system is necessary in order for any regulator to license the system.

All proposed advanced reactors are vastly different than the current fleet of light water reactors; many code suites will now be less valid due to physics simplifications. Similarly, the power generation cycle and structural materials will require modeling to determine their lifetime performance, especially with radiation damage and fatigue.

In this project, advanced lifetime modeling and simulation will be used to assess the current concepts and determine if they match regulations, meet physical requirements, and are feasible. An example this project addresses is the idea of an exportable, small modular reactor and the return of the cores at the end of life after they have been exported to and operated in foreign countries. To date, there has been no full study on whether the core will be too radioactive or structurally unstable for it to be shipped after over 10 years of operation. This investigation will help guide the future design and licensing of these novel reactor systems.

Summary of Accomplishments:

Several computer codes were benchmarked and/or validated and verified for use with advanced reactor systems, including the modified CINDER2008 transmutation code and the Serpent2 Monte Carlo code from VTT in Finland. These codes now allow Sandia and others to model advanced nuclear reactor systems that have long life or other advanced cores. CINDER2008 has been modified in-house to allow for dual incident neutral particles (neutron and photon), allowing full modeling of transmutation caused by both particles.

Significance:

These accomplishments, especially the CINDER2008 in-house extension, has already been applied to work in the national security mission at Sandia, as well as being utilized to help find better methods to minimize personnel dose at reactor facilities. Additionally, the work in benchmarking and validating has allowed Sandia to be positioned ideally for future advanced reactor systems, especially those that do not fit the current, light-water reactor mold.

Refereed Communications:

W.J. Martin, A.A. Hecht, and C.R.E. de Oliveira, "Reactor Fuel Depletion Benchmark of TINDER, *Annals of Nuclear Energy*, vol. 73, pp. 547-551, November 2014.

W.J. Martin, A.A. Hecht, and C.R.E. de Oliveira, "Dual Neutral Particle Induced Transmutation in CINDER2008," to be published in *Nuclear Instruments and Methods in Physics Research Section A.*

A.A. Hecht, R.E. Blakeley, W.J. Martin and E. Leonard, "Comparison of Geant4 and MCNP6 for use in Delayed Fission Radiation Simulation," *Annals of Nuclear Energy*, vol. 69, pp. 134-138, July 2014.

Time-Varying, Multi-Scale Adaptive System Reliability Analysis of Lifeline Infrastructure Networks

166143
Year 2 of 2
Principal Investigator: J. L. Gearhart

Project Purpose:

For a society's well being, one must be able to assess resilience of lifeline infrastructures against extreme events. Accurate risk prediction models can determine the systems-level resilience of an infrastructure from vulnerability models of its components. Since updates to these infrastructures often require many years to accomplish, it is essential that these models also capture the effects of infrastructure aging and deterioration. An accepted way to quantify post-disaster network reliability is to calculate the network disconnection probability. Several have attempted this measure using computationally expensive simulation approaches such as Monte Carlo simulation. The expense of simulation approaches increases significantly with lower levels of probability and larger network size. Some analyses use simplified component models, (e.g., HAZUS bridge fragilities). Others use simplified approaches to model the network response assuming statistical independence among component failures. Many full network time-variant analyses use oversimplified networks or are too computationally expensive. While the simplified models are computationally efficient, they may fail to realistically represent the infrastructure network.

This research aims to develop an analysis methodology for assessing network connection reliability that is realistic, time varying, computationally efficient, scalable, and non-simulation based. Realism is addressed by using real data to select and build time-variant component and network models. Such realism is absent from the majority of approaches used to address network resilience. The formulation of the network reliability analysis will allow system-level analysis with less iteration than sampling approaches. This work will also be the first time such flexible and accurate component models have been used in a non-simulation based approach. The multiscale approach used for this analysis will allow these methods to be used for large-scale infrastructure systems. This research will create a framework for practitioners to make risk-informed decisions that maximize network performance. This work is being done in collaboration with the University of Illinois Urbana-Champaign.

Summary of Accomplishments:

We developed an analysis methodology for assessing network connection reliability of infrastructure systems that are subject to deterioration and seismic hazards. This research addressed four key areas that were essential to the development of this methodology. First, we developed Bayesian inference-based techniques for updating infrastructure component information. This improves the accuracy and realism of the methodology by providing a mechanism for incorporating inspection data from the field. Second, we developed multiscale, clustering algorithms for assessing network connection reliability. These techniques allow larger networks to be analyzed, with less computational complexity than is possible with simulation-based approaches, such as Monte Carlo simulation. Third, we developed output metrics that make use of the hierarchical clusters identified by these algorithms. As the size of a network increases, it becomes increasingly difficult to assess the importance of individual components within that network. Group importance measures were developed to measure the importance of clusters of components at different levels of the hierarchy. These outputs were developed to help infrastructure managers develop maintenance and investment strategies, by identifying clusters of components and their associated importance. Finally, we extended these techniques to capture the effects of deterioration on network connection reliability. These techniques allow changes in component reliability, due to deterioration, to be used to understand how reliability of the system will change over time. They also provide output metrics that capture the time-varying nature of component and cluster importance. This allows for the development of infrastructure management strategies that incorporate the effects of deterioration. These research areas provide the necessary capabilities for performing efficient network connection reliability analysis on large-scale infrastructure systems that are subject to the effects of deterioration.

Significance:

Infrastructure reliability is critical to the national security of the US and the need for significant investment in aging infrastructure has been identified. This research provides several important capabilities for addressing this issue. First, the development of multiscale, clustering algorithms allow larger infrastructure systems to be analyzed than is possible with existing approaches. Second, the inclusion of deterioration improves the accuracy of analysis and allows the time-varying aspects of an infrastructure to be captured in the decision making process. Third, multiscale metrics facilitate the understanding of investment needs and the development of investments strategies for large infrastructures.

Refereed Communications:

H.-W. Lim, J. Song, and N. Kurtz, “Seismic Risk Assessment of Lifeline Networks using Clustering-Based Multi-Scale Approach,” to be published in *Earthquake Engineering and Structural Dynamics*.

N. Kurtz, and J. Song, “Cross-Entropy-Based Adaptive Importance Sampling using Gaussian Mixture,” *Structural Safety*, vol. 42, pp. 35-44, 2013.

Structural Health Monitoring for Impact Damage in Advanced Composite Structures using Virtual Sensor Grid

166149
Year 2 of 2
Principal Investigator: D. P. Roach

Project Purpose:

This ongoing research, which is in collaboration with Purdue University, is developing an in situ structural health monitoring (SHM) system for composite structures such as aircraft and wind-turbine blades by using a small number of passive and active transducers to identify impact loads and associated damage. Initially, a thorough review of the current state of the art was performed, initial simulations were carried out, further testing was planned, and proof of concept experimental tests were carried out and analyzed. By combining information regarding technical gaps in current technology with conclusions from prior Sandia efforts, we have found the needs that are not being fully met by existing technology and used these to focus ongoing research effort. In particular, we have found that thorough system integration between impact load and damage identification is currently not being implemented. To address this need for an integrated global impact load and damage identification system, we have tested the ability to identify impact locations and loads on a large structure (a wind-turbine blade) and developed methods to quantify the uncertainty associated with those load estimates. A damage identification technique, which uses an identified impact location to magnify the damage sensitivity, is being developed. Preliminary simulations showed the capability of this technique to increase the sensitivity to remote damage by over 40%. Initial experiments were consistent with simulation results, but more thorough and controlled testing is being planned to better assess the capability of this technique. Further system development will be guided by these test results, and a larger scale test will demonstrate the technology on a composite panel representative of current aircraft designs.

Summary of Accomplishments:

This work has developed structural impact identification technology by evolving a system that can detect the impact load location and magnitude in real time, while giving an assessment of the confidence in that estimate. Furthermore, we have identified ways by which impact damage could be more effectively identified by leveraging impact load identification information to better characterize the resulting damage.

The impact load identification algorithm was developed in this work by applying it to a commercial scale wind turbine blade and to bonded metallic plates that are representative of aircraft structures. Results from this study show the capability of detecting impact magnitude and location using a single accelerometer, regardless of sensor location. A technique for better evaluating the uncertainty of the impact estimates was developed by quantifying how well the impact force estimate meets the assumptions underlying the force estimation technique. This uncertainty quantification technique was found to reduce the 95% confidence interval by more than a factor of two for impact force estimates showing the least uncertainty.

Linear vibration based damage detection techniques were investigated in the context of structural stiffness reductions and impact damage. A method by which the sensitivity to damage could be increased for simple structures was presented and the challenges of applying that technique to a more complex structure were identified. The ability to detect damage through nonlinear dynamic characteristics was also determined, with a proposed technique that would leverage impact location estimates to enable the detection of impact damage. By further developing impact load identification technology and combining load and damage estimation techniques into an integrated solution, the challenges of deploying optimized composite structures can be effectively solved, thereby reducing costs, improving safety, and enhancing the operational readiness and availability of high value assets.

Significance:

Composite structures are increasing in prevalence throughout the aerospace, wind, defense, and transportation sectors, but the many advantages of these materials come with unique challenges, particularly in inspecting and repairing these structures. Because composites often experience subsurface damage which compromises the structure without clear visual indications, inspection of these components is critical to safely deploying composite replacements to traditionally metallic structures. Impact damage to large composite structures presents one of the most significant challenges. This work produced impact identification technology to enhance the ability to monitor the structural health of mission-critical composite structures.

Refereed Communications:

R.M. Bond, S.S. Underwood, D.E. Adams, and J.J. Cummins, "Structural Health Monitoring-Based Methodologies for Managing Uncertainty in Aircraft Structural Life Assessment," presented at the *International Workshop on Structural Health Monitoring*, Stanford, CA, 2013.

R.M. Bond and D.E. Adams, "Uncertainty in Impact Identification Applied to a Commercial Wind Turbine Blade," presented at the *Annual Conference of the Prognostics and Health Management Society*, New Orleans, LA, 2013.

C2R2: Compact Compound Recirculator/Recuperator for Renewable Energy and Energy Efficient Thermochemical Processing

170805
Year 2 of 3
Principal Investigator: I. Ermanoski

Project Purpose:

The purpose of this project is to develop and test a new type of heat exchanger, intended to recover heat between a hot and cold flow of packed particulate material. This will be achieved by demonstrating particle conveying between reaction volumes and heat exchange in a scalable package: the compact compound recirculator/recuperator (C2R2). To maximize productivity and the chances of success, key C2R2 features will be prototyped individually in order of increasing complexity.

While fluid to fluid and fluid to bulk heat exchangers are ubiquitous in today's world (from microelectronics to massive power plants), the challenging, yet promising field of heat exchange between packed particle beds remains almost entirely unexplored and undeveloped. Existing applications in need of this kind of heat exchange, such as cement manufacture, employ workarounds involving fluids to achieve satisfactory results. The need, however, has been steadily increasing in emerging technologies, such as solar coal and natural gas upgrade, solar thermochemical energy storage, water and CO_2 capture, or solar thermochemical fuel production, where workarounds would be difficult, if at all possible. These technologies will benefit significantly from the development of heat exchangers for packed particle beds. This critical need is especially well documented in the field of solar fuels.

Following the successful demonstration of "zero-profile" inlets, work was focused on designing, manufacturing, and testing specially shaped augers for vertical particle conveying that are compatible with heat exchange. In total, four geometries were tested extensively. Of these, two performed very well, one marginally, and one failed to meet requirements. The simpler and slightly better performing of the two successful geometries was chosen for final heat exchange tests. A second task was the design, build and test of a prototype-nested elevator, key to the compound design.

Development of High-Fidelity Models for Liquid Fuel Spray Atomization and Mixing Processes in Transportation and Energy Systems

170975
Year 2 of 3
Principal Investigator: R. N. Dahms

Project Purpose:

Significant inadequacies of current models for multiphase flows are a major barrier to rapid development of advanced high-efficiency low-emissions combustion devices. Liquid spray processes largely determine fuel-air mixture formation, which subsequently controls performance, emissions, and durability of a device. While substantial improvements in the design of advanced devices are possible, the processes are sensitive and require high levels of precision that can only be reached through development of advanced simulation capabilities. The present empirical understanding of sprays must be replaced by a new first-principles approach, and this need will only become more critical as requirements become more stringent. The objective of this research is to develop a first-principles approach in the context of high-fidelity large eddy simulation (LES). We propose to systematically develop a coupled system of advanced subgrid-scale models for LES aimed at treating liquid atomization and spray phenomena. Our primary focus will be on the stringent requirements of transportation, propulsion, and power devices. However, the models developed will have wide application to a variety of multiphase systems.

Predicting multiphase flow phenomena in modern liquid fueled combustion devices is widely recognized as a critical area of research for the design of advanced systems. These needs have been consistently highlighted over many years in a variety of industry, government, and academic forums. Needs and priority research directions emphasize the importance of establishing a basic science foundation for the development of advanced predictive models in this area. Developing such models requires a highly specialized effort that combines detailed theory, advanced simulation capabilities, and high-performance massively parallel computing.

Development of Quality Assessment Techniques for Large Eddy Simulation of Propulsion and Power Systems in Complex Geometries

170976
Year 2 of 3
Principal Investigator: G. Lacaze

Project Purpose:

Large eddy simulation (LES) is quickly becoming a method of choice for studying complex thermo-physics in a wide range of propulsion and power systems. It provides a means to study coupled turbulent combustion and flow processes in parameter spaces that are unattainable using direct numerical simulation (DNS), with a degree of fidelity that can be far more accurate than conventional engineering methods such as the Reynolds-Averaged Navier-Stokes (RANS) approximation. However, development of predictive LES is complicated by the interdependence of different subgrid-scale models, competition between modeling and numerical errors, model variability, and numerical implementation. Errors and ambiguities are multiplying, and control of accuracy has become a critical aspect in the development of predictive LES for design. When accuracy is not sufficient, results can be misleading and intractably erroneous due to factors such as poor numerics, poor grid quality, lack of appropriate spatial or temporal resolution, ill-posed boundary conditions, and inaccurate models.

The objective of this project is to create a comprehensive framework of metrics aimed at quantifying the quality and accuracy of state-of-the-art LES in a manner that addresses the myriad of competing interdependencies. The goal is to significantly increase confidence in the accuracy of a given solution while minimizing the time obtaining the solution. This goes well beyond the scope of isolated model development efforts and requires an integrated crosscutting approach. The planned approach will facilitate control of the tradeoffs between cost, accuracy, and uncertainties as a function of fidelity, models, and numerical methods employed. In a typical simulation cycle, only 20% of the computational time is actually usable. The rest is spent in case preparation, assessment, and validation. This approach will significantly improve this ratio by simultaneously reducing cost while increasing accuracy. Development of these metrics may have broad impact and significantly contribute to strengthening the role of high-fidelity simulations.

Quantifying Confidence in Complex Systems Models having Structural Uncertainties

170979
Year 2 of 3
Principal Investigator: C. S. Cooper

Project Purpose:

The primary challenge of this research was to identify principles and practices that lead to scientifically useful models. Too often as engineers, we focus on model-building details. Many of these details may not be truly important for furthering our understanding of the system the model is intended to represent. During the past 1.5 years, we have performed an in-depth inquiry into how to deal with model uncertainties and the theoretical limits of model predictivity. We have also highlighted the potential for multiple models to perform equally well (and thus be impossible to distinguish). This work has led us to identify and document several conceptual questions about models and the activity of modeling in general, which modelers must address. First, how well can models deal with potentially unknown external effects, even in principle? Second, how can disparate models which all fit observations be distinguished? What is required to have confidence in the projections of models outside of problem regimes we already understand well? The difficulty with such research is the tendency to become involved in the engineering details of a particular model or complex system, rather than establishing the usefulness and purpose of modeling itself. We have thus been able to address questions of model uncertainties, uniqueness, and predictivity within a controlled framework.

Summary of Accomplishments:

We have examined two aspects of structural uncertainties in models. First, we have explored in depth the theoretical limits of the predictivity of models. We have submitted a detailed report concluding that projections of models outside of the domain in which they are well tested is a very risky undertaking but is feasible for certain types of systems after rigorous validation processes. This is primarily a fresh discussion about sound modeling and validation practices in the face of deep uncertainties about possible external effects, as well as difficulties in establishing model uniqueness, both in practice and in principle. The discussion highlights the usefulness of models and the role of modeling as a part of the scientific method, despite the technical difficulties associated with constructing models and the uncertainties inherent in their predictions. It represents an incremental but nevertheless important advance in the theory of modeling uncertainties. Second, we investigated the differences between discrete and continuous modeling paradigms as applied to poorly understood systems, such as ecology, for which the underlying interactions may be unclear. For this effort, we developed software tools to integrate (and visualize the results of) discrete and differential equation sets for commonly used ecology models, such as the logistic equations and Lotka-Volterra. We have, furthermore, developed a formal framework to pose discrete-time models in a differential way with the goal of improving accuracy.

Significance:

Sandia's national security mission is evolving to include the modern-day threats of terrorism, energy surety, disease, climate change, and political instability. These threats are dynamic, complex, diverse, and adaptive. Understanding them requires the ability to model highly complex, interconnected systems, which consistently defy prediction. The investigations we performed here address foundational questions of complex systems' modeling, such as estimation of uncertainties, structural defects in models, model uniqueness, and the potential impacts of unknowable external effects. These new analysis capabilities will assist Sandia in developing, validating, and verifying models of new, real-world complex-adaptive systems critical for national security.

Use of Slurries for Salt Caverns Abandonment

171525
Year 2 of 3
Principal Investigator: G. Bettin

Project Purpose:

Abandoned underground storage caverns and mines create significant safety and environmental risks. Such abandoned openings are prone to collapse and thus contamination of near-surface groundwater aquifers and structural damage to surface facilities. For example, currently a cavern collapse in Louisiana has required the excavation of the Bayou Corne community for nine months due to natural gas venting. Current approaches to risk are limited to watchful monitoring and installation of alarm systems. Actual mitigation to stop or limit collapse is currently only a dream.

Conceptually, an approach would be to refill the underground caverns or mines with buttressing material (a process called backfilling). Especially for caverns, backfilling is currently not technically feasible. But conceptually, if the technology existed to emplace backfill as large-scale slurries through cavern wells, then we can finally mitigate the collapse of abandoned caverns and mines. The largest scale slurries to date were used to move coal from the Hopi Reservation to a coal power station near Lake Mead. But for a cavern, we need a process to move 500 million gallons of suspended particulate through two 20-inch diameter wells.

State government, natural resource departments, and environmental departments are responsible for the long-term stewardship of abandoned caverns and mines. This project seeks to create the scientific and technical basis for large-scale slurry emplacement.

The Effect of Proppant Placement on Closure of Fractured Shale Gas Wells

173076
Year 1 of 3
Principal Investigator: M. D. Ingraham

Project Purpose:

This project was undertaken to further our understanding of the interaction of proppant used in hydraulic fracturing processes with fractured host rock. Production declines in hydraulically fractured shale gas wells are far higher than conventional wisdom predicts and gas yields are low. By better understanding the placement of proppant in fractures and the interaction of the proppant with the formation, it may be possible to develop more efficient proppant placement methodologies and reduce production declines from fractured wells. For the security of the US energy economy, it is critical that all energy resources are exploited to their fullest; therefore, it is necessary to improve production from wells that are accessing 15% of the estimated gas in place at best.

To achieve this goal, a science-based approach to understanding proppant flow and proppant-formation interaction has been undertaken. We are in the process of conducting unique laboratory scale fracture and proppant-injection experiments to determine the location and condition of proppant after injection. With the information gleaned from these tests, a series of state-of-the-art multiphysics computational models capable of dealing with the multiphase flow are being utilized to model the flow, particle transport, and fluid-solid interaction within the fractured rock. A novel multiscale approach linking particle-scale to continuum modeling will be undertaken, greatly advancing the computational modeling of proppant flow. By parameterizing the model with experimental data, it should then be possible to optimize the proppant-injection process and particle type/size to ensure maintenance of fracture permeability over longer durations. Knowledge gleaned from this approach will advance the potential to design effective, low-water-use, fracking techniques with environmentally friendly materials thereby enhancing gas production and yield.

The Role of Real-Time Decision Making in Grid Resilience

173078
Year 1 of 3
Principal Investigator: L. Burnham

Project Purpose:

The transformation of the nation's distribution grid from a centralized system with a one-way flow of electricity, to a decentralized system with a bidirectional flow of electricity and information, is made possible by a sophisticated communications overlay that sends data in real time from field sensors and other devices back to the control center. This flow of data brings greater automation and intelligence to the grid, allowing for the growth of renewables, electric vehicles, faster restoration times, etc., but the transformation also represents a growth in complexity and abstraction that directly impacts system operators, the bulk of whose experience is rooted in traditional grid operations.

The purpose of this project is to analyze the impact of grid modernization on distribution operators and to identify the technological changes that affect base performance, as measured by the number and/or duration of outages. This study draws on Sandia's extensive experience in analyzing human reliability in high-consequence environments and also on our team's ability to combine cognitive analysis with machine learning techniques to predict the likelihood of human error. The research under way involves three parts: 1) an applied cognitive task analysis to extract information about the mental demands and critical-thinking skills required for each key task related to grid operations, 2) a critical-decision assessment to understand operators' situational awareness and decision making in non-routine (e.g., outage, situations), and 3) the development of a computational risk-based model of control-room decision making that will identify points of weakness and the potential for cascading failure.

This path-breaking study, the first to combine a cognitive approach with a risk-based model, will lead not only to a better understanding of the human factors underlying grid resilience, but to the development of tools to improve operator performance.

Next-Generation Global Atmosphere Model

173079
Year 1 of 3
Principal Investigator: W. Spotz

Project Purpose:

The DOE-sponsored accelerated climate modeling for energy (ACME) program and its components, such as the community atmosphere model (CAM), are developed from code bases that are well over a decade old, and in some cases, several decades old. Porting them to current and future computing architectures, such as multicore or many-core processing nodes, is arduous and time consuming. Adapting them to new purposes, such as interfacing to human impacts models, is also difficult, as they were not designed to work with anything but the most basic uncertainty quantification (UQ) and optimization methods.

Advancing polar simulation capabilities and assessing US security impact risks by modeling human response at the regional level both depend upon higher resolution global models and UQ support. Efficient high-resolution simulations require performance portable algorithms, and the most effective UQ algorithms require embedded logic. Neither of these capabilities is provided by ACME, and both are best implemented from the ground up.

Through this project, we will prototype a new atmospheric dynamical core, suitable for inclusion in ACME that will address these shortcomings. We will unite our expertise with Trilinos and CAM to develop a next-generation atmosphere model that promotes machine portability, and is designed from the onset to support embedded UQ. In addition to these features, we will use modern software engineering techniques, flexible design, advanced libraries, and support for multiple discretizations.

If successful, we will demonstrate what is possible in a modern climate model and provide the groundwork for using such a model in a policy and decision support role for enabling the mitigation of, or adaptation to, climate change impacts.

An Advanced Decision Framework for Power Grid Resiliency

173090
Year 1 of 3
Principal Investigator: J. Watson

Project Purpose:

The national power grid is the foundational infrastructure upon which our economy, national defense, health care, emergency response, and standard of living rely. Grid resiliency is, therefore, imperative. Grid control systems must prepare for and adapt to changing conditions and withstand and recover rapidly from disruptions, whether caused by deliberate attacks, accidents, or naturally occurring threats. Two key factors drive our need to boost grid resilience: the increasing frequency and magnitude of natural disasters, and tighter linkages with other infrastructures (e.g., cyber) driven by grid modernization efforts.

Current performance metrics for power systems address reliability boundaries, but they neither quantify resiliency nor consider delivery failure consequences. Without guidance from rigorous metrics, grid operators are ill prepared to anticipate and operate through large-scale cascading failures and blackouts, and lack comprehensive analytical capabilities to support restoration. We will develop foundational grid resiliency metrics and leverage state-of-the-art simulation and decision analysis tools to devise a novel control system to support operate-through and recovery-from system contingencies.

This research is high-risk and high-reward, and develops the core metrics and technologies that can substantially inform resilient grid infrastructures. Resiliency metric development is a complex, iterative process involving multiple stakeholders, with disparate interests. Metric acceptance by stakeholders is key to success, requiring social, institutional, and technical analyses. The planned grid control system requires integration of state-of-the-art analytic techniques, including uncertainty quantification, predictive simulation, state estimation, optimization, and high performance computing.

Fractal-Like Materials Design with Optimized Radiative Properties for High-Efficiency Solar Energy Conversion

173092
Year 1 of 3
Principal Investigator: C. K. Ho

Project Purpose:

This work will develop fractal-like structures and designs at multiple scales (millimeters to meters) that will maximize solar absorption while minimizing heat loss. Through our background research on radiative properties of surfaces, we have identified that self-similar feature of fractal structures over a large topological dimensional range will provide an effective trapping mechanism for solar irradiation. In addition, synthesis and design of fractal-like structures will be tailored to reduce reflective losses, local view factors, and thermal emittance at multiple scales. Novel radial and star-like patterns at the macroscale have been shown to reduce radiative view factors by up to 70% and total heat loss by 50%. Incorporation of these hierarchical features and designs at multiple scales are expected to significantly increase thermal efficiencies of solar energy receivers and a broad range of thermal collection devices for sustainable, lower-cost, high-efficiency energy conversion.

Solving the Longstanding Problem of Thermal Management in LED Lighting

173093
Year 1 of 1
Principal Investigator: W. L. Staats, Jr.

Project Purpose:

Nearly 14% of electricity is currently used for lighting in the US; according to DOE projections, the widespread adoption of solid-state lighting (SSL) technology over the next decade would reduce this figure to 7%, saving the US $250 billion in energy costs (for comparison, the installed capacity of all wind and solar power in the US is 3.1% of total generation). But the final obstacle of thermal management currently prevents SSL technology from being cost competitive; market penetration for SSL is currently 1%. The planned research seeks to overcome this thermal management roadblock by using a novel variant of the Sandia Cooler (Sandia's Air Bearing Heat Exchanger technology).

In this embodiment, light emitting diodes (LEDs) are mounted directly to the rotating heat-sink-impeller of the Sandia Cooler. Previous funding enabled the development of the Sandia Cooler to the point where its feasibility and value became self-evident. We seek to prove the effectiveness of the rotary cooled SSL concept.

Summary of Accomplishments:

We developed an overall model for the rotary-cooled solid-state lighting (RCSSL) system that predicts the operating point of the LEDs and includes the effect of thermal management on LED performance. Initially, we used computational fluid dynamics (CFD) to predict the performance of a heat-sink-impeller design tailored to the heat load of the rotating LEDs. We constructed a test platform to validate the thermal resistance of the heat-sink-impeller (using a resistive heater in place of each LED and a transient thermal decay test), which we measured to be 0.09 C/W. Next, we performed a test with LEDs and confirmed that the LED junction temperature was ~50 °C while delivering 10,000 lumens at 105 lumens per watt.

In addition, we developed a rotary transformer and driver circuit capable of providing mechanical-contact-free electrical power to the rotating LEDs. The driver circuit has a unique H-bridge push-pull excitation (20-80 kHz) architecture that runs directly off unfiltered, rectified three-phase power and was designed to have extremely low-cost and low-component count. We conducted experiments and confirmed that the entire driver circuit and transformer combination has an efficiency of over 99%, while delivering over 100 W of power to the transformer secondary (viz. the LED load).

Finally, we demonstrated a unique benefit of the RCSSL architecture: direct white light synthesis through rotational color mixing. We built a prototype system that has a ring of LEDs arranged in a repeating pattern of red, green, and blue LEDs. When rotating at 1800 rpm, the array of color LEDs appears to be a ring of flicker-free white light. This demonstrates a simple and effective solution to the LED color-mixing problem and ensures that improvements in red and green LED technology can be used effectively in achieving high luminous efficacy area lighting.

Significance:

With the groundbreaking thermal performance of RCSSL, LEDs can be driven to full output without overheating, meaning that fewer LEDs can deliver a desired light output. This reduces upfront cost significantly and leads to greater market acceptance. Additionally, rotational color mixing allows future designs (with improved color LED technology) to achieve a ~25% increase in theoretical efficiency through elimination of phosphors inherent in white LEDs.

Proliferation of solid-state lighting addresses Sandia's energy and climate security missions. Office of Energy Efficiency and Renewable Energy expects that solid-state lighting could reduce domestic energy consumption by 300 TW-h annually (equivalent greenhouse gas emissions of 40 million cars).

The adoption of SSL represents a rare opportunity for significant energy savings, with consequences to energy and climate security that have a direct bearing on Sandia and DOE's missions. We believe that, in addition to expediting widespread adoption of SSL, this research could also stimulate the development of US-based SSL businesses.

Measurements and Modeling of Black Carbon Aerosols in the Arctic for Climate-Change Mitigation

173094
Year 1 of 3
Principal Investigator: H. A. Michelsen

Project Purpose:

Growing evidence suggests that black carbon (BC) particles contribute significantly to global climate change and are largely responsible for the enhanced warming of the Arctic (~twice that of the global rate). Because of the relatively short atmospheric lifetimes of particulates compared to CO_2 and the large radiative forcing of BC aerosols (~65% that of CO_2), BC reductions are being considered as a viable near-term climate-change mitigation approach. Assessing the effectiveness of such a strategy, however, will require better estimates of BC climate forcing, which are hampered by large uncertainties associated with a paucity of atmospheric observational constraints, particularly in the Arctic, and poorly represented BC physical and optical properties in climate models. This project aims to reduce the uncertainties of Arctic climate forcing of BC by combining Arctic field observations, laboratory experiments, and modeling. Specifically, we plan to: 1) deploy instrumentation to characterize the abundance of BC-containing aerosols in the Arctic, 2) combine laboratory experiments and modeling to improve the parameterizations of BC processes in current atmospheric chemistry and climate models, and 3) assess the improved parameterization on climate-forcing estimates for Arctic climate predictions.

This project embodies a unique combination of: 1) Arctic field-instrument deployment, which leverages Sandia's expertise in Arctic measurements and instrument development, 2) controlled laboratory experiments, which exploit Sandia's unique capabilities in BC particle diagnostics, and 3) detailed process modeling to investigate BC radiative properties and improve BC parameterizations in the state-of-the-art community earth system model (CESM), which includes the new spectral element community atmospheric model (CAM-SE) developed at Sandia. Risks include uncertainties in the performance of BC field instrumentation, deployment of instruments in extreme environments, and addressing the complexity of BC properties and implementing parameterizations in CESM. Impacts include resolving large discrepancies between modeled and measured atmospheric BC, leading to a new understanding of BC in the global and Arctic atmosphere.

Classifier-Guided Sampling for Complex Energy System Optimization

173494
Year 1 of 2
Principal Investigator: P. Backlund

Project Purpose:

Design and configuration of modern energy distribution systems are complex engineering problems. Integration of traditional fossil and renewable sources, unpredictable loads, and the inclusion of energy storage elements are only a few of the factors that contribute to the complexity of such problems. High-fidelity computer models of such systems are invaluable resources for accurate evaluation of system performance. However, computational expense limits their usefulness for optimization and decision space exploration, because prevalent optimization methods require numerous evaluations of the expensive model to identify acceptable solutions. The goal of this project is to leverage an emerging optimization paradigm known as classifier-guided sampling (CGS) to develop a novel optimization method that is capable of solving large, complex, computationally expensive, multi-objective optimization problems. CGS reduces expensive evaluations of high-fidelity models by using an inexpensive classifier to predict the qualitative performance of candidate solutions. Successful completion of this project will address current limitations of existing optimization methods and will drastically reduce the time required to solve complex energy infrastructure optimization problems.

Preliminary studies on small test problems have shown that CGS has great potential to solve computationally expensive optimization problems. However, significant mathematical developments are needed before CGS will be suitable for application to real-world optimization problems. Dedicated research efforts are needed to develop CGS into a robust algorithm that is a viable alternative to existing methods. The developments that result from this project will be validated by applying them to large-scale energy infrastructure problems, but the primary goal is to develop mathematical underpinnings that can be applied to a broad variety of problem domains.

Electrostatic Coating with Naked Copper Nanoparticles

173495
Year 1 of 3
Principal Investigator: T. J. Boyle

Project Purpose:

In collaboration with the University of Arizona, low-cost nanoinks for interconnect applications will be developed, focusing on nano-copper (Cu) inks. Current methodologies are of limited applicability to the development of flexible electronic devices, due to stress-induced delamination between conductive and insulating layers. Therefore, an alternative coating method that allows for conductive film formation on a variety of substrates is desirable, both as an alternative to conventional conductive thin-film processing as well as the emerging field of flexible electronic and photovoltaic devices. Physical vapor deposition methods are approaching their size limitation for performance in device fabrication. Other work focused on using aqueous solutions but necessitated complexing agents and polymers to prevent agglomeration. In conventional approaches, a metal catalyst is used that can be both expensive and increases the resistance of interconnect lines. An alternative approach to the formation of Cu thin films is electroless deposition (ELD).

The ELD process applies the use of colloid suspensions of metallic nanoparticles attracted to a substrate surface and allows for a number of bottom-up tailoring options to conductive pathway formation. The requirement for a rudimentary coating of metal nanoparticles (NPs) is hypothesized to be that the substrates maintain a partial-positive electrical surface charge. Nanophase particles offer feature resolution that is dependent on controllable physical properties, and their electrochemistry may be tailored to eliminate grain growth catalysts. The use of NPs over a bulk phase allows for the bottom-up creation of electric paths that conform to the local shifts in position of the underlying layer and are formed at moderate (<673K) temperature. ELD films may conduct current in low-thermal budget applications, where the substrate undergoes macroscopic flexing. The combination of the ELD process with flexible substrates is an innovative opportunity. The proposed research may lead to applications in flexible electronics, bottom-up device creation, and environmentally sustainable/ benign electronic device manufacture.

Predictive Engineering Tools for Novel Fuels

173664
Year 1 of 3
Principal Investigator: C. A. Taatjes

Project Purpose:

The development of advanced "next-generation" biofuels that can be efficiently obtained from lignocellulosic biomass may introduce fuels with different properties than traditional petroleum distillate fuels. These new fuels could be disruptive or they could be enabling for emerging clean efficient engine technologies. A key technology to implement cooperative evolution of fuel discovery and engine innovation is a rapid but reliable means to assess the performance characteristics of novel fuels based simply on their molecular structure. This project is in collaboration with University of California, Berkeley and will develop and expand predictive engineering models, employing artificial neural networks and predictive data analysis tools to infer quantitative structure-performance relationships. These relationships will serve as a first sorting tool for more detailed and fundamental structure activity investigations. In addition, the project will explore new high-efficiency engine concepts such as the argon power cycle, an ultra high efficiency diesel cycle using argon as the working fluid. This project will include engine analysis to determine its feasibility and scalability; the argon cycle could dramatically improve engine efficiency.

Understanding Photo-Induced Oxidation Mechanisms of Volatile Organic Compounds

176312
Year 1 of 3
Principal Investigator: D. L. Osborn

Project Purpose:

Understanding of the photo-induced oxidation mechanisms of volatile organic compounds (VOCs) in the troposphere is crucial to human health and well being. Atmospheric modeling relies on well-known oxidation mechanisms to interpret the changing global environment and assess the health risks associated with climate change. Oxidation of biogenic and anthropogenic VOCs leads to the formation of photochemical smog, yet insufficient data exists on the initial oxidation steps that occur in polluted and pristine environments. The purpose of this project is to address this deficiency with two approaches. The first uses pulsed-laser-photolysis near-infrared cavity ringdown spectroscopy to study the peroxy radicals formed by chlorine-initiated oxidation of isoprene. The second uses multiplexed photoionization mass spectrometry (MPIMS) coupled to the Lawrence Berkeley National Laboratory Advanced Light Source to understand the products formed by oxidation of hydrocarbons in the troposphere.

Our work, in collaboration with Caltech, studies the product branching in the reaction of acyl peroxy radicals with hydroperoxy radicals. Our goal is to understand this reaction, which is a potential missing source of atmospheric oxidants that would have important implications on our understanding of isoprene oxidation in tropical regions. Isoprene represents about one third of the hydrocarbons released into the atmosphere and can be important to the chemistry associated with air pollution. Atmospheric chemistry is spectacularly complex, involving reactive species at low concentrations, governed by reaction mechanisms that are, in many cases, poorly understood. This research seeks to discover reaction pathways in the oxidation of isoprene that either promote or are benign to the formation of photochemical smog. If successful, this innovation would place models of smog formation on a more sound scientific footing and increase fidelity of model predictions.

Low-Cost Solar Simulator Development for High-Flux Materials Testing and Accelerated Aging Studies

178921
Year 1 of 1
Principal Investigator: J. Yellowhair

Project Purpose:

In concentrating solar power applications, high temperatures (>700 °C) are required to achieve high power cycle efficiencies. Novel materials are being developed to absorb highly concentrated solar fluxes (10-100W/cm^2) while maintaining low heat losses. The extreme conditions in which these materials operate trigger specific aging mechanisms, which alter their performance, requiring aging tests. However, accelerated aging under high solar fluxes and well-controlled environments is difficult, time-consuming, and expensive using conventional outdoor solar furnaces, which are subject to weather fluctuations and use during daylight hours only. We propose to design a low-cost, indoor, high-flux solar simulator to be used in place of the sun. Ideally, it will allow day and night operation in the flux range of 10-100W/cm^2, with a cost of <\$10K. Different kinds of materials will be exposed to either constant or variable solar fluxes under controlled conditions to artificially accelerate aging. Characterization methods will then be used to assess their durability.

Several existing high-flux solar simulators (PSI in Switzerland, DLR in Germany, and University of Minnesota) are capable of reaching high fluxes (>100W/cm^2), but at significant costs (>\$100K) and limited functionality due to their large size and customized components. Massachusetts Institute of Technology built a solar simulator for less than \$15K, but their peak flux was less than 10W/cm^2 due to the use of poor concentrating reflectors. We propose to use high-intensity filaments with electroformed nickel-based silver elliptical reflectors to achieve higher concentrations. Our work will develop a ray-tracing model coupled with a unique optimization routine to maximize the concentration with consideration of the focal length and aim points of each reflector. A unique carousel-design for the sample holder will allow automated flux variation, thermal cycling, and high throughput of sample treatment. The development of a highly functional, low-cost, high-flux solar simulator will allow Sandia and other DOE research institutions to cost-effectively study and develop needed materials for concentrating solar power applications.

Summary of Accomplishments:

We designed a low-cost, flexible, indoor, high-flux solar simulator to be used in place of the sun. The cost was kept low by using commercial off-the-shelf (COTS) components. The solar simulator uses four high-intensity metal halide arc lamps (1800 watts) with four electro-formed nickel-based, silver-coated elliptical reflectors (32-inch inter-focal distance) to achieve high concentrations. The beams from the lamp-reflector systems will be overlapped at the reflector focus. Our work developed a ray-tracing model coupled with a unique optimization routine to maximize the concentration with consideration of the focal length and aim points of each reflector. Our models were validated with experimental results. For characterization studies, we integrated a single lamp with the reflector. After alignment of the lamp and reflector and taking safety precaution to mitigate risk hazards, we measured a peak irradiance of 34W/cm^2 and peak temperature of 1000 ºC, at the max output, at the focus of the reflector where the lamp output is highly concentrated. The single lamp characterization allowed us to predict the performance of the full four-lamp system. Since the lamp source is incoherent, we summed the irradiances from the four lamps. Assuming the performances of the four lamps are similar, we can achieve greater than 1200 kW/m^2 or 1200 suns equivalent.

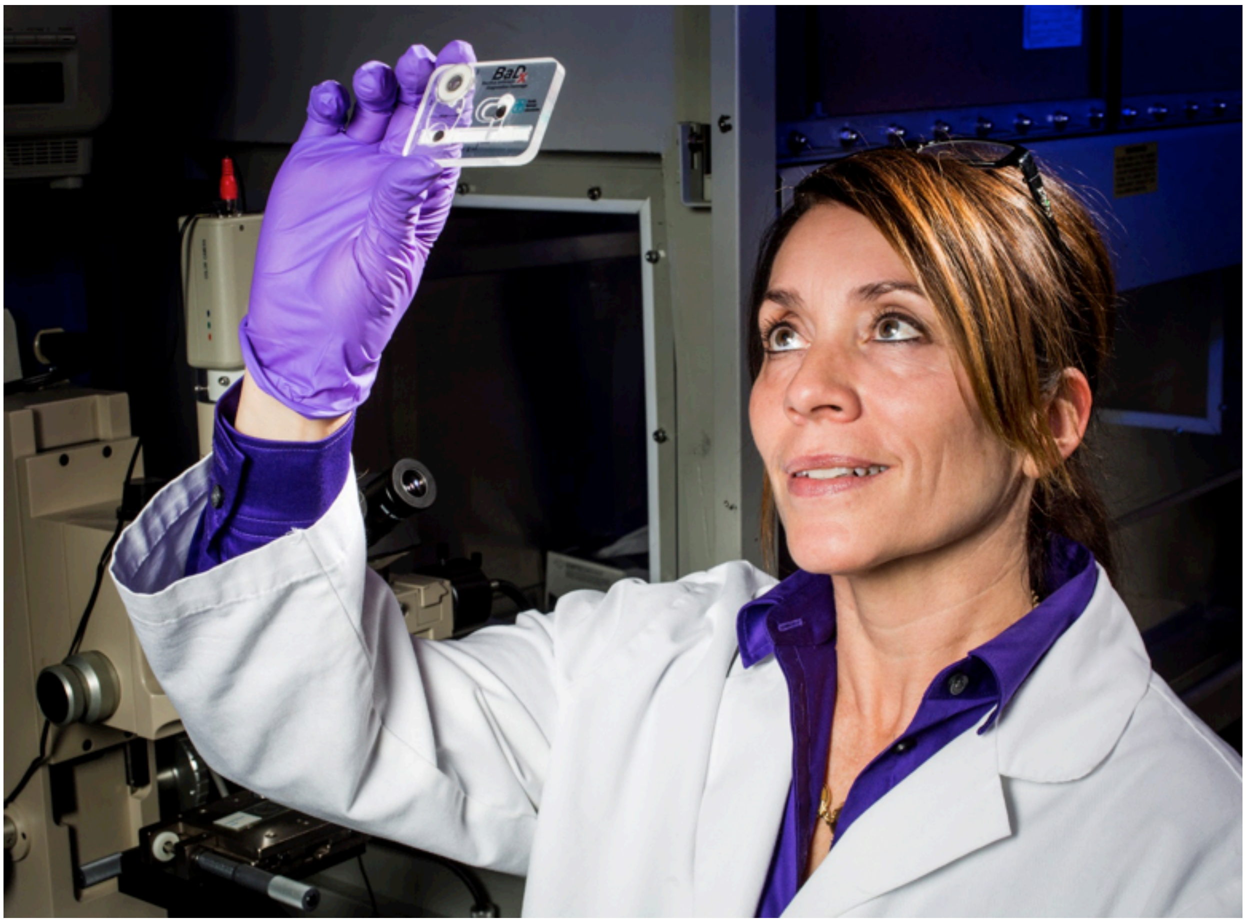
The solar simulator will allow day and night operation in the flux range of 10-100W/cm^2, with a cost of less than $15K. Upon completion of the solar simulator, different kinds of materials will be exposed to either constant or variable solar fluxes under controlled conditions to artificially accelerate aging. Characterization methods will then be used to assess their durability.

Significance:

The low-cost solar simulator can reach >1200 suns and >1000 ºC at the focus of the reflectors. Products from the solar simulator may potentially contribute to DOE's strategic plans for renewable energy and SunShot goals of reaching $0.06/kW-h. The solar simulator will be used to study materials used in high-temperature components for solar receivers. Assembled components (e.g., receivers) will also be tested. Going to higher temperatures may lead to improved efficiencies of the solar thermal power cycles in CSP systems. Cooperative research and development agreements (CRADAs) are being put in place to support CSP companies. The goal with this new test capability is to also increase opportunities for WFOs.

INTERNATIONAL, HOMELAND, AND NUCLEAR SECURITY

A vital US national security concern is that various adversaries who want to acquire power, support, and legitimacy are attracted to weapons based on nuclear, radiological, chemical, biological, cyber and explosives threats, or some combination of these threats. As the threat becomes more sophisticated and creative, we must identify effective solutions that mitigate current and future risks. We are seeking research that enables creative solutions in international and domestic risk reduction against these threats.



A portable diagnostic device for *Bacillus anthracis* detection in ultra-low resource environments developed at Sandia. The device does not require any power or extra equipment to store, operate or read; users need minimal training; and a built-in feature sterilizes the device after each use. (Project 158813)

INTERNATIONAL, HOMELAND, AND NUCLEAR SECURITY

Development of a Sustainable Anthrax Diagnostic Test for Countering the Biological Threat

158813
Year 3 of 3
Principal Investigator: M. Finley

Project Purpose:

Anthrax poses a significant threat to US national security as demonstrated by the 2001 terrorist attacks targeting the US Postal Service and Senate Hart Building. The causative agent, *Bacillus anthracis*, is ubiquitous, and more importantly, found in countries harboring terrorists. Anthrax outbreaks commonly occur in livestock, and consequently, the agent is routinely isolated, propagated, and maintained in laboratories by indigenous populations to diagnose the disease. This practice drastically increases laboratories' repositories of *B. anthracis*, and escalates the risk that the agent can be stolen for nefarious purposes. To mitigate this risk, we propose to develop a sensitive diagnostic assay that will significantly reduce the amount of *B. anthracis* maintained in laboratories. The assay will use the sensitivity and cost effectiveness of culture, without producing viable cultures; samples will be automatically decontaminated after testing is complete. The project is driven by Sandia's technologies for biodetection to address global critical issues in biological threat reduction and will develop a practical and deployable diagnostic assay that minimizes *B. anthracis* handling, isolation, propagation, and storage.

The goal of the proposed work is to develop a portable diagnostic device for *B. anthracis* for use in low-resource environments where the biological threat is elevated. In contrast to the relatively high expense and maintenance of currently available diagnostics, our proposed device will cost <$5 per assay (including a positive control for assay validation), will be operable by individuals with little technical training, and apply chemical and phage technology to sterilize the contents of the culture following detection assay — a critically important aspect to minimizing malfeasant use. Moreover, the self-contained device will combine microculture methods to amplify *B. anthracis* with plasmon coupling among metal nanoparticles for target detection, and not require any instrumentation/equipment.

Summary of Accomplishments:

We designed and created a self-contained and self-sterilizing diagnostic device to detect *B. anthracis* in low-resource environments, and at the same time, improve laboratory diagnostic methods and biosecurity. The credit card sized platform consists of a microculture chamber, a lateral flow assay, and a decontamination system. Because isolation and culture are the gold standard for diagnosis, the platform was designed around the microculture chamber optimized to support the isolation and growth of *B. anthracis*.

We developed a method of the synthesis and functionalization of gold nanoparticles for the selective detection of three virulence factors (protective antigen [PA], lethal factor [LF], edema factor [EF]) excreted by *B. anthracis*; gold nanoparticles were synthesized by the reduction of gold salt, and subsequently, functionalized with polyethylene glycol (PEG) monolayers to minimize nonspecific adsorption and covalently linked antibodies to the particles. We used enzyme-linked immunosorbant assay (ELISA) to characterize the time-dependent excretion of PA, LF, and EF in traditional as well as on-chip microculture; and demonstrated that culture conditions and competitive organisms may, in some cases, decrease the expression of these factors. We developed a lateral flow assay (LFA) that uses antibody-functionalized gold nanoparticles for the visual detection of PA and LF following microculture. This approach is advantageous as it detects antigens directly related to the pathogenicity of *B. anthracis*, rather than other commercial LFA strips that do not detect virulence factors.

We tested and optimized the use of dichloro-s-tranzinetrione (dichlor) as the included decontamination method. We modified the device to accommodate pressure increases that occurred with the mixing of media and dichlor, to ensure maintenance of the valve and closed system.

Significance:

The created diagnostic device has the potential to enhance US national security by promoting laboratory biosafety, reducing the opportunity for acquisition of *B. anthracis* from legitimate laboratories in low-resource environments, and enhancement of biosurveillance efforts to help characterize *B. anthracis* globally. The platform can be adapted to detect other pathogens, and as a result, could more broadly advance the fields of diagnostic medicine, biosurveillance, and biosecurity.

Refereed Communications:

J. Harper, M. Finley, B. Carson, G. Bachand, T.G. Edwards, W. Arndt, and J. Lovchik, "Portable Diagnostic Device for the Detection of *Bacillus Anthracis* in Ultra-Low Resource Environments," presented (invited) *Lab-on-a-Chip World Congress*, San Diego, CA, 2013.

J. Harper, M. Finley, B. Carson, G. Bachand, T.G. Edwards, W. Arndt, J. Lovchik, J. Murton, A. Carroll-Portillo, and B. Ricken, "Portable Diagnostic Device for the Detection of *Bacillus Anthracis* in Ultra-Low Resource Environments," presented (invited) *Gordon Research Conference*, Newport, RI, 2014.

J. Harper, M. Finley, B. Carson, G. Bachand, T.G. Edwards, W. Arndt, and J. Lovchik, "Portable Diagnostic Device for the Detection of *Bacillus Anthracis* in Ultra-Low Resource Environments," presented (invited) *Micro Total Analytical Systems (mTAS)*, San Antonio, TX, 2014.

J. Harper, M. Finley, B. Carson, G. Bachand, T.G. Edwards, W. Arndt, and J. Lovchik, "Portable Diagnostic Device for the Detection of *Bacillus Anthracis* in Ultra-Low Resource Environments," presented (invited) *Mátrafüred International Conference on Electrochemical Sensors*, Visegrád, Hungary, 2014.

J. Harper, T.G. Edwards, M. Finley, B. Carson, G. Bachand, J. Lovchik, and W. Arndt, "Portable Diagnostic Device for the Detection of *Bacillus Anthracis* in Ultra-Low Resource Environments," presented (invited) *PITTCON 2014 Conference & Expo*, Chicago, IL, 2014.

J. Harper, M. Finley, B. Carson, G. Bachand, T.G. Edwards, W. Arndt, and J. Lovchik, "Portable Diagnostic Device for the Detection of *Bacillus Anthracis* in Ultra-Low Resource Environments," presented (invited) *SPIE Chemical, Biological, Radiological, Nuclear, and Explosives (CBRNE) Sensing XV*, Baltimore, MD, 2014.

Advanced Diagnostic and Sample Preparation Platform for Early Threat Surveillance

158814
Year 3 of 3
Principal Investigator: S. Branda

Project Purpose:

Emerging infectious diseases present a profound threat to global health, economic development, and political stability, and therefore, represent a significant national security concern for the US. The increased prevalence of international travel and the increase in globalized trade further amplify this threat. The key to preventing an outbreak before it goes global is to establish a biosurveillance network that effectively reaches even the most remote regions and provides a network-integrated, location-appropriate, diagnostic capability. At present, the two main factors that prevent the extension of biosurveillance activities beyond centralized laboratory facilities are the lack of a deployable rapid-response diagnostic platform and a method to safely and consistently process infected samples in the field for analysis.

To minimize serious global outbreak events, modern surveillance requires both coordination and investment in infrastructure at the international level to enable rapid response to pathogens as they emerge. The first critical steps in the surveillance process (clinical observation, sample collection, and preliminary diagnosis) typically fall to first responders around the world. However, the facilities, technology, and protocols they use can vary widely depending on the available infrastructure, which complicates efforts for a globally coordinated biosurveillance scheme. This project proposes to address this identified capability gap by delivering an automated clinical sample processing platform integrating a universal sample collection and preparation protocol with a comprehensive diagnostic strategy. This will require: 1) the creation of a fieldable advanced diagnostic and sample preparation (ADSP) platform to safely and cost-effectively automate the extraction of pathogen nucleic acids (NA) from potentially infectious clinical samples for analysis, 2) the on-platform integration of a multiplex polymerase chain reaction (PCR) array for initial point-of-care diagnostic screening and the implementation of on-platform NA formatting for subsequent off-platform microarray or next generation sequencing analysis, and 3) the transfer of the ADSP technology to identified biosurveillance collaborators for testing and integration into real-world pathogen detection and surveillance workflows.

Summary of Accomplishments:

We first developed an end-to-end sample-processing pipeline (blood –> RNA –> cDNA ready for quantitative PCR [qPCR] and next-generation sequencing [NGS]), using bench scale manipulations potentially compatible with microscale implementation. This pipeline uses fresh human whole blood (25-100 µl, equivalent to fingerstick yields) as the starting material. Intermediate and end products were tested extensively for yield, quality, and purity.

Once this bench scale sample-processing pipeline was established and validated, we engineered three microfluidics-based modules individually capable of executing the key work units at microscale dimensions.

The first module isolates total RNA from whole blood. It depends upon a novel solution for interfacing large volume samples (here, 100 µl blood plus 280 µl RNA extraction reagents; in concept, >10 ml samples could be handled similarly) with digital microfluidics (DMF) devices. In essence, the large volume sample is continuously passed through a small volume droplet (here, 10 µl) located on the DMF device, and RNA-binding magnetic beads are used to recover the RNA into the small volume droplet.

The second module (the DMF device itself) further purifies the RNA and carries out first strand cDNA synthesis. An air-matrix DMF device is used for convenient integration with the first and third modules. This required a novel solution for managing evaporation of microscale droplets during heating steps (e.g., 95 ºC for 3 min).

The third module, a rotary-zone PCR (rzPCR) wheel, carries out second strand cDNA synthesis and PCR. This novel device uses low power, compatible with in-field operation (e.g., powered by a motorcycle battery).

We have experimentally verified that the output of each module meets the requirements for input into the next module, and have demonstrated end-to-end processing using the set of three modules, though with manual intervention at some transitions.

Significance:

Our first iteration system demonstrates a clear path forward for development of a fieldable sample preparation device to support rapid detection and characterization of pathogen containing clinical specimens in infectious disease hot zones. Such a device would greatly improve our capabilities in responding to disease outbreaks and conducting routine surveillance at sites of potential emergence, for protection of US interests. In developing our system, we achieved several technical breakthroughs that have advanced the biomedical and biotechnology fields. Our work has also cross-pollinated other microfluidics-based sample preparation efforts at Sandia (e.g., for applications in nuclear forensics and in-flight environmental monitoring for NASA).

Refereed Communications:

M.J. Jebrail, A. Sinha, S. Vellucci, R.F. Renzi, C. Ambriz, C. Gondhalekar, J.S. Schoeniger, K.D. Patel, and S.S. Branda, "A Novel World-to-Digital-Microfluidics Interface Enabling Extraction and Purification of RNA from Human Whole Blood," *Analytical Chemistry*, vol. 86, pp. 3856-3862, January 2014.

Multi-Target Camera Tracking, Hand-Off, and Display

158819
Year 3 of 3
Principal Investigator: R. J. Anderson

Project Purpose:

Central Alarm Station (CAS) alarm monitors can be overwhelmed by multiple simultaneous targets during emergency operations. For operators, the manual tracking of intruders takes focus and attention away from overall situational awareness (SA). By combining automated tracking algorithms that share target information across multiple cameras, we can simplify the human/machine interface and shift the cognitive focus from manual operation of the system to command and control. Rather than focusing on the cameras systems, which generate alarms per motion event within a single video image, our approach generates alarms per target. Active targets are displayed on a single coherent display system that links tracked intruders in a compound to the respective video feeds. Applications include fixed infrastructure sites and tactically deployed surveillance systems.

We have advanced a number of key component technologies and algorithms necessary for making multi-camera tracking of multiple intruders possible. This includes a precise and rapid image distance calculations using indexed color spaces, an in situ camera calibration technique using color laser scans, fast statistical template based tracking using graphical programming units (GPUs), and an advanced region of interest (ROI) method for segmenting and clustering targets. It has proven its ability to automatically isolate, identify, and track multiple targets simultaneously and in real time.

Summary of Accomplishments:

We developed a new system for multiple target tracking that is based on a number of software and algorithm innovations.

To overcome the problem of rapidly calibrating cameras in a 3D space, a new calibration scheme was developed that integrates 3D laser scanning equipment with video projections inside a game engine model.

To improve background segmentation for color cameras, a new indexed color table method was developed that combines precise metrics with rapid distance computations via table lookups. This indexed color scheme could also be adapted to remove sensitivities to shadows.

To reduce image size without distorting or blurring color information, we developed an image reduction technique that maintains color information. This method uses multiple copies of the sampled color to effectively represent color uncertainty along an edge.

In order to rapidly track dynamic human targets, a new sampled template method was developed and implemented. This method maintains multiple sampled representations of a moving target that can be used for dynamic real-time tracking and as an input for learning systems.

We developed a more sophisticated method for describing a targets' ROI, and then used this method to carve out target polyhedrons in a 3D space.

Finally, we integrated all of these component technologies into a system that can simultaneously communicate with multiple IP cameras, segment out the moving foreground targets, determine the location of these targets within the 3D space with respect to a model of the facility, and then display the results to an operator monitoring the site.

Significance:

The current approach to security systems for DOE has reached an impasse. Advanced IP cameras keep getting cheaper, but the cost to display, record, monitor, and respond to camera based alarms is too high. Adding more motion-detection cameras to a monitored sector will result in more alarms, and likely more confusion, workload, and cost. The work in this project provides a basis for changing this dynamic, providing a method that improves operator awareness while reducing costs. The technology has been implemented in indoor and outdoor test environments using commercial off-the-shelf video and computing hardware. It can readily be adapted to existing installations. This capability is relevant wherever cameras are being used for security, and rapid response is critical: subways, airports, DOE sites, etc.

Intrinsic Material Elements Seal

158821
Year 3 of 3
Principal Investigator: H. A. Smartt

Project Purpose:

Seals are widely used for identifying, securing, and monitoring items. They must be unique, non-counterfeitable, tamper indicating, robust, easily applied, and low cost. Unfortunately, US development efforts for seals ended in the 1990s — in spite of the emergence of new technical requirements such as compatibility with complex geometries, hostile environments, and remote interrogation. Currently, there is nothing in the global inventory of seals that adequately addresses all these needs. Presently, employed systems for reflective particle tags suffer from slow and cumbersome readouts and require mounting of the camera system on the item being verified. Using newer technologies, better seal designs, and readout options are possible. State-of-the-art cameras, modern image analysis, and new illumination approaches can be combined to produce a faster, user-friendly, noncontact readout system. This will allow more frequent verification, minimizing the time that inspectors spend in restricted or environmentally unfriendly locations.

We are developing a seal technology based on microscopic, randomly located, and oriented reflective elements that possess planar optical cavities that vary from particle to particle. Each particle's reflectance spectrum depends on its cavity parameters, the local orientation of the particle, and the incidence angle of the interrogating beam. Designed to be easily applied in a coating or paint, this seal will be compatible with flat surfaces as well as complex rough geometries. Interrogation of the seal will include illumination from multiple incidence angles, and will lead to features and images that can be analyzed using efficient image analysis algorithms.

Summary of Accomplishments:

We successfully designed, built, and tested a non-contact (approximately 10 cm from the seal) reader for reflective particle tags. There were two major components to this work: 1) design and development of an optics system that could supply sufficient illumination (in terms of brightness and uniformity) and acquisition of high-resolution images at a high frame rate (all while maintaining compactness), and 2) development of algorithms/code to align the reader with the tag in free space over multiple image acquisitions.

The optics system comprised three high-power LED illuminators mounted to a lightweight but rigid frame with handles. A high frame rate four-megapixel complementary metal-oxide semiconductor (CMOS) camera was mounted along the axis of the frame and focused at a location 10 cm below the ring (at the tag). After alignment of the optics system with the tag, the illuminators were sequentially strobed and nearly 100 full resolution frames were captured (illuminated from each of the three directions of the LEDs).

We performed testing of the registration/alignment system and it worked as described in the following example: an "inspector" manually centered the tag in the view of the camera — the code began locating focus measures and image features (features that would be used in the algorithm for alignment). The system would save the focus measures/image features and acquire images. The inspector would leave and return at a later time. The inspector repeated the process and, again, the system calculated focus measures and image features. This time, however, the system guided the inspector in alignment using on-screen fiducials. Once the inspector was within a defined range of tolerances, the system acquired images. The images would then be processed (using similar algorithms) to further determine if the tags match, although if the inspector were able to match the fiducials, confidence would be high that the tags match.

Significance:

The reflective particle tag (RPT) system is currently considered a robust, low-cost, hard-to-counterfeit passive tagging system for treaty verification/international safeguards applications. However, the current RPT system suffers from drawbacks that limit potential applications. These limitations can be overcome by the development of a non-contact handheld tag reader. Such a system would not require physical contact of the reader with the tagged item, be compatible with complex geometries, and minimize the time that inspectors spend in harsh or environmentally restricted locations. In addition, such a system could allow for automation in repetitive tasks. This research into new seal technologies directly supports any application requiring integrity of monitored items.

Modeling the Contents of Radiological Devices in Real Time

161869
Year 3 of 3
Principal Investigator: G. G. Thoreson

Project Purpose:

Modeling how radiation is emanated and transported through complex radiological sources has been limited to supercomputers in the past. This makes portable computing devices such as a laptop prohibitively slow in modeling 3D objects in reasonable time. This project's purpose was to discover new ways to approximate this solution quickly on a personal computer. Decreasing the computation time by orders of magnitude is an ambitious task. However, we have achieved this by applying existing radiation transport algorithms in new ways and precomputing data as much as possible. We can now compute results equivalent to a traditional 3D radiation transport approach thousands of times faster.

Summary of Accomplishments:

We have successfully completed two major milestones by implementing and testing two radiation transport techniques for the modeling of 3D radiological sources.

The first milestone of this project is the successful approximation of 3D photon scattering in the environment surrounding the source and radiation detector. Scattered photon radiation is computed via a Green's Functions approach. In this method, the transformation in energy, space, and direction of photons scattering from a surface is reduced to a set of stored transport kernels. The contribution of scattered photons from all the surfaces in the environment, such as a laboratory space, is integrated into the radiation detector. This requires less than a second on a personal computer. This method has been benchmarked against a wide range of experiments with good agreement.

The second major accomplishment is the development of the new method for 3D transport within the radiological object. A complex object is decomposed into a set of simpler geometries. The radiation transport is approximated as a series of 1D models to generate a volumetric source term for the entire object. This 3D source term is then ray-traced to the radiation detector. The entire process requires less than a minute of computation time on a personal computer. For many cases, the results of this new method match or exceed the accuracy of a traditional 3D transport code, thousands of times faster. This has revolutionized how we model complex sources and created new capability that can be applied to many new projects.

Significance:

This work can potentially benefit the mission of national radiological emergency responders, providing the ability to better model and analyze complex radiation sources on a personal computer and allowing them to make decisions quickly in scenarios where time is valuable. Furthermore, this new capability can be used to train and improve their skills by creating simulated data based on hypothetical radiological devices.

Compressive Sensing for Nuclear Security Applications

161870
Year 3 of 3
Principal Investigator: B. J. Gestner

Project Purpose:

Special nuclear material (SNM) detection has applications in nuclear material control, treaty verification, and national security. The neutron and gamma ray radiation signature of SNMs can be indirectly observed in scintillator materials, which fluoresce when exposed to this radiation. A photomultiplier tube (PMT) coupled to the scintillator material is often used to convert this weak fluorescence to an electrical output signal. The fluorescence produced by a neutron interaction event differs from that of a gamma ray interaction event, leading to a slightly different pulse in the PMT output signal. The ability to distinguish between these pulse types (i.e., pulse shape discrimination (PSD)), has enabled applications such as neutron spectroscopy, neutron scatter cameras, and dual-mode neutron/gamma ray imagers.

Realizations of these applications are based on conventional digitization of PMT output signals, followed by PSD and statistical processing. Given that currently these pulses are sampled at 200MHz-8GHz, an enormous amount of data must be processed in real-time or stored for off-line processing. Clearly, this approach is not feasible in a resource-constrained, remote-deployment setting, such as a wireless sensor network. Therefore, reduced-data sampling and processing techniques specifically for PSD must be developed.

Compressive sensing (CS) has emerged as a mathematical method for efficiently representing and reconstructing signals. There has been considerable work in this area at Sandia for radar applications, but compressive sensing has never been applied to PSD. This research is the first application of compressive sensing to radiation detection.

We will use compressive sensing to guide the development of novel mixed-signal hardware for PMT output signal acquisition. We will explore smart digitizers that extract sufficient information for PSD while requiring a considerably lower sample rate than conventional digitizers. Given that we will determine the feasibility of realizing these designs in custom low-power analog integrated circuits, this research will enable the incorporation of SNM detection into wireless sensor networks.

Summary of Accomplishments:

We first demonstrated that a hybrid analog/digital approach has the potential to reduce the cost of a radiation detection system in the areas of monetary cost, power consumption, and data storage requirements. Such a system would be initially triggered by a level-sensitive threshold circuit or a suitable computational fluid dynamics (CFD) circuit. Once triggered, the system would extract information in the analog circuit domain throughout the duration of the PMT output pulse. Rather than continuous digitization of the pulse signal, the resulting output of the analog circuit would be digitized only after the duration of the pulse passed. This fundamental difference is the key driver for the overall cost reduction of the potential system.

The compressive-sensing framework appeared to be a suitable technique for realizing this hybrid system. As a first step toward utilizing this framework, we explored sparse signal representations of PMT output signals. We discovered an efficient representation of these signals in the Discrete Haar Wavelet domain. We demonstrated that when a PMT output signal segment is transformed to the Discrete Haar Wavelet domain, the majority of the resulting wavelet coefficients have a magnitude close to zero. We then further demonstrated that only a small number of Discrete Haar Wavelet coefficients were required to reconstruct a PMT output signal that contained sufficient pulse energy, pulse location, and PSD information.

Encouraged by these results, we then developed and implemented a compressive-sensing framework based on representing PMT output signals in the Discrete Haar Wavelet domain. We found that while the compressive-sensing framework could be easily mapped to our originally proposed hybrid analog/digital acquisition system, the compressive samples did not contain sufficient PSD information. We did demonstrate, however, that a low number of compressive samples are sufficient to extract sufficient pulse energy and pulse location information.

Significance:

National and international security customers in both government and private sectors are continually seeking tools with new capabilities for detecting radiological threats. The effort in our research enables a new capability, remote distributed SNM detection, in addition to reducing the complexity of existing PMT-based radiation detectors. In the DOE Strategic Plan, this capability supports Goal 3 — enhance nuclear security through defense, nonproliferation, and environmental efforts. In the DHS Strategic Plan, this capability supports Goal 2 — protect our nation from dangerous goods. Clearly, a successful project outcome could uniquely position Sandia to address radiological threats at US borders and within the US.

Development and Field Testing of a Diagnostics Platform for Global Syndromic Disease Surveillance

165676
Year 2 of 3
Principal Investigator: M. Finley

Project Purpose:

Infectious disease epidemics continue to threaten the homeland and international security landscape. Global biosurveillance programs are critical for detecting and mitigating outbreak scenarios due to natural, emerging, or engineered biological threats. However, many agencies lack the infrastructure and resources to implement effective disease surveillance, particularly in low-resource settings. Public health and veterinary professionals lack the necessary skills to provide an accurate clinical diagnosis; therefore, many incidents of infection with high-consequence agents go undetected, and thus, unreported. New tools are urgently needed to meet the stringent operational and economic requirements for biosurveillance, including cost, speed, ease of use, field portability, and reliability. Furthermore, disease surveillance activities may be streamlined by shifting from traditional diagnosis to syndromic-based testing, in which the diagnostic tool screens for a panel of high-priority pathogens and diseases based on clinical symptoms.

We plan to meet these needs with the development of novel syndromic-based assays and an accompanying device based on Sandia's proprietary SpinDx diagnostic platform for global disease surveillance. The inherent advantages of our approach (low cost, ultra-sensitivity, easy to use, no sample preparation, broad assay menu, and a novel syndromic approach) differentiate us from other conventional biosurveillance methods. Another key advantage of our approach is that, rather than focus on particular pathogens, we will develop a syndrome-based screening allowing access to useful, actionable information faster. Field-portable assays for most of the diseases that we plan to target do not exist; hence, the first task will be to develop assays to diagnose a panel of high-priority zoonotic diseases. Disease of focus will be sudden death and hemorrhagic syndrome in cattle or gastro-respiratory in small ruminants. The assays will be developed in collaboration with the Veterinary Diagnostic Laboratory (VDL) and Biosecurity Research Institute (BRI) at Kansas State University. This work merges Sandia's expertise in point-of-care diagnostics and biosecurity in low-resource settings to uniquely address this need.

Processing Radiation Images behind an Information Barrier for Automatic Warhead Authentication

165679
Year 2 of 3
Principal Investigator: C. W. Wilson

Project Purpose:

The purpose of this project is to develop enabling technologies and options that could facilitate future arms control treaty negotiations. Future arms control treaties may not be possible without the ability to utilize nuclear measurements to count warheads on delivery systems and/or measure weapon signatures to verify nuclear weapon type or status. A consensus within the arms control verification community agrees that sophisticated radiation imaging, never before used in this environment, offers the ability to measure new types of signatures of treaty-limited nuclear weapon systems or components. However, to protect sensitive information, information barriers (IB) must be used with any imaging systems. Analysis of the images behind an IB is a complex task that must be performed reliably, without human assistance. The image processing problem is far more complex, and to date, no one has demonstrated a functional system for reliable image verification behind an IB.

New radiation imaging techniques, such as the Oak Ridge National Laboratory (ORNL)/Sandia's fast-neutron coded-aperture imager, and ORNL's neutron tomography system are just becoming available. The quality, characteristics, and measurable features available in the images they produce are still uncertain. While other techniques such as radiography imaging are mature, exploration of the image features available from any of these techniques is at a very early stage. Many new and advanced feature extraction algorithms have been developed but have not yet been applied to radiation images of nuclear weapons. The risks are high but the potential result is a game-changing advance in the way that arms control treaties are verified.

RGB+D for Biometrics and Physical Security

165681
Year 2 of 2
Principal Investigator: J. D. Bradley

Project Purpose:

Many existing and future critical physical security concerns will rely upon standoff biometric identification and tracking systems that are accurate, and logistically and economically feasible. Success in this area would transform multiple areas of physical security with a science- and research-based approach. Recent development of inexpensive (~$150) RGB+D (red, green, blue. and depth) sensors, such as the Microsoft Kinect has enabled research incorporating depth information into traditional data streams. These sensors, when combined with a suite of software tools, provide a game changing set of capabilities and inspire research concepts that were prohibitively difficult and expensive to pursue. We plan to develop algorithms and analysis tools, which unlock the unique new capabilities enabled by commercial off-the-shelf (COTS) RGB+D sensors within the arena of physical security. We will develop methods and algorithms which would facilitate:

- An inexpensive system for biometric identification using 3D gait analysis and kinematic template matching
- A system to detect the same person from multiple, geographically distributed, RGB+D sensors.
- A robust multi-modal interior volumetric sensor for physical security that significantly improves probability of detection and successful assessment at a much lower cost.

We propose to perform gait analysis and biometric identification using a model-based paradigm, driven by the RGB+D sensor data. We have not found anything in the literature to suggest this type of research has been done. Such an approach offers a number of advantages, namely, the ability to provide our research an idealized human skeletal model. We will explore which shape and motion elements of the model are most useful for biometric identification.

Summary of Accomplishments:

We prototyped a volumetric video motion detection system, which robustly alerted based on the presence of novel objects in its viewshed. The prototype optionally uploaded imagery and other information about the intrusion via HTTP to a web-server display.

We properly identified individuals, out of a population of 66, with 95% accuracy. We believe this result to be quite good in comparison to current video-based gait biometric studies. We investigated the sensitivity to differing footwear and found our system held to roughly 85% accuracy.

We prototyped a tracking system which could correlate observations of an individual based on body geometry and clothing colors over non-overlapping sensor viewsheds.

Significance:

Like most other biometric systems, our accuracy is insufficient to play the role of authentication or identification, but could be useful as an authentication layer, especially given its standoff nature. Categorizing people within multiple RGB+D streams based on their appearance, skeletal segment lengths, gait kinematics, and clothing would allow for automatic tracking of individuals throughout a facility. The prototyped volumetric video motion detection system could provide enhanced alarm capability. The individual tracking prototype could be used to index individuals for after-event review of video, or enforce two-person rules in high security areas.

Radiography Signature Science of Homemade Explosives

165682
Year 2 of 3
Principal Investigator: J. E. Parmeter

Project Purpose:

The purpose of this project is to determine x-ray radiographic properties for credible threat formulations of key families of homemade explosives (HME) (i.e., x-ray attenuation parameters that bound all credible threats). This is a critical national security issue based on the need to use x-ray radiography to detect explosives in aviation security applications. Credible threat formulations are those that are detonable and can be readily prepared by an adversary. In this project, characteristic x-ray radiographic (attenuation) properties of key types of HME, including both hydrogen peroxide (HP)/fuel and potassium chlorate (KC)/fuel formulations will be determined. These radiographic properties will also be compared to those of various benign materials in order to gauge the ease of discrimination using x-ray radiography; hence, the likely impact of nuisance alarms resulting from benign materials in screened baggage. The work performed includes a combination of experimental measurements and computational studies. Detailed characterization of x-ray source output and detector response has served as an important prerequisite to the experimental investigations of HME x-ray radiographic properties and constitutes an important part of the project. Development and documentation of safety procedures for working with small quantities of HME is also critical. Once data have been acquired, experimental and computational results can be compared and both experimental and computational techniques can be refined. The theoretical work will provide a better understanding of the experimental results, and if excellent agreement between theory and experiment can be demonstrated, additional calculations can be carried out to obtain x-ray radiographic properties of HME formulations. We do not have adequate time or funding to investigate these experimentally. Theoretical work involves not only the application of existing codes to compute x-ray attenuation parameters, but also the development of new mathematical methods and algorithms for improved extraction of these parameters from experimental data sets.

Distinguishing Bioengineering from Natural Emergence in Biothreat Genomes

165683
Year 2 of 3
Principal Investigator: K. P. Williams

Project Purpose:

Identification and characterization of engineered biological agents (EBAs) is an unsolved biosecurity challenge. Technical expertise required to generate EBAs with new gene combinations exists worldwide. Current EBA detection approaches target toolmarks of classical bioengineering (cloning vector sequences); however, advanced technology allows omission of such toolmarks. Further complicating EBA identification, novel pathogenicity gene combinations and contexts also arise naturally through horizontal gene transfer (HGT). Fortunately, biological limitations on HGT exist that enable discrimination between EBAs and HGT products. Three categories of genomic sequence information support EBA identification: 1) intrinsic gene properties (function, composition), 2) gene phylogeny, and 3) neighbor-gene context. Two aspects to our EBA identification plan are: ruling in genetic engineering by detecting its genomic signatures, and ruling out a possible natural origin of the organism by comparison with the gene context characteristics of naturally emerging genomes. Current nucleic acid-based assays (polymerase chain reaction [PCR], microarrays) yield limited intrinsic gene data and no gene context data; the anticipated increased use of high-throughput sequencing (HTS) for biodetection enables EBA identification methods that exploit gene content and context.

So that appropriate measures can be enacted in the event of an outbreak, this work will provide decision makers with tools yielding statistical evaluations of positive evidence of unnatural sequences and pathogenic potential (engineering rule-in), along with the probability that the organism emerged naturally (non-engineering rule-out).

EBA detection via the (omittable) toolmarks of bioengineering is unreliable. Our approach probes much more deeply into the feasibility of natural emergence of the disease-relevant gene combinations found in a query pathogen. The general approach to EBA detection will directly analyze content of pathogenicity genes and their phylogenetic and gene-neighbor contexts. This will yield a naturalness score (N) for a candidate EBA, parameterized through machine learning, and a confidence level derived by comparison with the distribution of N-scores for thousands of known non-engineered genomes.

Jam-Proof Wireless Communications

165685
Year 2 of 3
Principal Investigator: D. A. Perea

Project Purpose:

This project will perform fundamental R&D for a robust and secure distributed wireless networking technology. Wireless technologies are vulnerable to denial of service (DoS) or jamming attacks, and for this reason are not allowed at nuclear weapons sites to communicate sensor or imager information from security perimeters. A few seconds of disruption in communications could make the difference in high-consequence scenarios.

The project plans a solution through the combination of advanced physical layers, detection, and cognitive networking to produce a new form of "jam-proof" wireless communications that will meet high security needs. DOE and DoD policy currently impose the exclusion of wireless networking, even though policy does not yet exist that defines the "wireless threat." This is a testimony to the progressive ideas behind this concept. It is only a matter of time before DOE and DoD address the void/absence of a definition of the wireless threat that sites will be required to mitigate.

The technologies required to create a cognitive robust and secure networking topology that is scalable to many nodes and sensors requires research and development of cognitive network controllers that can act intelligently and autonomously, since the wireless threat environment is dynamic and unpredictable. The networked system requires advanced approaches in hardware/software actor-based frameworks to realize the many complex tasks of managing incoming intrusion detection data, and ensuring reliable communications of networked resources. It shall incorporate attack detection and triangulation as an active component of the cognitive network, providing real-time data and geo-location of possible threats and allowing specific action to be taken by the end user. Advanced physical layer technologies at Sandia will be enhanced to allow many types of phenomenology and network layers to work as one in an adversarial environment, allowing the network to mitigate multiple attacks while providing data on the attack to system users.

Using Electroencephalography (EEG) and other Methods to understand Domain-Specific Visual Search

165686
Year 2 of 3
Principal Investigator: A. Speed

Project Purpose:

Often, national security problems demand rapid decision making in uncertain, risky situations. In such circumstances, consequences of false positives and misses can both be significant, yet high-consequence decisions are often made using "instinct," or implicit processes, as much as explicit facts. Furthermore, how an expert analyst processes incoming information is as much a stimulus-driven process (i.e., bottom-up) as it is driven from past experience (top-down). In the first two years of this project, we attempted to identify experts making errors using EEG. However, due to large variability in accuracy between individuals, there was significant noise in the EEG data. Thus, it became clear that we needed to first understand the nature of this variability.

As there exist multiple populations of experts making similar decisions (e.g., Transportation Security Officers (TSOs), cyber analysts), understanding common characteristics across domains and understanding the blend between top-down and bottom-up processes influencing these risky, uncertain decisions provides significant advantage in selection and training of these experts. Numerous measures (e.g., eye tracking, reaction time) offer mechanisms for characterizing implicit processes (e.g., number of eye fixations can predict likelihood of error). We will test the hypotheses that experts across multiple similar domains share some common features and that factors influencing their decision making are regularly patterned. We will continue to work with TSOs and will collaborate with other projects (e.g., PANTHER) to test these hypotheses. If successful, we could significantly improve risky, ambiguous decision quality in numerous domains including transportation security, imagery analysis, and materials characterization.

Improved Pulse Shape Discrimination in a Multicomponent Water/Organic System

165687
Year 2 of 3
Principal Investigator: J. G. Cordaro

Project Purpose:

Active interrogation for sensitive nuclear materials (i.e., ^{235}U) and reactor monitoring for treaty verification are critical for the security of our nation. The development of organic-based scintillators, motivated by their intrinsic sensitivity to neutrons and particle discrimination (PSD) has proceeded rapidly based on this need. PSD, using liquid scintillators, finds widespread application for direct detection of fast neutrons, although these organic materials perform poorly in high radiation fields due to the pile-up of long-lifetime pulse tails. Development of new materials is needed for efficient PSD on short timescales.

We have been developing a water-based organic-inorganic scintillator for the improved discrimination of fast neutrons. Enhanced PSD will be achieved by selectively quenching the rate-limiting 'background' emission from the organic scintillator, and by comparing the ratio of fast organic (<10ns) to delayed inorganic (<60ns) luminosity. This combination will not only increase the maximum practical count rate for the material, but will also significantly improve PSD due to differences in the particle-specific luminescence response that are significantly larger than in current PSD materials. Based on known values, an organic scintillator and $CeCl_3$ combination is expected to show a 76% difference in the prompt versus delayed components — more than three times greater than what is observed for traditional organic scintillators alone.

If successful, this new system will show enhanced performance compared to current PSD organic scintillators. Organic and inorganic scintillators in an amphiphilic polymer matrix or hydrogel provide a low-cost and large-scale solid-state scintillator system that exhibits superior fast neutron discrimination capabilities.

Identification of Nucleic Acid Biomarkers of Infection in Blood

165767
Year 2 of 3
Principal Investigator: S. Branda

Project Purpose:

Infectious disease surveillance and outbreak mitigation require rapid, accurate, and reliable means of distinguishing infected vs. healthy individuals, to enable rational use of countermeasures (diagnostics, therapies, and quarantine). Screening populations based on direct detection of the causative pathogen can be problematic, because readily accessible specimens such as blood often contain little or no pathogen, particularly at pre-symptomatic stages of disease. However, host response to the pathogen is rapid, robust, and evident in blood throughout the course of infection. Thus, screening populations based on host response biomarkers in blood and other readily accessible specimens is an attractive approach, especially if the biomarkers are nucleic acids (NA), as these can be efficiently recovered from tiny specimens (e.g., fingerstick draws) and detected with tremendous sensitivity and specificity via polymerase chain reaction (PCR). Proof-of-concept studies have not been definitive, however, largely because use of sub-optimal sample preparation and detection technologies has precluded comparative analysis of specimens with sufficient sensitivity, specificity, and throughput.

Sandia has developed new methods and technologies for: 1) selective isolation of NA that are unique to, or shared between, specimens, and 2) highly efficient preparation of NA for second generation sequencing (SGS). We are using this sample preparation pipeline to carry out high-throughput, high-quality screens for both universal and pathogen-specific NA biomarkers of infection. Specimens from three different sources (human burn patients who become septic; human primary cells infected with biodefense-relevant pathogens, and rodent models of infection) are fractionated (e.g., DNA vs. RNA), and each NA pool converted into an SGS-compatible library. Molecular suppression of libraries preceding SGS enables identification of rare NA that segregate with infection state. Biological and statistical interactions between candidate biomarkers are identified through pattern recognition and network/pathway analyses. A predictive framework based on pathway activation signatures is generated via supervised classification methods. Through this systematic and comprehensive approach, we are identifying and verifying robust, predictive panels of NA biomarkers of infection.

Toward Interactive Scenario Analysis and Exploration: A Study on Simulation Technology Optimization and Scalability with Big-Data Analysis and their Applications

167008
Year 2 of 2
Principal Investigator: T. R. Gayle

Project Purpose:

Existing and future change will drive many national security solutions with need for a rapid tactical analysis response in ways that traditional modeling and simulation (M&S) cannot address. Issues around large data, computational requirements, delivery mechanisms, and deep analyst involvement are already challenging; any use in the field is not viable. While current solutions require hours to days to compute, rising expectations to address analysis with more depth and breadth for larger and complex scenarios will only increase difficulty. Some solutions using traditional high performance computing (HPC) have been considered, but progress is slow and tactical response is impractical. To overcome many of these challenges, we envision a next-generation computational paradigm for M&S that efficiently divides the computational and storage requirements while supporting the shuttling of results between field operators, back-end analysis, and data sources. By coupling innovations in M&S software with emerging advances in cloud computing, big-data methodologies, and existing HPC, we will provide an approach that is fast (seconds to minutes), offers unique delivery options, enables a degree of rapid analysis iteration not available today, and applicable to a variety of problems for DOE, DHS, and DoD. To allow a tractable scope and effort, we will focus on force-on-force and sensor analysis in physical security as driving application domains.

Our hope is that the results of this work drive innovations and applications across several domains. Along with innovations in the underlying M&S software technology, novel technical solutions are expected in the coupling of the simulation architecture with a cloud-like resource environment that should apply to related problem spaces. Analysts will be inspired and enabled by an approach that allows fast iterative feedback on complex scenarios, allowing for rapid, deep, and broad analysis results that can be delivered in numerous ways. This type of work could enable a new class of solutions for our most important national security challenges.

Summary of Accomplishments:

This study investigated the effectiveness of simplified “parallel multi-simulation” (i.e., running many possibly diverging “scenarios” at the same time) in 3D M&S applications. This study focused on building such a platform and then adapting existing M&S solutions and building novel applications to use it.

First, we designed and developed a generic “cloud” platform built on horizontally scalable (performance scales with the number of machines) open technologies for parallel multi-simulation. The “cloud” aspects, coupled with open technologies aimed to minimize the effort necessary to deploy and manage the platform while simultaneously ensuring it, is easy to use. Since each component was horizontally scalable, we can easily grow this “cloud” with minimal reconfiguration and achieve expected performance results. We demonstrated that it is easy to set up and capable of performing multi-simulation with different M&S tools simultaneously. As anticipated, we showed that performance of the system is limited either by available cloud resources or by the speed of the slowest scenario run.

This approach and its utility were highlighted through several applications based on the Umbra Simulation framework. A cloud-enabled “Dante Batch Manager” leverages the cloud for its tens to thousands of scenario runs. We show that this easily accelerates the compute processes required for analysis. Next, we integrated the cloud directly into the Dante Scenario Editor. This allows analysts or scenario designers to more immediately see results and potential outcomes, thus providing a novel way to explore and experiment with scenarios. Finally, we built a novel “pathways analysis” prototype tool that automatically explores a “space” of potential attack paths and uses the cloud to evaluate each path. The computation involved would be intractable and complicated without our parallel multi-simulation environment.

Significance:

The solutions developed apply to existing 3D M&S applications; results could ultimately benefit a number of mission goals across different agencies, particularly those related to physical security and requirements planning, emergency response, missions requiring response to rapid threat and situational changes, and asset protection. Furthermore, the developed applications provide additional ways to explore and experiment over a given scenario where it is otherwise unfeasible with existing tools. Finally, the platform can serve as a model for developing and deploying compute resources in an easy to use and scalable fashion.

High Fidelity Forward Model Development for Nuclear Reactor Spent Fuel Technical Nuclear Forensics

170995
Year 2 of 3
Principal Investigator: M. R. Sternat

Project Purpose:

Spent nuclear fuel (SNF) is an attractive material for a nuclear terrorism event, and with processing, reactor grade plutonium can be recovered from SNF. Nuclear forensics is a major pillar of nuclear security efforts to reduce the risks from this threat. One of the key requirements of a credible nuclear forensics capability is accurate and timely characterization of questioned material that is interdicted outside of regulatory control. In previous work, Oak Ridge ORIGEN (Oak Ridge Isotope Generator) model was utilized in a SNF forensics system to reconstruct reactor information from spent fuel characteristics. This basic forward model does not use any geometric or non-fuel material characteristics that may be recoverable from an interdicted item and relies on predefined cross-section libraries to predict Sandia characteristics. These libraries only exist for well-known power reactors and cannot accurately simulate research or other reactor types.

Utilizing previous work as a proof of concept, this project increases the accuracy of reconstruction of pre-irradiation characteristics from a spent fuel sample by developing and implementing a methodology for increasing the fidelity of the forward model within a forensic inverse analysis. The project focuses on two primary methods for higher fidelity forward models. The first involves developing new one-group collapsed cross-section libraries for reactors and the second involves implementation of a 2D/3D reactor depletion code as the forward model in the inverse analysis instead of the zero dimensional ORIGEN model.

This work is innovative and unique as it expands the boundaries of nuclear forensics science and establishes a predictive technique for SNF forensics. Creativity will be required to develop a practical predictive system, including the implementation of higher fidelity forward models that work with limited amount of information recoverable from an interdicted SNF sample.

Radar Detection of Personnel Obscured by Foliage

170996
Year 2 of 3
Principal Investigator: K. J. Pascoe

Project Purpose:

The purpose of the project is to create and demonstrate foliage-penetration radar for physical security, and to combine the radar with other sensors via a data fusion algorithm. This system will improve intruder detection and response force timeliness, thus increasing security at key facilities.

We conducted a study of radar clutter stability in ultra high frequency (UHF) band and L-band. This study involved both outdoor measurements and computer simulations to determine how much clutter varies over short time periods. The simulations used computational electromagnetic codes to provide the most realistic solutions to radar scattering from targets and clutter. Measured data included windy and non-windy conditions. Clutter was found to be sufficiently stable to allow the planned system to work effectively. Targets were visible in clutter at realistic ranges indicating that a useful system is possible.

We developed algorithms to convert data into usable form, transform and smooth it, remove clutter, detect targets present in the data, virtually steer a beam by manipulating data to get better azimuth resolution, combine radar data with other sensor data, and track targets. Development continues on some of the algorithms.

We designed the transmitter and receiver architecture for the demonstration radar unit and procured most of the components. Component assembly is under way.

We have started field test planning including test site selection, request for frequency allocation, and safety planning.

Combinatorial, Microscale Fuel/Oxidizer Formulations for the Systematic Determination of HME Properties

173105
Year 1 of 2
Principal Investigator: P. J. Hotchkiss

Project Purpose:

The countless combinations of precursors that can be used in homemade explosive (HME) formulations make them difficult to study. Conventional single-batch formulation is slow and hazardous and does not allow for adequate study of the properties that govern detection and identification; disconcerting given the rapidity with which new HME formulations appear. We plan to implement a combinatorial, microscale (<10 mg per sample) approach to studying emerging HME threats that increases speed and safety and reduces cost in their formulation and increases efficiency in analysis of their properties.

Current research on HMEs has focused on the explosive properties of the material to understand their effects and safety in handling, both of which require large amounts of material (grams to kilograms). Chemical and physical properties are not always studied. As such, the idea of formulation strictly for chemical and physical property determination has yet to be developed, though it is these properties that govern materials signatures that are available for detection and identification. In contrast to military explosives, which are well characterized, HMEs are used only for illicit purposes, thus much of this fundamental data is absent.

The ever-increasing use of HMEs in improvised explosive devices (IEDs) necessitates the development of rapid and definitive ways to characterize these materials. A combinatorial approach applied to HME formulations has not been tried and the overall approach would greatly enhance the way in which these materials are made and studied in the future.

The applications of the planned capability extend beyond counter-IED applications; this approach to rapid microscale energetic materials deposition would be highly beneficial in nuclear weapons development and stockpile surveillance activities by allowing for more efficient study of materials' aging and compatibility.

Decontamination of Radiological-Contaminated Materials using Magnetotactic Bacteria

173106
Year 1 of 2
Principal Investigator: M. D. Tucker

Project Purpose:

Decontamination of radiological-contaminated materials is a difficult task. Unlike toxic chemicals or biological organisms that can be neutralized or killed, radiological contaminants must be physically extracted from a material. This is especially difficult if the radionuclide particle has penetrated into porous materials such as concrete or limestone. Traditional approaches use chelating agents that chemically bind to the radionuclides. These methods have been largely unsuccessful because there is not an efficient method to extract the radionuclide/chelator from the subsurface. This leaves surface removal or surface scouring as the preferred option for decontamination, which is very expensive, labor intensive, and generates large volumes of hazardous waste. We are investigating a technology for radionuclide decontamination based on the use of magnetotactic bacteria (MTB). MTBs have the capability to bind to and/or adsorb radionuclides. After deployment of MTBs onto a material, the bound radionuclide can then be extracted from contaminated materials using separation techniques that utilize the magnetic properties of the bacteria. By reducing the need for removal of contaminated material surfaces, we could enhance our nation's resilience to a disruptive radiological dispersal device (RDD), an improvised nuclear device (IND), or an accidental release from a nuclear power plant (e.g., Fukushima). The study is designed to exploit the natural characteristics of MTB (i.e., magnetism, high specific surface area of reactive particles, and the ability to migrate toward a magnetic pole) as the basis for developing new technologies for sequestration/separation of radionuclides. The primary objective is to identify MTB cell surface functional groups and metabolic functions involved in the complexation of radionuclides. A secondary objective is to investigate magnetic separation techniques for retrieval of radionuclide-bearing MTB biocolloids from subsurface environments and building materials. This will be achieved by studying sorption properties of MTB with a contaminant highly relevant to the national security mission.

Tamper-Indicating Materials using Microvascular Networks

173107
Year 1 of 2
Principal Investigator: H. A. Smartt

Project Purpose:

We intend to research materials that provide an inspecting agent the ability to readily recognize that penetration into the material has been attempted without providing adversaries the ability to repair damage. Such material can significantly enhance the current capability for tamper-indicating technologies, used to support treaty verification regimes by maintaining continuity of knowledge regarding information or materials of concern. Many tamper-indicating technologies attempt to secure entry points of enclosures, and some attempts have been made at designing approaches for securing whole volumes; however, some challenges include: 1) enclosures are non-standard in size and shape, 2) enclosures are both host and facility owned, 3) it may be cost-prohibitive to secure entire enclosures, 4) tamper attempts must be detectable, 5) solutions must be robust, and 6) a technology may be found that can indicate penetration but it may be difficult to prevent adversaries from repairing that penetration. We will investigate several solutions including two types of dispersed microencapsulated liquid dyes that exhibit a ”turn-on” fluorescence response upon fracture of the encapsulated material, and a method based on electroless deposition of metal. These approaches are intended to address the stated challenges by allowing flexibility in application, creating materials that are low-cost, and providing a secure technology by working iteratively with Sandia’s vulnerability review team.

While we believe we can develop materials that generate a tamper-indicating response, it is challenging to scale and maintain a robust response in such a manner that adversaries cannot remove it. Sandia has particular expertise relevant in this area, from the development of tamper-indicating technologies to material science to vulnerability analysis.

We envision ultimate application for treaty verification regimes; however, these materials also are applicable in the commercial sector for general tamper-indication of various sized enclosures or objects (e.g., pharmaceuticals, cargo shipments, and food industry).

VMD Fused Radar (VFR) — The First Volumetric Ultra-Low NAR Sensor for Exterior Environments

173108
Year 1 of 2
Principal Investigator: J. L. Russell

Project Purpose:

Due to recent events at the Y-12 National Security Complex, the issue of excessive nuisance alarm rates (NAR) has surfaced as a major issue for high security sites. Sites can experience a high number of nuisance alarms per day. It is believed that DoD sites also experience elevated NAR because they use the same sensors. DHS has also suffered from excessive NAR, as demonstrated by the sensors deployed in the failed Southern Border Initiative. The purpose of this project is to create a new sensor system that will significantly reduce NAR in an outdoors environment, yet provide reliable detection.

Traditional sensors possess detection envelopes 1-6 feet wide and generate an alarm at a single point. The proposed solution will integrate volumetric sensors possessing detection envelopes as wide as a PIDAS (physical intrusion detection and assessment system), 30-130 feet wide. Video motion detection (VMD) and radar sensors have been selected for this effort, each capable of generating an “alarm-track” consisting of 5-100 alarm points within a PIDAS. Our belief is that analysis of many points will allow vastly superior discrimination between intruder and NAR sources, yet maintain reliable detection. If successful, we will create a highly reliable intrusion detection capability with an ultra-low nuisance alarm rate.

The most significant challenge in this effort is the creation of a reliable ultra-low NAR algorithm. One approach being considered is a Bayesian methodology that provides a mechanism where prior beliefs are converted into posterior beliefs when new data becomes available. This is ideally suited for analysis of “alarm-tracks” consisting of spatially and temporally correlated alarm points. A novel feature of the algorithm is a spatially applied “and”/“or” logic, exploiting the strengths of both “and”/“or” logic. Our goal is a maximum NAR of 1 every 10 days and at stretch goal of 1 every 100 days during all weather conditions, still meeting required detection performance.

Development of a Novel Nanoparticle Delivery Vehicle for Pre-Treatment with Nerve Agent Countermeasures

173110
Year 1 of 3
Principal Investigator: C. E. Ashley

Project Purpose:

Nanotechnology promises to revolutionize the prevention and treatment of organophosphorus (OP) nerve agent poisoning through encapsulation of OP scavengers and acetylcholinesterase (AChE) reactivators in nanoparticles that can improve their pharmacokinetics and enhance their efficacy. However, many existing nanoparticle delivery vehicles, including liposomes and polymerosomes, suffer from limited capacities, uncontrollable release profiles, and complex, specialized synthesis procedures that must be re-adapted for each new cargo molecule, leading to drug- and application-specific approaches. To address these limitations, we will develop mesoporous silica nanoparticle-supported lipid bilayers ('protocells') for encapsulation and controllable delivery of OP scavengers and AChE reactivators. In this effort, we will demonstrate that protocells can be loaded with high concentrations of OP scavengers and AChE reactivators, administered to mice via Sandia-developed polymer microneedles, and achieve either broad, systemic distribution or targeted accumulation within the central nervous system in order to prevent or reverse effects of poisoning by the OP nerve agent simulant, paraoxon. Importantly, we will also demonstrate that protocells administered prophylactically (i.e., in advance of paraoxon exposure) confer protection against OP nerve agents, a result that has not yet been achieved due to the poor inherent pharmacokinetics of nerve agent countermeasures and the inability of existing nanoparticle delivery vehicles to stably encapsulate or controllably release cargo molecules.

No existing nanoparticle delivery vehicle has demonstrated prophylactic efficacy, primarily due to uncontrollable biodistribution and biodegradation. In contrast, we have designed protocells to be highly modular, which enables us to independently control loading capacities, release rates, biodistribution, and biodegradation. This effort will have an immediate high impact by conclusively demonstrating that nanoparticles can alter the innate pharmacokinetics of a therapeutic molecule, thereby enabling prophylactic administration or extended therapeutic applications. The project will also further develop Sandia's polymer microneedles as an alternative to intravenous injection that avoids the need for skilled medical personnel and limits the generation of biohazardous materials.

Real-Time, Autonomous Field Surveillance for Vector-Borne Pathogens

173111
Year 1 of 3
Principal Investigator: R. Meagher

Project Purpose:

Mosquito-borne viruses (arboviruses) such as West Nile virus, dengue virus, and Rift Valley fever virus are among the most significant emerging (and re-emerging) pathogens worldwide. The recent spread of West Nile virus to the western hemisphere provides a striking example of how quickly a vector-borne disease can spread across borders and oceans, and become endemic across entire continents within a few years. Arboviruses represent an acute threat to military personnel stationed overseas, particularly in tropical regions, and they are also potential agents of bioterrorism, directed either against humans or economically important livestock. Vaccines and therapeutics are largely unavailable for these (primarily) RNA viruses, leaving vector surveillance and control as the only effective strategy for preventing or stopping arboviral disease outbreaks. Detection of arboviruses in adult mosquitoes can provide warning of an impending outbreak days or weeks prior to widespread transmission to humans or animals, but conventional vector surveillance is a low-throughput process dependent upon skilled labor and detailed laboratory analysis by trained entomologists. Novel approaches are required to improve the spatial and temporal resolution of vector surveillance to better combat the spread of vector-borne viral diseases.

We plan to develop and deploy a new generation of rugged yet inexpensive “smart traps” to perform autonomous field surveillance of arboviruses, with daily assays and wireless data reporting. Our approach represents a revolutionary advance in vector surveillance, which presently relies upon skilled labor and minimal technology for data collection. Long-term, our smart traps will reduce costs by reducing the labor bottleneck in vector surveillance, but to encourage adoption in the short term, the smart traps must be simple, reliable, accurate, and inexpensive to deploy. Creating a reliable, accurate device within these constraints requires creative new approaches to engineering autonomous systems, emphasizing simplicity of design in place of costly, complex components.

Online Mapping and Forecasting of Epidemics using Open-Source Indicators

173112
Year 1 of 3
Principal Investigator: J. Ray

Project Purpose:

Fast, dependable forecasting of disease activity can revolutionize medical planning and response. Collection of public health (PH) data, traditionally used for this purpose, is slow and thus not useful for effective response. Due to its voluntary nature, epidemiological reporting typically has irregular and incomplete spatial coverage. Thus, real-time mapping and forecasting of epidemiological activity is still not feasible.

Online, open-source indicators (OSI) of disease activity (e.g., disease-related searches, media reports etc.) and meteorology can serve as strong covariates and leading indicators of outbreaks. They are readily available, timely, and have far superior spatiotemporal resolution than PH data, especially in developing countries. Currently, there are no data assimilation (DA) methods that can fuse disparate datastreams to compensate for delayed/unavailable PH data, nor meteorology-driven disease models for accurate forecasting. We intend to develop the methods and models and integrate them into a DA framework. Such a framework would be invaluable for disease tracking in the US and globally.

Our key hypothesis is that OSI are sufficiently rich to calibrate a high-resolution spatial representation of disease activity, modeled on weather patterns. Within the DA framework, the spatial model will interpolate sparse disease data. OSI are noisy datastreams, and the spatial model will allow noise suppression by pooling of information across monitored sites (generally large cities). The spatial model, along with the meteorology-driven disease model, will allow OSI-calibrated forecasts in regions outside OSI coverage. Scalable ensemble Kalman filters will provide the mathematical underpinnings of data fusion so that the framework can be applied to country-sized problems.

The game-changing potential of data assimilation has not been applied to disease forecasting because it has relied on sparse PH data. OSI, and our data assimilation framework, would be a novel development with impact in data-poor regions. We will demonstrate this by tracking the evolution of the annual dengue outbreak in India using OSI data from HealthMap.

Single-Volume Neutron Scatter Camera for High-Efficiency Neutron Imaging and Source Characterization

173113
Year 1 of 3
Principal Investigator: E. Brubaker

Project Purpose:

The neutron scatter camera (NSC), an imaging spectrometer for fission energy neutrons, is an established and proven detector for nuclear security applications such as weak source detection of special nuclear material (SNM), arms control treaty verification, and emergency response. Relative to competing technologies such as coded aperture imaging, time-encoded imaging, neutron time projection chamber, and various thermal neutron imagers, the NSC provides excellent event-by-event directional information for signal/background discrimination, reasonable imaging resolution, and good energy resolution. Its primary drawback is very low detection efficiency due to the requirement for neutron elastic scatters in two detector cells. We will develop a single-volume double-scatter neutron imager, in which both neutron scatters can occur in the same large active volume. If successful, the efficiency will be dramatically increased over the current NSC cell-based geometry. If the detection efficiency approaches that of coded aperture imaging, for instance, the other inherent advantages of double-scatter imaging would make it the most attractive fast neutron detector for a wide range of security applications.

The key technical hurdle for this concept to be successful is the ability to resolve two proton recoils in a single scintillator volume at spatial and temporal separations of order 1 cm and 1 ns, respectively, via the scintillation light isotropically emitted from the two interaction points. This central task would not be possible using traditional photomultiplier tubes, but recent advances in photodetection technology have made it conceivable. With photodetector timing resolution of 10-100 ps, and ~1 mm spatial resolution in two dimensions, we will reconstruct the wavefront of optical photons emitted in the prompt part of the scintillation pulse. This will present significant technical challenges, especially when resolving nearby scatter events, but no fundamental arguments preclude its success. A calculation of the achievable improvement in effective area is at least an order of magnitude. The detector footprint will also be greatly reduced.

A Complex Systems Approach to More Resilient Multi-Layered Security Systems

173114
Year 1 of 3
Principal Investigator: K. L. Adair

Project Purpose:

In July 2012, protestors cut through security fences and reached the exterior of the Highly Enriched Uranium Materials Facility at the Y-12 National Security Complex. This identified an issue with what was believed to be a highly reliable, layered security system. The configuration of layered security measures is at the center of efforts to protect a range of systems from high-value facilities to large-scale infrastructures.

Historically, analyses of security systems have been performed using directed graph and path analysis tools like adversary sequence diagrams. However, there are many dimensions in the design space of a security system, including selection of technologies, alternative locations/configurations, different threats, and competing cost limitations. The dimensionality of this problem makes it effectively impossible to evaluate all permutations of potential system architectures. The experience of the individuals configuring the system drives the careful examination of a small subset of architectures.

The key goal of this project is the creation of a consistent, robust mathematical framework using complex systems analysis algorithms and techniques to better understand the emergent behavior, vulnerabilities, and resiliency of layered security systems subject to budget constraints and competing security priorities. Because there are several dimensions to security system performance and a range of attacks that might occur, the framework must be multi-objective for a performance frontier to be estimated. Since security measures can fail for a range of reasons, this research will also explicitly include resiliency as a dimension of system performance.

The innovation is in modeling a multi-layered security system as a complex system and the integration of what are likely multiple dynamic and stochastic algorithms to represent each element of the problem, including an optimization model to suggest optimal security architectures. Hence, this project will develop a rigorous mathematical/computational framework, sufficiently flexible to be appropriate to a wide range of layered security system design instances, including complex system behaviors like emergence and resiliency.

Denial of Use of Bulk Chemical Agents and their Precursors

173115
Year 1 of 2
Principal Investigator: M. K. Kinnan

Project Purpose:

Rapid bulk neutralization and/or the ability to rapidly render at-risk stockpiles unusable and/or safe for transport elsewhere are high-priority, high-visibility needs. Past and present research projects have focused their efforts on the surface decontamination of chemicals of interest (COIs) leaving a gap when it comes to bulk neutralization. Current technologies for bulk neutralization of COIs require heavy equipment and/or significant quantities of materials resulting in major logistical burdens. This includes incineration, the explosive destruction system, and the field deployable hydrolysis system. The purpose of this research is to develop bulk neutralization technologies that are irreversible, rapidly deployable, broad spectrum, and solidify a variety of COIs.

This project is demonstrating effective neutralization/solidification of bulk COIs without the use of high quantities of materials. For example, batch reactor-based neutralization can require up to a 100:1 dilution ratio of solvent (e.g., water with bleach) to COI. That introduces logistical burdens due to the high quantity of neutralizing materials required that will inevitably generate a significant amount of waste. The chemical pathways used in this research have utilized small quantities of materials and no solvents. In this work, the neat (undiluted) COI solution is consumed during the neutralization, which inherently changes the properties of the solution that can alter the reaction performance. Other technical challenges include performing the reactions at room temperature with no mixing.

To date, we have demonstrated on selected COIs gelation from 15 minutes to seven days depending on the chemical pathway. Quantities of additives ranged from 5% to 31% by volume of the quantity of COI to neutralize.

3D Imaging with Structured Illumination for Advanced Security Applications

173492
Year 1 of 2
Principal Investigator: G. C. Birch

Project Purpose:

High value assets are typically secured via numerous sensing devices. A critical component of these security systems is a 2D camera that feeds visual information to a user in a command environment. These 2D camera devices have advanced in consumer markets such as casinos and banks. However, the needs of high value security devices have begun to drift away from the commercial direction of the current security camera companies. This drifting apart will present further challenges in the next decade as consumer technology becomes available that enables confusing, camouflaging targets, or disabling 2D security cameras, using simple components.

This research will develop a structured illumination, real 3D imaging device designed to function in outdoor environments. We will develop a new illumination system that projects an active structured intensity pattern with irradiance greater than that of natural sunlight over a narrow spectral band while maintaining eye safety. This system will take measured 3D point clouds and use algorithms developed in this research project to perform data fusion with 2D security cameras. This will reduce counter options for threats, and non-linearly increases the complexity of developing camouflage to defeat both devices simultaneously.

This project is the first known use of outdoor 3D imaging using structured illumination for target detection applications such as perimeter security. The outdoor environment poses many challenges for active 3D imaging systems. Developing this system will be a significant advancement for 3D imaging devices in security and open many opportunities in image processing, data fusion, and video software analytics.

The potential value of this project is great because it will solve numerous shortcomings in many physical security systems. It will deliver real-time 3D information that can reduce false alarms and nuisance alarms when coupled with traditional imagers, lay the groundwork for a 3D command environment, and significantly increase the difficulty of defeating the security system.

Deployable Molecular Assays for Biosurveillance

173661
Year 1 of 1
Principal Investigator: S. A. Langevin

Project Purpose:

Globalization has significantly altered the infectious disease landscape and increased the ability of human pathogens to cause epidemics in previously undocumented regions of the world. Integrated national disease surveillance programs are critical to monitor endemic infectious diseases and to detect the introduction of novel human pathogens into susceptible populations. There is a recognized international responsibility for all countries to track and characterize locally circulating human pathogens and inform global public health agencies when highly pathogenic microbial agents are causing significant disease to mitigate pandemics. However, countries that have the greatest human disease burden, mainly in tropical/subtropical geographic regions worldwide, lack the infrastructure and resources to implement effective disease surveillance systems. Novel pathogen detection tools and disease surveillance strategies are needed to strengthen existing biosurveillance infrastructures and improve homeland security against microbial threats domestically and abroad.

This work is aimed at designing pan-genome detection reagents to rapidly screen and identify viral pathogens at the genus level in a single reaction utilizing LAMP (loop-mediated isothermal amplification) polymerase chain reaction (PCR) technology. This work could ultimately aid in the need to strengthen domestic/international biosurveillance programs in the early detection and prevention of pathogenic viral outbreaks.

Summary of Accomplishments:

We compared culex mosquito RNA-Seq libraries with and without hydroxyapatite chromatography (HAC) normalization (HACN) to determine the viral sequence enrichment when utilizing this methodology. In all viral genomes analyzed (n=33), HACN treatment of the mosquito samples increased the raw number of reads that mapped to viruses and the overall mean coverage across each virus genome when compared to untreated mosquito RNA-Seq libraries generated with 3-5 times more sequence reads.

We evaluated the overall microbial composition of culex mosquito species collected from four distinct geographic locations (Coachella, Kern, Greater Los Angeles, and Sacramento, California). We determined sequence homology by blast, genome structure, and genome size for all the viral contigs generated using virominer. Known endemic California arboviruses such as West Nile virus, Culex flavivirus, Umatilla virus, Negev virus, Hart Park virus, and Culex pipiens pallens densovirus were found circulating in California culex mosquito populations. In addition, Nam Dinh virus, a member of the genus alphamesonivirus, previously isolated from Vietnam and China, was identified in California culex mosquitoes. No evidence of virus recombination events due to the de novo assembly were observed, the mapped sequences were evenly distributed across the viral contigs, and each virus genome had at least 10X sequence coverage (10X to 1000X range) for any given nucleotide position.

Significance:

Mosquito surveillance to monitor vector-borne pathogens circulating in geographically defined regions allows for rapid and targeted vector control measures to lower mosquito populations; therefore, minimizing the organism's epidemic/epizootic potential. The early detection and prevention of viral outbreaks in countries with high disease burden will mitigate the spread of disease strengthening our national security. This work potentially addresses objectives in the DHS Strategic Plan by enhancing our biodefense capabilities to prepare for, monitor, and promptly respond to intentional or accidental outbreaks of emerging infectious disease.

Advanced Imaging Algorithms for Radiation Imaging Systems

173669
Year 1 of 3
Principal Investigator: P. Marleau

Project Purpose:

The diversion of special nuclear material (SNM) is a central concern in nuclear security and safeguards communities. As such, radiation-imaging devices are desirable due to their ability to detect and localize radioactive sources. Because of their low natural background, difficulty to shield, and unique association with SNM, fast-neutron imaging provides a promising means for the detection of SNM. Several fast-neutron imaging systems are under development including the dual-particle imager being developed at the University of Michigan as well as the neutron scatter camera and coded aperture neutron imaging system being developed at Sandia.

A key feature to the success of these projects is the development and implementation of robust image reconstruction algorithms. To date, simple backprojection, match filtering, and maximum likelihood expectation maximization (MLEM) have been demonstrated. Backprojection can be implemented quickly but can suffer from poor resolution. MLEM is a statistically based, iterative reconstruction technique that can provide higher resolution at the cost of larger computation time. However, it is limited by its need for a priori knowledge of a system's response which may include attenuation and/or scattering from the environment; information not readily available prior to a measurement.

Depending on the application, radiation-imaging systems may be exposed to measurement scenarios that experience variability in source parameters such as distance, material distribution, energy spectrum and shielding. Improvements will be made to both simple backprojection and MLEM reconstruction techniques that will make imaging systems more robust to these various detection scenarios. Such improvements will include the development of algorithms capable of modifying a generalized MLEM system response matrix to more accurately model a specific measurement scenario. Once developed, these advanced image reconstruction algorithms will be applied to existing imaging systems and used as a basis for designing and optimizing novel imaging techniques. This work is in collaboration with the University of Michigan.

Building the Scientific Basis for Cyber Resilience of Critical Infrastructure

179224
Year 1 of 3
Principal Investigator: M. J. Hutchins

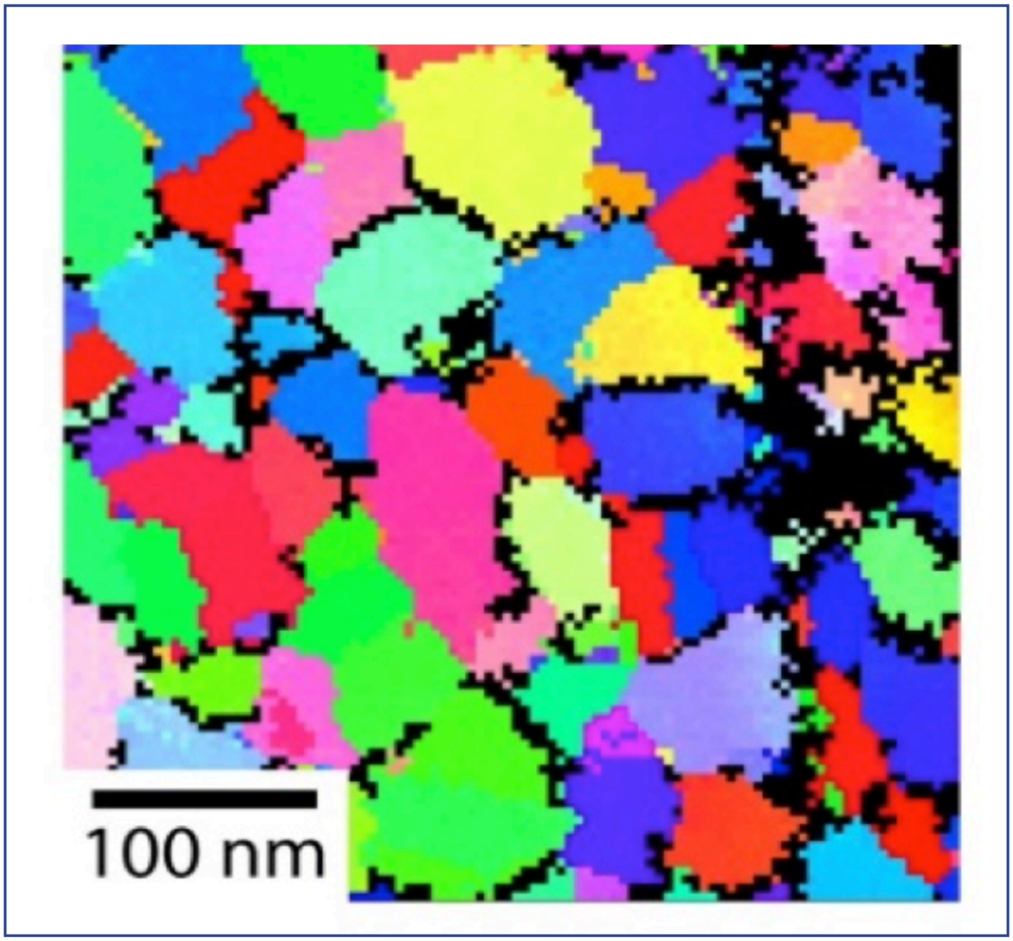
Project Purpose:

Through this research, we will develop new mathematically rigorous algorithms and models for quantifying, measuring, and increasing the cyber resilience of critical infrastructure. Vulnerabilities in the existing global digital information and communications infrastructure (i.e., "cyberspace") may be exploited by an adversary, which places critical US systems at risk (e.g., financial, energy, transportation, and security). The number of vulnerabilities is large and increasing in number, the attack surface is changing over time, and the problem combines technical and non-technical factors. Given this complex and dynamic landscape, mitigating risk is an important strategy. It is necessary to ensure that critical infrastructure is resilient, that is, able to efficiently reduce both the magnitude and duration of the deviation for targeted system performance levels.

Scientifically rigorous approaches to addressing cyber resilience are in the nascent stages; further research is required to develop the algorithms that accurately represent the full complexity of real world systems and threats. The goal of this project is to further the science for cyber resilience through design and modeling of critical infrastructure (CI). This effort will extend existing efforts, such as those put forth by NIST and Caralli et al., by researching and developing mathematical models and algorithms that facilitate the design of resilience enhancing countermeasures for specific CI (i.e., energy delivery systems). We will identify the operational and design factors that affect cyber resilience of CI, and create systems models that represent dynamic interplay between these factors and the cyber threats that CI face.

NUCLEAR WEAPONS

The primary goal of the Nuclear Weapons (NW) Investment Area is to support Sandia's strategic objective of excellence in our NW mission through investments in leading-edge science and the incubation of new technologies and capabilities. These investments are intended to promote exceptional innovation in our core products to meet future mission needs, to develop new tools and technologies for design, qualification and surveillance, and to nurture the seamless integration of science and engineering in all we do. They are also intended to enable risk-taking in innovation that may not be acceptable under a weapon development effort.



A scanning electron micrograph depicting the nanograin structure of an alloy designed to produce electrical contacts that are non-segregating, environmentally robust and wear resistant. (Project 158856)

NUCLEAR WEAPONS

Chemical Enhancement of Surface Kinetics in Hydrogen Storage Materials

158853
Year 3 of 3
Principal Investigator: D. Robinson

Project Purpose:

In much of the temperature range where palladium alloy powders store hydrogen, the rates of hydrogen uptake and release are limited by chemical reactions at the surface. A stable surface hydride forms that has an undesirably high barrier to transport into the bulk metal or back into the gas phase. To transport hydrogen more quickly than this allows, a hydrogen storage or separation system that uses palladium would require extra material, and/or higher pressure drops. Overcoming kinetic limits could thus improve cost, volume, and weight efficiency.

This project tested the hypothesis that enhanced kinetics can be achieved by destabilizing the surface hydride so it more closely matches the stability of the bulk hydride. Prior modeling by others has suggested that near-surface alloys — submonolayers of alloy elements at or just below the palladium surface — can cause the adsorbed states to be energetically equivalent to the bulk states, facilitating transport of hydrogen between them. We have a newly developed capability, electrochemical atomic layer deposition that allows us to make these surface alloys. We have extended our experience with film substrates, conformally applying layers of alloy elements to micrometer-scale palladium powders. Our hypothesis was tested through measurement of hydrogen isotope exchange rates.

Summary of Accomplishments:

We first performed electrochemical studies of planar films to develop atomic-layer deposition procedures and measure hydride kinetics. We created samples where the surface and bulk hydriding reactions give similar signals, varying film thickness to distinguish surface from bulk. We used scanning tunneling microscopy to verify film structure. Electrochemical measurements of hydriding kinetics showed that about one monolayer's worth of rhodium or platinum significantly improves reaction rates. Thicker layers are less beneficial.

We applied our understanding of films to invent two scalable methods for deposition on powders. One is electrochemical, where electrical contact is made to the sample, and deposition controlled by applied voltage. The other is electroless, where the deposition is chemically induced. Film structure was verified by electron microscopy and x-ray photoelectron spectrometry (XPS).

Through numerous hydrogen isotope exchange experiments, we discovered that the traditional cleaning procedure for such experiments as reported in the literature was inadequate. Through further XPS experiments, we identified that the traditional method removed surface oxide, but did not remove carbon. Electrochemical experiments informed us that several oxidation-reduction cycles effectively clean liquid-immersed electrodes. By performing similar cycles in the gas phase, we significantly reduced the XPS signal of carbon and improved isotope exchange rates of all of our samples, including unmodified palladium. Gas-phase experiments showed the same trends as the electrochemical experiments: about one monolayer's worth of rhodium or platinum significantly improves isotope exchange rates.

For a more quantitative understanding of our hypothesized link between surface-state thermodynamics and gas-to-bulk reaction kinetics, we numerically modeled the isotope exchange reaction, accounting for surface intermediates, as well as processes such as diffusion that could obfuscate kinetic measurements. We performed neutron-imaging experiments that reveal the isotope distribution within the solid as the reaction proceeds. These efforts added confidence that our exchange experiments are measuring meaningful kinetic information.

Significance:

This project has broken through a fundamental performance barrier in hydrogen storage and separation materials imposed by palladium surface chemistry. It has provided a material that performs reliably over a wide range of pressures, temperatures, and timescales. The new materials and methods are expected to be of value to diverse engineering applications related to hydrogen storage, separation, and energy conversion, as well as selective catalysis of hydrogenation or oxidation of organic materials.

Refereed Communications:

L.B. Sheridan, V.M. Yates, D.M. Benson, J.L. Stickney, and D.B. Robinson, "Hydrogen Sorption Properties of Bare and Rh-Modified Pd Nanofilms Grown via Surface-Limited Redox Replacement (SLRR) Reactions," *Electrochimica Acta*, vol. 28, pp. 400-405, May 2014.

P.J. Cappillino, J.D. Sugar, F. El Gabaly, T.Y. Cai, Z. Liu, J.L. Stickney, and D.B. Robinson, "Atomic-Layer Electroless Deposition: A Scalable Approach to Surface-Modified Metal Powders," *Langmuir*, vol. 30, pp. 4820-4829, April 2014.

M. Salloum, S.C. James, and D.B. Robinson, "Effects of Surface Thermodynamics on Hydrogen Isotope Exchange Kinetics in Palladium: Particle and Flow Models," *Chemical Engineering Science*, published online http://dx.doi.org/10.1016/j.ces.2014.09.001, September 2014.

Impact of Crystallization on Glass Ceramic to Metal Bonding

158855
Year 3 of 3
Principal Investigator: S. X. Dai

Project Purpose:

The purpose of this project is to develop a fundamental materials and process science basis that can subsequently be employed to pursue high performance and reliability glass-ceramic (GC) to metal seals in stockpile components. Dissection of these headers indicates weak or no bonding at the glass-steel interface. Examination of as-received GC pressed powder preforms revealed the existence of multiple crystalline phases. Early experiments indicated that the amorphous GC wet and bonded to SS well while pressed powder preforms (PPPs) with pre-existing crystalline phases did not.

A robust GC to metal seal must have: 1) a strong chemical bond between GC and metal and 2) a controlled coefficient of thermal expansion (CTE) match between GC and metal for long-term structural integrity. Recrystallizable GCs have been extensively studied and widely used for such sealing applications because of their controllable CTEs by process conditions. However, while it is well known that the precipitation of multiple crystalline phases in a recrystallizable GC substantially changes the chemistry of the residual glass, the effects of residual glass chemistry on the wetting and bonding at the GC/metal interface remains largely unexplored.

We studied the interface between the GC and the metal, and the effects of crystallization in the G-C on the bond strength. The study represents a major step forward from current knowledge on glass-metal seals that is predicted primarily on controlling the crystallization in the GC to achieve CTE match to the metal. The goals were to: 1) understand the interfacial reduction-oxidation (redox) process that is essential for a strong chemical bonding, 2) investigate the change of glass chemistry from crystallization and its effect on the redox process, and 3) explore paths that enhance the interfacial redox for improved glass-metal bond.

Summary of Accomplishments:

Oxides with lower Gibbs free energy than P_2O_5 in the Ellingham diagram were added to GC to study whether the dopants could be reduced over P_2O_5 for interfacial redox (reduction-oxidation), with Cr, Mn and Si being oxidized from the SS, in GC-SS seals. The modified GCs compositions include oxidants AgO, CuO, PbO, CoO, NiO, MoO_3, FeO, WO_3 and SnO. Wetting of GCs on SS were characterized by sessile drop test. GC-SS bonding was assessed on SS pins using a pin-GC-pin configuration. Cross sections of GC-SS were examined extensively by scanning electron microscope (SEM) and transmission electron microscope (TEM) to study the bonding oxide layer from the interfacial redox.

A comprehensive survey on the feasibility of forming bonding oxide layer via redox at the GC-SS interface was completed. Key findings are: 1) reducing atmosphere inside a graphite fixture competed with the intended GC-SS interfacial redox for the added oxidation agents in modified GCs, 2) for CuO-doped GCs, CuO was reduced at the GC surface rather than the GC-SS interface, and 3) for CoO-doped GCs, interfacial redox overtook the surface reduction and an interfacial bonding layer was established. However, the redox was limited by slow diffusion of Co^{++} ions in GC.

The reduction of surface CuO for CuO-modified GCs could be suppressed in favor of interfacial redox in a sealing atmosphere with trace oxygen. Strong bonding between GC-SS was established as an interfacial Cr_2O_3 layer emerged from the redox. The results could be used to form strong glass-ceramic to metal joints.

Significance:

The current project established a critical perspective on fundamental materials and process sciences on the interaction and chemistry at the GC to metal interfaces. The outcome can be employed to design, develop, and manufacture high performance and reliability GC to metal seals for mission critical devices and applications.

Synthesis of Wear-Resistant Electrical Contact Materials by Physical Vapor Deposition

158856
Year 3 of 3
Principal Investigator: S. V. Prasad

Project Purpose:

The major focus of the work will be on the development of gold (Au) nanocomposite films in the 0-2vol.% zinc oxide (ZnO) range, as these showed promise for electrical contact applications. Films will be subjected to accelerated aging followed by cross-sectional microscopy to assess their materials aging behavior relative to electroplated hard Au. We will also evaluate the electrical contact resistance (ECR)-friction behavior in self-mated contacts (i.e., with Neyoro G pins coated with Au-ZnO composite) to minimize diffusion of elements (most notably copper, Cu) from the pin to the coating. Subsurface microstructural and chemical changes induced by the combined action of friction and passage of current through the contact will be evaluated by electron backscatter diffraction (EBSD) and aberration-corrected transmission electron microscope (AC TEM) and automated expert spectral image analysis (AXIA). We will then perform nano-ECR measurements on wear surfaces to evaluate the mechanical and electrical response of near surface regions that would not be discernible by bulk measurements alone. We will continue the ion beam activities by optimizing the helium (He) implantation of Au as well as self-ion irradiation to develop a robust nanostructure without incorporating ceramic particles. Finally, we propose to develop analytical and finite element models of electrical contact resistance for thin composite and layered architectures comprising of conducting and ceramic pairs.

Summary of Accomplishments:

Notable accomplishments include the synthesis of Au-ZnO nanocomposite films by electron-beam evaporation (E-beam hard Au) and He ion-implantation of Au. Using the E-beam deposition system, Au-ZnO nanocomposite films with wide range compositions (from pure Au to 100% ZnO) were synthesized. Bulk electrical resistivity was shown to increase monotonically with increasing ZnO content, falling into three regimes of behavior associated primarily with: 1) grain boundary electron scattering due to grain refinement at ZnO volume fractions (vf) below 0.3; 2) percolation theory for ZnO volume fractions at and above the percolation threshold, vf = 0.85; and 3) a transition region between these where resistivity was influenced significantly by the formation of Au-Zn complexes. A model incorporating electron scattering and percolation theory describing the composition dependence of electrical resistivity was developed. Thermal annealing with in situ electrical resistivity measurements were used to glean information about dynamic grain growth and activation energy for grain boundary mobility. EBSD analysis revealed that a significant reduction in grain size can be achieved even at 0.1 vol. % ZnO. Sliding electrical contact resistance measurements with simultaneous friction data acquisition were made in regimes relevant to surety mechanism contacts using a spherically tipped Au-Cu alloy pin. Composites with 2 vol. % ZnO were found to have practically no measurable wear, offering potential alternatives to electroplated hard Au. We demonstrated that significant improvements to the tribological behavior of Au (i.e., reductions in friction coefficients from ~1.5 to ~0.5 and specific wear rates from ~$4x10^{-3}$ to ~$1x10^{-4}$ mm^3/N, without compromising the electrical contact resistance) can be achieved by He ion beam implantation. E-beam hard Au has been applied on engineering parts with complex geometries as a demonstration of the proof-of-concept of the technology. Two invention disclosures were filed.

Significance:

Electrical contacts in electromechanical devices for national security missions use electroplated hard gold. It is difficult to achieve reproducibility with electroplated hard gold coatings due to inconsistencies in preparation and aging of plating baths. Compounded by the rapidly shrinking supply due to stringent OSHA regulations on the use and disposal of toxic chemicals in electroplating baths, gold-ceramic nanocomposite coatings described here present a path toward a higher performance, higher reliability, and more ecologically conscious solution. This is the first practical engineering implementation of a nanocrystalline metal-matrix nanocomposite where grain boundaries are stabilized using highly dispersed ceramic particles rather than alloying.

Refereed Communications:

J.-E. Mogonye, K. Hattar, P.G. Kotula, T.W. Scharf, and S.V. Prasad, “He Implantation for Improved Tribological Performance in Au Electrical Contacts,” to be published in the *Journal of Materials Science*.

R.L. Schoeppner, D.F. Bahr, H. Jin, R.S. Goeke, N.R. Moody, and S.V. Prasad, “Wear Behavior of Au-ZnO Nanocomposite Films for Electrical Contacts,” *Journal of Materials Science*, vol. 49, pp. 6039-6047, 2014.

S.V. Prasad, “Nanostructured Materials for Solid Lubrication,” presented at the *European Symposium on Friction, Wear and Wear Protection*, Karlsruhe, Germany, 2014.

S.V. Prasad, “Friction Behavior of Nanocrystalline Metals,” presented at the *RF Mehl Medal Symposium on Frontiers in Nanostructured Materials and their Application*, San Diego, CA, 2014.

S.V. Prasad, “Tribology of Au-Nanocomposites for Sliding Electrical Contacts,” presented at the *Materials Science and Technology Conference and Exhibition*, Montreal, Canada, 2013.

Extension of Semiconductor Laser Diodes to New Wavelengths for Novel Applications

158857
Year 3 of 3
Principal Investigator: M. H. Crawford

Project Purpose:

Extension of laser diodes (LDs) to the deep ultraviolet (DUV) is, thus far, unrealized but would be a major technological breakthrough. Over the past decade, advances in AlGaN semiconductor alloys have led to the first DUV light-emitting diodes. However, demonstration of DUV LDs has been thwarted by a lack of fundamental insight and solutions to formidable AlGaN materials science challenges.

Our effort combines Sandia's state-of-the-art AlGaN growth and fabrication capabilities with advanced modeling to overcome these challenges. Innovative approaches to p-type doping include band structure engineering to dramatically reduce acceptor activation energies. Mitigating extended crystalline defects will involve Sandia's recently demonstrated patterned overgrowth process to promote defect annihilation. New insight into non-radiative, atomic-scale defects will be gained using deep-level optical spectroscopy, a technique mastered by few groups worldwide. Sandia-developed laser models will be used to guide AlGaN band structure engineering for maximizing material gain. Finally, LD development will include exploration of a novel laser architecture that has the potential to overcome long-standing challenges in AlGaN LD design.

Summary of Accomplishments:

This project focused on overcoming major materials roadblocks to achieving AlGaN-based deep-UV laser diodes. Notable progress was made in the development and optimization of novel reduced-defect-density AlGaN templates by applying overgrowth of submicron-patterned features in high-defect-density AlGaN/AlN/sapphire templates. We employed these templates in the growth of laser heterostructures and demonstrated optically pumped lasing at 346 nm with low thresholds of 50-200 kW/cm^2. A major accomplishment of this project was the further demonstration of ridge waveguide lasers with room-temperature pulsed-current lasing in the 352-356-nm region. We evaluated two distinct designs that explored trade-offs between carrier injection and optical loss. Both designs yielded lasing up to 60 ºC and had threshold current densities of ~21-25 kA/cm^2. Future efforts to improve device performance and further advance this technology were identified. In parallel, we performed numerous materials studies to advance higher-Al-content AlGaN alloys relevant to shorter wavelength UV laser diodes (< 280 nm). We identified open-core threading dislocations as the origin of current leakage that limited diode performance and discovered material growth conditions to mitigate such defects.

Significance:

The 352-nm laser diode demonstration is notable as few groups worldwide have demonstrated laser diodes in the < 360 nm UV region and commercial technology is presently limited to > 365 nm. Our success was enabled by advancing the state-of-the-art in reduced-defect AlGaN templates in addition to other AlGaN materials accomplishments. Extending laser diode technology to UV wavelengths has the potential to benefit numerous national security missions. Applications including fluorescence-based bioagent sensing and portable water purification systems would be enabled by robust semiconductor laser diodes in the UV and deep-UV region.

Refereed Communications:

M.E. Zvanut, W.R. Willoughby, U.R. Sunay, D.D. Koleske, A.A. Allerman, K. Wang, T. Araki, and Y. Nanishi, "The Effect of Growth Parameters on the Mg Acceptor in InGaN:Mg and AlGaN:Mg," *Physics Status Solid C*, vol. 11, pp. 594-597, April 2014.

M. Moseley, A.A. Allerman, M. Crawford, J.J. Wierer, Jr., M. Smith, and L. Biedermann, "Electrical Current Leakage and Open-Core Threading Dislocations in AlGaN-Based Deep Ultraviolet Light-Emitting Diodes," *Journal of Applied Phys*ics, vol. 116, p. 053104, August 2014.

Inherent Secure Communication using Lattice Based Waveform Design

161862
Year 3 of 3
Principal Investigator: M. O. Pugh

Project Purpose:

The wireless communication channel is susceptible to eavesdropping due to the broadcast nature of the electromagnetic medium. Traditional approaches to combat these insecurities have included encrypting the data via cryptographic methods, hiding the data in the noise floor as in wideband communications, or nulling the signal in the spatial direction of the adversary, using array-processing techniques.

Recent advances in signaling constellation design have shown that an additional level of security exists at the physical layer. By appropriately designing communication waveforms, the ability of an eavesdropper to correctly demodulate the intended secure signal can be hindered while maintaining successful communications with the desired receiver. This process increases the eavesdropper's bit error rate (BER) and inhibits successful decoding of the secure signal. This method has only been theoretically verified for simple point-to-point channels.

This research will target the design of secure communication waveforms in more complicated and realistic channels such as multipath (fading) channels and multiple antenna environments with multiple possible eavesdroppers. The effects of system constraints such as peak power consumption on the code design will also be researched.

The design of secure wireless channels has primarily focused on encryption, spread-spectrum and/or beam forming techniques. Achieving enhanced secrecy at the physical layer through the design of communication signals is orthogonal to these existing methods. It has the following benefits: 1) unlike other secrecy techniques that either require changes to existing systems such as additional bandwidth or the need for more antennas, this technique can be implemented with minimal changes and 2) this method is broadly applicable in all environments. This has the potential to improve secrecy in all military and national security wireless communications, including satellite applications, fleet command and control, and even short range tactical communication.

Summary of Accomplishments:

We analyzed the effects of scaling lattices to meet a probability of successful transmission in a point-to-point additive white Gaussian noise channel with an eavesdropper. We discovered a modified Newton's method algorithm that enables the computation of the required probabilities that is much faster computationally than previously suggested methods. We analyzed the simplest of lattices, the integer lattice, to try to better understand key features of the system. Closed-form solutions were derived for this case that could be well approximated computationally. Construction A random lattices were then analyzed to try to improve performance. Monte Carlo simulations were conducted to analyze the statistical performance of this class of lattices for small dimensions. Optimization techniques were applied to the problem to try to find the best possible lattices. Specifically, semi-definite programming was used to discover the best lattices in small dimensions.

Significance:

Probability over lattices is a relatively new area of research that has many applications in cryptography, secure communications, and other potential uses relevant to national security missions.

Impact of Materials Processing on Microstructural Evolution and Hydrogen Isotope Storage Properties of Pd-Rh Alloy Powders

162522
Year 3 of 3
Principal Investigator: C. W. San Marchi

Project Purpose:

Palladium and its alloys are optimal storage media for tritium due to high volumetric capacity at low pressure, rapid kinetics of absorption and desorption, and resistance to poisoning. As such, development of synthetic and materials processing methods that yield reliable, optimized material is critical. Preliminary investigation of atomized palladium-rhodium (Pd-Rh) powders has shown that post-processing methods have significant influence on the physical properties and dimensions of Pd-Rh powders, which in turn impacts isothermal pressure-composition-temperature (PCT) curves of Pd-Rh materials. These effects are particularly noticeable in the hydrogen (H)-storage capacity, plateau pressure slope and hysteresis loop upon H-cycling. The material synthesis and processing methods that have been investigated include gas atomization, cryomilling of atomized powder and electrochemical precipitation. Further investigation using these techniques will be supplemented by spark plasma sintering (SPS) as well as other processing methods to explore the effects of texture and porosity on hydrogen isotope storage kinetics and thermodynamics.

In Pd/Pd alloys, the connection between hydrogen isotope storage properties and physical properties such as particle morphology, particle size and micro- and nano-structural aspects such as grain size, defect density and porosity remains to be fully understood. The combination of state-of-the-art facilities for alloy syntheses, a suite of cutting-edge materials characterization techniques and the ability to measure hydrogen isotope storage behavior provides an opportunity to break new ground in understanding this relationship. Feedback between these aspects should facilitate the tailoring of hydrogen storage properties to suit a given application. The work is in collaboration with UC-Davis.

Summary of Accomplishments:

Cryomilling is a powerful mechanical milling process for modifying the microstructure of metals or alloys by severe plastic deformation. In the current project, we used cryomilling to induce severe plastic deformation of Pd-Rh atomized powders with the aim of probing the effect of microstructure on hydrogen sorption characteristics. We completed the experimental test matrix for cryomilling, microstructure characterization and measurements of the pressure-composition (PC) isotherms to characterize H absorption and desorption behavior for the UC-Davis produced atomized Pd-Rh powders. The analytical approach and measurement plus transmission electron microscopy (TEM) imaging enabled us to establish correlation between microstructure evolution and H-storage. We found that the milling-induced dislocations, subgrains, and high surface area have a great impact on PC behavior, in particular the hysteresis loop associated with sorption-desorption. Severe mechanical milling refined the deformation-induced subgrain structure and narrowed the PC hysteresis loop. The most severe milling conditions (64:1 ball to powder ratio and milling 16 hours) result in dense dislocation structures, very fine equiaxed subgrains, and structures that appear to consist of a high density of nanopores. There is some evidence suggesting these severe milling conditions also promote phase separation in the Pd-Rh system. These structures are significantly different from those developed with less severe milling conditions, which results in greater hysteresis. Preliminary results also suggest substantial microstructural evolution during subsequent cycling that widens the hysteresis loop of material subjected to the most severely milled condition. By developing a more comprehensive understanding of the microstructural effects on hydrogen sorption characteristics in Pd-Rh alloys, we advance our knowledge of hydrogen-metal interactions and enable the design of H-storage materials.

Significance:

Establishing a fundamental understanding of the relationship between microstructure and hydrogen-metals interactions contributes to the leading edge of scientific advancements in hydrogen energy technologies, which are a critical feature of long-term energy security and stability.

Refereed Communications:

N. Yang, J.K. Yee, Z. Zhang, L. Kurmanaeva, P. Cappillino, V. Stavila, E.J. Lavernia, and C. San Marchi, "Hydrogen Sorption Characteristics of Nanostructured Pd-10Rh Processed by Cryomilling," to be published in *Acta Materialia*.

Developing Software Systems for High-Assurance Applications

164661
Year 3 of 3
Principal Investigator: G. C. Hulette

Project Purpose:

Ordinary development practices for digital logic and embedded sensing and control programs yield unpredictable and indeterminate results. While the positive function (what we intend for the system to do) is often at least partially testable, the negative function (what we don't want it to do) typically is not. We must analyze the digital system itself as a mathematical object in order to reason about what it is capable of doing under the broad circumstances that high-assurance systems require. Ascertaining negative function is particularly important in high-consequence applications such as nuclear weapons.

Conventional development practices for digital systems yield programs with large spaces of negative function. If code cannot be analyzed, providing assurances against negative function is typically impossible. This project will develop a language in which digital hardware or software can be created that is specifically designed to be analyzable. Writing code in this language is unlikely to be as easy as in an unconstrained language like C, but the results will provably conform to pre-defined surety constraints. Of course, there can be no guarantee of complete safety or security outside of what the designer has specified. However, an important artifact of the proposed methodology is that, even after the digital system is complete and in use, it will remain analyzable, and a posteriori newly discovered constraints can still be checked, and in the case that new faults or vulnerabilities are discovered, proposed mitigations can be proven.

Tools for developing formally verified digital systems have the potential to revolutionize high-assurance applications, enabling engineers to hold digital products to an entirely new sort of confidence — the same confidence we place in verified mathematical proofs.

Summary of Accomplishments:

This project has explored the technical issues inherent in comprehensively verifying digital systems, and resulted in the following scientific achievements:

1) We have shown that testing, which is the traditional approach to verification and the only method in widespread use within Sandia today, does not scale to support verification of crucial safety and security properties for all high-consequence digital systems.
2) We have identified formal, computer-checked proofs of correctness, based on formal logic with quantification over higher-order terms, as the "gold standard" approach to digital system verification.
3) We have demonstrated that such proofs are difficult to construct in practice after a design is complete. We have identified a plausible alternative, wherein proof of correctness is incorporated into the design and implementation process. This approach can be realized using certain kinds of dependently typed functional programming languages. Verification can then exploit the well-known theory of "Curry-Howard correspondence," which connects logical predicates and specifications to types, and proofs to well-typed programs.

4) Existing dependently typed programming languages are complex and oriented towards theoretical applications, limiting their potential adoption for practical use. We designed and developed a prototype implementation of a simplified language amenable to formal verification.
5) We demonstrated the utility of our language through examples. Prototype implementations of this work are ongoing, now with NW program sponsorship.
6) We explored the challenges of verifying certain kinds of requirements, where the model involves continuous variables interacting with discrete transitions. We demonstrated how our novel approach to resolving these issues could be realized within a dependently typed programming language.

Significance:

The results of this project move Sandia closer to the goal of delivering digital designs with very high assurances of correctness, enabling mathematical proof high-level, complex safety, and security requirements. This capability will allow our designs to be provably free from flaws that may be exploitable by adversaries or triggered unexpectedly in unforeseen environmental conditions. Achieving this goal is critical to ensuring the safety and security of digital components within nuclear weapons, as well as other critical national infrastructure, such as power grids, avionics, and communications networks, which increasingly rely on digital components.

Understanding H Isotope Adsorption and Absorption of Al-Alloys using Modeling and Experiments

165724
Year 2 of 3
Principal Investigator: D. Ward

Project Purpose:

The aging performance of austenitic stainless steel reservoirs for hydrogen (H) isotopes can be limited by time-dependent H-metal interactions (e.g., embrittlement). Aluminum (Al) alloys, alternatively, have very low solubilities for H-isotopes and no evidence of embrittlement in dry H environments, suggesting improved resistance towards aging vulnerabilities. Unfortunately, the long time scales associated with effects of H-isotopes make solely experimental investigations impractical. Therefore, robust simulation tools need to be developed to strengthen our understanding of Al/H-isotope interactions and guide accelerated testing. A continuum level model capable of capturing aging of the material does not exist. Such a model requires a fundamental understanding, at the atomistic level, of H-isotope interactions with Al-metal/oxide surfaces and crystalline defects (e.g., dislocations, precipitates).

This work focuses on H interacting with binary Al-Cu containing a surface oxide. Copper is a common alloying element in Al-alloys and is the primary source of strengthening in candidate alloys such as Al2219. This project includes numerous innovations. First, we are developing the first-ever chemical-reaction-simulation-enabling high fidelity quaternary bond-order-potential (BOP). The fidelity of the BOP is achieved by extensively benchmarking with high quality density function theory (DFT) calculations and validating with experiments. The BOP is then used in molecular dynamics (MD) and Monte Carlo (MC) simulations to study atom trapping energies and absorption mechanisms. Second, we are developing a defect dynamics (DD) model, informed from atomistics and experiments, to study effects of hydrogen and precipitates on the motion of dislocations within the binary system. Our model will be the first to combine the interactions of precipitates and the effects of H on dislocations in three dimensions. In addition, the corresponding experiments to explore H on oxidized binary surfaces and trapping in Al-Cu will both be firsts in the field.

Carbon Composite MEMS Accelerometer

165725
Year 2 of 3
Principal Investigator: C. Dyck

Project Purpose:

Our highest deliverable is to develop a carbon composite microelectromechanical systems (MEMS) accelerometer as a possible future replacement for the Bell XI accelerometer. The Bell XI is aging and will require robust, inexpensive replacement technology on an adaptable platform. The motivation is to understand a unique carbon-carbon blend developed at Sandia, which leverages graphene sheets embedded in an amorphous carbon backbone and development of the material to a highly sensitive 10^6 dynamic range accelerometer. Fundamentally, the graphene sheets are in random orientations (flat/folded), however, their direct interactions suggest double bond carbon-carbon templates (sp2 basal plane alterations) made during processing and needs further understanding. Recently, carbon cantilevers using graphene stiffeners demonstrated a tunable Young's modulus of 65% using 2 wt.% graphene and a 2X increase in conductivity. From literature, graphene materials show improved strength, low density (~1.4 g/cm^3), good ductile behavior, and linear responses under force. The carbon accelerometer will be designed towards a proof mass architecture for optimal displacement and view impedance vs. G-force and should require little or no dampening to the proof mass due to the low density.

A carbon composite MEMS accelerometer using graphene stiffeners drives new materials and devices into MEMS to improve dynamic range, sensitivity, lifetime, and functionality when compared to state of the art MEMS technology. The planned carbon composite structure is a replacement for single crystal/metal MEMS beams, flexures, struts, etc., at a fraction of the expense. These materials are less prone to stiction under high G-force loading and have tremendous resilience under extreme mechanical deformation and shock. The exact understanding of the science and engineering required to build a carbon composite device does not currently exist. This project will increase the technical readiness level by tuning the capability of carbon composite MEMS.

Organosilicon-Based Electrolytes for Long-Life Li Primary Batteries

165726
Year 2 of 3
Principal Investigator: K. R. Fenton

Project Purpose:

We aim to develop new lithium primary power sources designed to have wider operating temperatures using inherently safe materials to increase the performance and safety of power sources used in nuclear weapons (NW) testing applications. The Achilles' heel of organic electrolytes used in Li primary and secondary batteries is their instability at elevated temperatures and safety concerns including fire and explosion. In order to eliminate flammability concerns at elevated temperatures, we propose to develop a new class of 'organosilicon' electrolyte materials with high temperature stability, high ionic conductivity, which are nonflammable, nontoxic, and have low viscosities (~1.4 cP). Informed by new density functional theory (DFT) models, these compounds will offer both high temperature (>75 °C) and low temperature (-40 °C) performance in a nontoxic, nonflammable electrolyte solvent. We will fabricate CF_x (carbon monofluoride)-based Li-primary cells with these optimized electrolytes, employing advanced packaging concepts and focusing on safe, high energy density primary batteries.

Organosilicon electrolytes exhibit several important properties for use in lithium cells that include: 1) high conductivity/low viscosity and 2) thermal/electrochemical stability. The systematic manipulation of the silicon oxide backbone geometry and repeat unit length as well as the appended ethylene oxide moieties allows for fine-tuning of the thermal and electrochemical properties of the electrolyte. These manipulations also allow for incorporation of innovative functionalities such as anion binding agents (ABAs), which dramatically change the electrochemical properties of the electrolyte and bind the fluoride anion (a byproduct of discharge) leaving lithium ions available for incorporation into the electrolyte. This work will enable the design of unique multifunctional, thermally stable organosilicon compounds with a wide variety of tunable properties. The knowledge developed in this project is expected to have an immediate impact on battery technology, but is more broadly relevant to other applications, which range from semiconductor manufacturing materials to drug delivery agents where organosilicon is being investigated.

The Use of Degradation Measures to Design Reliability Test Plans

165729
Year 2 of 2
Principal Investigator: J. W. Lane

Project Purpose:

Many nuclear weapon system components display some measure of degradation. For example, solder strength on a circuit board and neutron generator output both degrade over time. In each case, a measurable attribute dependent on component usage or age is related to the reliability of the component. In this project, reliability will be understood to mean the reliability with respect to a performance measurement and its associated specification limit, sometimes called margin reliability.

Our technical goal is to create robust reliability test plans for components subject to degradation. That is, given a component subject to degradation, a measure of success would be the development of an efficient reliability test plan and, if appropriate, development of replacement and maintenance plans. Models and methods may be well developed for components with significant historical data. However, additional models and methods are needed to optimize test plans for components with little or no existing data. Our goal is to design new test plan strategies for components that display degradation and have limited data. This will require extending current methodology as well as developing new theory. These new test plans will seek to optimize both time and resources needed to demonstrate reliability goals with respect to performance specifications. This approach builds on the present emphasis on quantification of margin and uncertainty (QMU) for the nuclear weapons stockpile. A related goal of testing using degradation measures is to improve component replacement and preventative maintenance strategies. The methods developed will be illustrated using actual nuclear weapons component data as well as simulated examples.

Summary of Accomplishments:

We compared the use of quantile regression with confidence bounds to tolerance bound methodology to analyze independent degradation data, demonstrating the benefit to using this nonparametric method when analyzing data with an unknown, non-normal distribution. We finalized methodology to develop test plans for degradation data with normal coefficients and applied it to a real major component (MC). We then extended that methodology to develop test plans for degradation data with coefficients with unknown distributions. To do this, we applied nonparametric methods to our previous methodology, namely median regression and kernel density estimation. This allows us to design robust test plans for degradation data whose path parameters do not come from a normal distribution and may have some random errors along the degradation paths. We tested this method using simulated data, particularly simulated degradation paths whose intercept coefficients were non-normal, and also demonstrated the robust design of a test plan for a real MC. Because of the use of non-parametric methods, the robust test plans are not as reduced as the test plans designed using the assumption of normality. However, in situations where that normality assumption is not valid, the robust test plans provide a more accurate assessment of the state of health of the degrading component.

Significance:

The methods developed will reduce the time and resources required to demonstrate component margin reliability goals, as degradation measures can be used to demonstrate high margin with limited testing. Further, by increasing our knowledge of degrading components, the life of these components can be extended through the use of optimized replacement policies and improved preventative maintenance scheduling. The impact will be felt especially in the weapon life extension programs, helping us to maintain a highly reliable stockpile. This is especially relevant to the DOE's mission to maintain a safe, secure, and effective US nuclear stockpile.

Lithium Thiophosphate Compounds as Stable, High Rate Li-Ion Separators: Moving Solid Electrolytes into High Rate Applications

166148
Year 2 of 2
Principal Investigator: C. A. Apblett

Project Purpose:

Lithium ion (Li^+) batteries require an electrolyte to support transport of Li^+ between electrodes during operation of the cell. This electrolyte is typically a liquid with a dissolved salt. Liquid is preferred due to the high mobility of the ion in solution, which allows the cell to support high currents with little over potential loss. However, these liquid solvent/salt electrolytes suffer from being highly volatile, pose health risks, and are highly flammable, making them a concern for implementation into larger scale systems such as vehicles and stationary storage. Solid phase electrolytes exist, but they are typically several orders of magnitude lower in ionic mobility than their liquid counterparts, limiting the utility of these systems to niche applications. Improving the ionic transport of Li^+ through a solid phase electrolyte up to the mobilities of liquid systems would enable a new class of batteries that would be safer, easier to manufacture, and perhaps cheaper than existing vehicle and grid solutions.

We are investigating a new class of highly conductive Li^+ solid phase conductors. This work is in collaboration with the University of Colorado-Boulder to support research into physical vapor deposition (PVD) of these materials, and mapping the stoichiometry/morphology space and understanding the effects of these on the transport performance and long term stability of the resultant materials. Battery separators based upon lithium thiophosphate ($LiPS_4$) have previously been demonstrated at UC Boulder, but the thickness of the separators was too high to be of practical use in a lithium ion battery. The separators are solid phase, which makes them intrinsically less prone to thermal runaway and thereby improves safety. Results of attempting to develop sputtered thin film layers of this material by starting with targets of pure Li, Li_2S, and P_2S_5 are reported. Sputtering rates and film quality and composition are discussed, along with efforts to use Raman spectroscopy to determine quantitative film composition. The latter is a rate limiting step in the investigation of these films, as they are typically thin and require long times to get to sufficient thickness to be analyzed using traditional methods, whereas Raman is particularly well suited to this analysis, if it can be made quantitative.

Summary of Accomplishments:

Efforts to sputter thin films containing P and S resulted in very low deposition rates and significant impact to the Li targets and the chamber in general. Moving to the lithia/silica/lithium system allowed for more controlled deposition. Analysis of the deposition rate from sputtered lithia indicated that reasonable thicknesses and deposition rates of samples could be generated under moderate power conditions. Lithia sputter rates ranged from 2000A/hr for 20W power, up to 10000A/hr at 40W. In contrast, SiO_2 sputtering rates were significantly slower, with deposition rates roughly 100A/hr for 20W up to 300A/hr at 40W. Since the intent is to control relative ratios of Si/Li inclusion in the film, either the Li_2O sputter rate must be suppressed or the SiO_2 sputter rate must be increased. The intent now is to keep the sputter rate of Li_2O at 20W (the lowest power at which a stable plasma can be maintained and good quality films are obtained), and further increase the power of the SiO_2 target to 60W-80W range. Since we would like to be in the Si rich region, it may be necessary to change the stoichiometry of the SiO_2 target to SiO, or even Si, and then rely on oxygen content from the Li2O system to provide the remaining oxygen to form the silica tetrahedra.

Initial efforts to understand these films using Raman spectra showed good promise to isolate both Si containing bonds as well as Li containing bond absorptions, allowing elemental analysis more simply than the current method of inductively coupled plasma — optical emission spectrometers (ICP-OES) on the solvated samples.

Significance:

The increased powers accessible with the Li_2O and SiO_2 targets are showing much more promise towards a rapid, stable film growth that plagued the early thiophosphate work. Learning made in studying the Li-Si-O system may be more broadly applicable to the high rate systems, and can lead to further work in durability of these systems.

Development of new, thin film Li-ion batteries with higher rate capability than currently existing systems allows for a host of new applications to grow from this foundational work. Thin film batteries find use in powering continuous low power sensor networks for national security, and high rate solid-state batteries would provide an alternative to the current work in transportation grade batteries with a higher margin for safety. Lastly, thin film solid batteries can support higher temperature operation, making them attractive for grid storage energy at the highest volumes.

Cognitive Data Science for Neutron Generator Predictive Pattern Analysis

173153
Year 1 of 3
Principal Investigator: R. A. Roach

Project Purpose:

Our project is a multi-technology, multi-pronged research effort focused on the performance of neutron generators where waveforms of data are collected as performance assessments relative to requirements. Human visual pattern recognition and interpretation by experienced operators are the primary assessment methods. One of our primary research challenges is to assess whether expert visual pattern recognition on tester waveform images can be captured and integrated into automated models of product performance patterns (failure/success); and, together with models of the underlying data, provide leading indicators for future product performance. The development of these cognitively informed models of waveforms is a decidedly unique and novel approach in product engineering data analysis. In addition, the integration of the interrelationships and combinations of the waveform data and cognitive models to leverage the strengths of both human expertise and algorithmic methods offers the potential to discover new insights that each method in isolation might overlook.

Recycling Scandium and Erbium from Nuclear Weapon Manufacturing Operations

173156
Year 1 of 3
Principal Investigator: R. F. Hess

Project Purpose:

The main goal of this project is to establish a scientific basis for the dissolution and deposition of lanthanides using ionic liquids (ILs). Initial efforts will focus on isolating scandium (Sc) metal from process generated coated tungsten (Sc-W) crucibles as a benchmark. The separation of Sc^{3+} from other metal ions using solvent extraction techniques has been demonstrated but relies heavily on the use of concentrated acid and organic solvents similar to the PUREX process for actinides. In contrast, the IL dissolution of lanthanides has been relatively unexplored. ILs have low vapor pressures and larger electrochemical windows that will allow for the reduction of Sc^{3+}/Er^{3+}. We will develop tailored IL materials to selectively electrochemically dissolve scandium metal from the crucible and determine the conditions necessary to electroplate scandium metal. This novel IL solution route will also enable the more delicate instrumentation to be 'washed'. After the Sc is solubilized, select electrochemical deposition of Sc(0) will be necessarily developed from the IL. Little information is available to direct these fundamental electrochemical studies but literature reports support this as a reasonable approach. In addition, we will study the separation and recovery of Ln^{3+} from process solutions containing large amounts of cerium, which itself will be recovered for further use. Technical risks that may be encountered include potential difficulties in crystallizing IL-metal complexes, which make structural characterization problematic, and challenges in achieving high product purity after electrodepositing the Sc and Er metals.

The study of the dissolution and electro-winning to produce pure lanthanide metals has not been explored in depth. The development of a benign separations process will yield the fundamental scientific information necessary to produce a long-term cost savings and enable the recycling of other lanthanides from products (i.e., fluorescent lights, magnets).

Compressed Sensing to Support Reduced Flight Testing

173180
Year 1 of 3
Principal Investigator: J. Helms

Project Purpose:

We are using compressed sensing (CS) as a low-complexity/low-power on-board compression algorithm in telemetry systems that would support the reduction of flight tests. In telemetry, there is a drive to quantify margins and uncertainties. This drive requires an increase in sensor data by an order of magnitude, yet there is no corresponding available increase in the telemetry bandwidth. In addition, the reduced number of flight tests makes it imperative to maximize the amount of data to be collected per flight test. Traditional compression methods prove inadequate, as they require an increase in onboard complexity resulting in greater power consumption and volume. Complex onboard processing introduces latency, limiting the capability for end-event measurements. Additionally, using the same compression algorithm for various telemetry signals may not be possible. The cost and complexity of multiple algorithms based on traditional compression make this approach unfeasible.

Compressed sensing offers compression ratios comparable to traditional methods without significant increases in cost, on-board processing or complexity.

CS is a new, fast-growing field that fundamentally changes data acquisition. It allows for sampling at much lower rates than Nyquist. Our research will provide insight on how to implement concepts of CS theory in telemetry systems. We will show that CS has comparable compression performance compared to traditional compression, while offering the following additional benefits:

- Decoupling of compression and decompression: we can change decompression without changing the compression process
- Robustness: each coefficient is a linear combination of random samples of the signal, such that even if some coefficients are dropped the information contained is not completely lost
- Security: unless the sensing matrix is known, it is almost impossible to recover the signal
- Low cost and low computational on-board complexity: low power requirement
- Flexibility: new sensors can easily be added
- Applicability to hi-fi flight tests: due to the low complexity, CS based algorithms can be used for lightly instrumented hi-fi tests

Organic Semiconducting Materials for Thin-Film Optoelectronic Devices

173183
Year 1 of 3
Principal Investigator: J. G. Cordaro

Project Purpose:

Next-generation photonic and electronic devices require new materials with tunable optical and electrical properties. Detection in the information rich 900-2,600 nm spectral regions can only be achieved using conventional solid-state inorganic based systems, such as those based on Ge and alloys of $Ga_xIn_{1-x}As$. These suffer from limited modularity, intrinsic fragility, cooling requirements for reasonable performance, and incompatibilities with silicon complementary metal-oxide-semiconductor (CMOS) processes. These features restrict the application of inorganic photodetectors for various applications and for the development of advanced optoelectronic technologies particularly where low-power and high speed may be required. Organic materials are promising because of their large linear and nonlinear absorption cross-sections, semiconducting attributes, mechanical properties, chemical modularity and processing versatility. Despite significant research efforts, there exists no strategy to modulate the properties of these materials precisely and the lack of understanding of the features that govern performance in these systems precludes their broad utilization. Recent synthetic advances to generate semiconducting polymers have been developed where we can systematically influence the electronics, sterics, aromaticity and degree of intermolecular coupling in the solid-state. These features have been shown to directly influence the optoelectronic and physicochemical characteristics of the resultant materials, nature and properties of transient species, inter- and intramolecular charge transfer properties of holes and electrons, and corresponding device performance parameters. We have demonstrated that first-principles calculations can reliably predict key electronic properties allowing only promising synthetic targets to be pursued. Preliminary performance measurements of our materials match or exceed state-of-the art materials. This development affords a unique opportunity to systematically understand the features governing performance in organic based devices and to advance new electronic technologies.

Electro-Syntheses of Intermetallic Couples as Thin-Film Heat Sources for Advanced Thin-Film Thermal Batteries

173184
Year 1 of 3
Principal Investigator: C. A. Apblett

Project Purpose:

We will develop low-cost, high-energy electroplated heat sources based on nickel-aluminum (Ni-Al) intermetallic formation that can be rapidly formed into shape for use in advanced thermal batteries and for fast brazing, joining, and energetic components. Current heat sources of this type use alternating nanostructured layers of reactive metals made by sputtering, a process requiring thousands of iterations, high capital investment, and expensive shaping to fabricate the heat sources. We will electroform the couples as an alternative. Using pulse electrodeposition, we will achieve an equivalent structure on a preformed substrate, eliminating both slow sputtering and expensive shaping. This will result in a smaller, faster, and cheaper heat source for both current and future thermal battery systems.

We will develop a process for electrodepositing compositionally modulated metal multilayers (CMMMs) using aprotic solvent/electrolytes. Tailoring the concentration and deposition mode of the noble material allows tuning thickness and resolution of the CMMMs. We will investigate continuous dispersion electroplating processes — electrochemical deposition while simultaneously electrophoretically co-depositing a colloidal solid that is then intimately bound to the substrate with the metal. Rather than layer formation, inclusions of one reactant will be embedded into a matrix of the other reactant, which allows for oxide exchange reactions to be developed. The use of aprotic solvent/electrolytes to deposit these reactive chemistries is in its infancy, and while there have been reports of several candidate elements deposited from aprotic solvent/electrolytes, no one has yet synthesized a discrete laminar or dispersion matrix of constituents to make a reactive heat source.

Engineered Composite Materials Science and Technology for Next-Generation Glass-to-Metal Seals

173186
Year 1 of 3
Principal Investigator: K. G. Ewsuk

Project Purpose:

Steadily increasing demands on nonnuclear components in nuclear weapons (NW) have pushed critical properties like the strength of traditional glasses in glass-to-metal (GtM) seals to their limits, eliminating margins critical to predictable performance and reliability. Glass-ceramics (GCs) in GtM seals have improved tolerance to cracking/chipping, but at the expense of robust manufacturability, and with unresolved hermeticity issues attributable to poor interface bonding. New materials and technology are needed to resolve conflicting design, manufacturing, performance, and reliability requirements for GtM seals in NW components. The solution is novel, interface-engineered, advanced composites comprised of two or more chemically compatible materials that take advantage of the desirable attributes of the constituent materials while circumventing their deficiencies.

Particle-filled glass composites (FGCs) will be developed as new sealing materials to make improved performance and reliability GtM seals. FGCs offer enhanced manufacturability, performance, and reliability by combining the processing robustness and thermodynamic stability of a traditional glass, with the physical stability, design flexibility, and enhanced performance of a crystalline solid. Compared to the process sensitive GCs targeted to replace traditional sealing glasses, lower entropy FGCs afford more robust processing and greater control of microstructure and physical properties. FGC GtM seals are being developed using a combination of materials engineering and fundamental materials science, employing: 1) experimentally validated molecular modeling to develop new glasses with controlled chemistry and structure to improve interface bonding and seal reliability; 2) property and process modeling to optimize FGC design, manufacturability, and performance; and 3) interface engineering to produce metal surfaces/interfaces that are thermodynamically more stable. Coupled modeling and experiment will be employed to optimize GtM interface bonding through understanding and control of critical glass chemistry-structure relationships.

Reconfigurable Matching Networks for High-Efficiency GaN Power Amplifiers

173187
Year 1 of 3
Principal Investigator: M. M. Elsbury

Project Purpose:

Modern radar transmitters under development are based on single-chip gallium arsenide (GaAs) power amplifiers (PAs) capable of producing unprecedented levels of radio frequency (RF) power and integration. Unfortunately, because these PAs are designed to cover wide bandwidths, they operate with low power-added-efficiency (PAE), resulting in tremendous waste heat. The thermal management problem created by this high power dissipation is a daunting technical challenge.

Gallium nitride (GaN) is a new RF semiconductor technology capable of operating at much higher voltages and temperatures than conventional GaAs. Recently, researchers have exploited the high-voltage capability of GaN to design highly efficient, switching-mode RF PAs. Unfortunately, the maximum practical bandwidth of these switching mode PAs is too low for many applications. This project will create a switching mode PA design utilizing narrow-band high-efficiency matching networks reconfigurable to operate in any one of multiple sub-bands.

State of the art high-efficiency class-C/E/F power amplifiers can typically achieve only a few percent bandwidth. Creating a reconfigurable high-power output-matching network to enable high-efficiency operation across a large bandwidth will significantly reduce the thermal design complexity while maintaining the required application bandwidth. For example, in a 100 W amplifier, increasing PAE from 30% to 50% cuts the dissipated power from 230 W to 100 W, thus significantly relaxing the requirements and manufacturing complexity of the thermal design. Such improvements require an increase in electrical design complexity with a corresponding large initial investment of research and development time and resources. If successful, creating band-reconfigurable PAs will not only be an enabling technology for future fuzing radars, but will yield technology broadly applicable to multi-band commercial communications, software-defined radios, and other defense-related applications.

Welding of Advanced Shape Memory Alloys

173188
Year 1 of 2
Principal Investigator: J. Rodelas

Project Purpose:

Shape memory alloys (SMA) represent a group of metallic materials with the ability to be deformed and returned to original shape simply by heating above a specific temperature. Conventional SMAs such as Nitinol used in arterial stents, eyeglass frames, orthodontic wire, etc., change shape at relatively low temperatures (e.g., <100 ºC). Applications in which materials operate at temperatures >100 ºC require the use of more metallurgically complex high temperature shape memory alloys (HTSMAs), including Ni-Ti-Hf/Pt/Pd alloys currently under development at Sandia.

Eventual SMA/HTSMA application in weapon components, aerospace, energy, etc., requires joining. However, a fundamental understanding of SMA/HTSMA weld microstructural evolution is lacking despite promising avenues for application. Non-equilibrium melting and solidification associated with welding destroys the highly engineered starting microstructure and can result in diminished or non-existent shape memory effect, loss of mechanical properties, and/or formation of cracks. This project will develop a fundamental, science-based understanding of the solidification behavior and solid-state microstructural evolution in simple binary systems to enable successful SMA/HTSMA joining.

The research represents a first-of-kind study of the weld solidification behavior and weld microstructural evolution of binary SMAs and ternary HTSMAs that will serve as the scientific foundation for development of kinetic (i.e., process) and compositional techniques for weld microstructural control. This research aims to characterize weld microstructure/property relationships using highly dynamic thermomechanical simulation and advanced electron microscopic techniques. Ultimately, the science-based tools developed for the weld microstructure control will be of use not only for joining, but also for other SMA/HTSMA melt process fabrication techniques.

Process-Structure-Properties Relationship of Electrodeposited Au Thin Films used in Thermoelectric Power Generation Device

173666
Year 1 of 2
Principal Investigator: D. Banga

Project Purpose:

The purpose of this project is to develop Sandia's S&T knowledge base of gold (Au) electrodeposition for thermal mitigation and contact of the next-generation high performance thermoelectric power source device by fundamentally understanding the mechanisms whereby microstructure, grain size, crystallographic texture influence mechanical and optoelectronic properties in gold electrodeposits. Au coatings are mission-relevant to NNSA for its extensive use throughout the stockpile. We will combine quantitative electrochemical measurements, x-ray diffraction, and surface and bulk microscopies to understand how grain structure affects properties and performances of Au electrodeposits, and then use such understanding to develop electrodeposition conditions favorable for the growth of films with controlled and stable microstructure which are critical to the performance and reliability of many technologies relevant to national security. This work will culminate with the production of low emissivity and electrically conductive Au films containing twin boundaries. Because of their electron scattering coefficient that is one order of magnitude lower than that of other high angle conventional grain boundaries, twin boundaries are effective in increasing strength without negatively affecting conductivity. We will introduce nanosized twin boundaries in electrodeposits by controlling deposition conditions including reduction rates of the precursors by the use of pulsed electrodeposition. Technical challenges to the success of this project include: 1) the difficulty of capturing the actual Au nucleation and growth processes by the use of electrochemical techniques due to side reactions and 2) the effects of bath chemistry and additives. To solve 1), in addition to the electrochemical current transient technique for instantaneous and progressive nucleation models, we developed in situ electrochemical scanning probe microscopy (EC-SPM) for dynamic observations of evolving surface morphology and structure. To address 2), we have chosen a cyanide bath with no added additive and have limited ourselves to one primary bath chemistry, placing our primary experimental emphasis on deposition parameters influencing the rates of mass and energetics incorporation.

Effects of PSA Measurements on Device Reliability

176309
Year 1 of 2
Principal Investigator: P. Tangyunyong

Project Purpose:

The power spectrum analysis (PSA) technique is an electrical technique developed at Sandia to detect electrical differences in devices. The goal of this project is to determine whether PSA creates any latent damage in the test device and to evaluate the long-term reliability of PSA measurements.

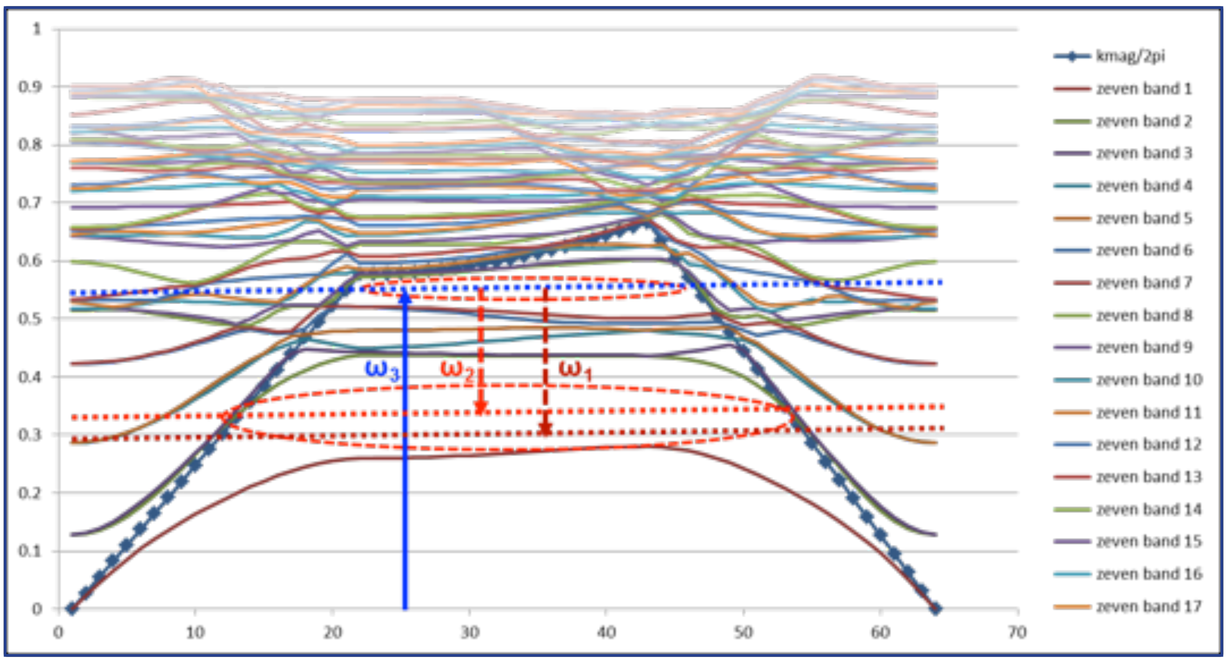
The devices selected for this study were commercial off-the-shelf (COTS) products. To evaluate the reliability of the test devices, the samples were subjected to both elevated-temperature and elevated-voltage accelerated testing. After each accelerated testing cycle, electrical testing was performed on the test devices to see if there were failures.

After several accelerated testing cycles, no failures occurred, indicating that PSA had little or no impact on the reliability on the test devices. Statistical analysis indicated that the reliability of the devices that have been subjected to PSA measurements was at least 0.999.

CYBERSECURITY

The Cybersecurity Investment Area intends to address the daunting national security challenge of securing the information technology infrastructure essential for crucial government, military, economic, and critical infrastructure functions. Its research goal is to help establish, develop, and advance the scientific foundations for cybersecurity to enable much more robust approaches for addressing and mitigating the significant cyber vulnerabilities we face today and in the future.

The work applies aspects of computer science, physical science, mathematics, and social sciences, and is exploring novel and near-term applications of quantum information technologies and quantum algorithms that support national security needs.



The 3D band structure of a photonic crystal showing transverse electric bandgaps and cavity modes, studied in the exploration of new models for quantum computing. (Project 158782)

CYBERSECURITY

Memristor Evaluation and Optimization for Cybersecurity

158740
Year 3 of 3
Principal Investigator: M. Marinella

Project Purpose:

Dynamic random access memory (DRAM) and flash memory technologies are nearing physical scaling limits and are starting to require significant switching energy compared to other components of modern computing systems. Excitement surrounding memristor (or ReRAM) technology led Sandia to begin investigating possible applications of this device, which led to the following conclusions: 1) government customers are interested in using this device for security related applications, and 2) we found that these applications require devices to have several electrical and physical characteristics that are not of interest to companies involved in memristor technology development, and thus, have not been thoroughly studied. Sandia has the necessary expertise, infrastructure, and partners to evaluate and optimize this technology. In this research, Sandia will continue to develop a state-of-the-art memristor process, design a memristor controller (application specific integrated circuits) ASIC, and develop a robust set of characterization methods to evaluate these properties.

Sandia is uniquely positioned to carry out this research. We have the necessary facilities and expertise to fabricate and characterize memristors, a cooperative research and development agreement (CRADA) with leading researchers which has provided a significant background knowledge set, and the necessary infrastructure to perform sensitive work related to national security.

Summary of Accomplishments:

A brief summary of the key accomplishments follows:

1) We developed a technique to deposit and characterize metal-oxide switching films tuned to form high yielding devices. We focused on the fabrication of complementary metal-oxide semiconductors (CMOS) compatible TaOx/TiN memristors, but also made devices with AlN, TiO2, and SiO2 switching films.
2) Ultra scaled (<20 nm) vertical and lateral memristor structures were developed.
3) We developed, demonstrated, and published results on the electrical characterization of the devices we fabricated, with particular attention given to characteristics needed for security applications. DC current-voltage (I-V) characteristics, endurance, and pulsed analog capabilities were measured. Automated testing provided information on the statistical variation of the forming, on and off resistances. Performance and reliability trade-offs were assessed for different materials systems with regard to exemplar applications. For instance, certain material systems are better suited for analog behavior, whereas others have improved retention.
4) We developed, designed, and demonstrated a CMOS controller ASIC bonded to our memristor crossbar, with custom circuitry to assess the properties of memristors for government use.
5) We discovered a two-state variable operation in our TaOx memristors. Specifically, we modeled the resistance of our TaOx memristors as a function of both the switching filament radius and its conductivity. When the device is being transitioned to the low resistance state, the conductivity is being altered, but

when it is being transferred to the high resistance state, the radius is changing. This has the important consequence that for each resistance state, there are multiple internal configurations possible that can make up that state — which may provide a path to a high-density memory.

Significance:

This work has provided a fundamental understanding of memristor properties that will facilitate potential use of this technology for government applications. We have an understanding of the trade-offs that make a material system suited to an application field. For example, longer retention and faster switching can be obtained by the use of a metal-oxide device (e.g., TaO_x), but more precise analog tunability may be possible with an electrochemical device (such as SiO_2/Ag). The two-state model discovery has provided an interesting new set of capabilities, which may be possible with TaO_x devices using the degenerate resistance states.

Refereed Communications:

A.J. Lohn, P.R. Mickel, and M.J. Marinella, "Dynamics of Percolative Breakdown Mechanism in Tantalum Oxide Resistive Switching," *Applied Physics Letters*, vol. 103, p. 173503, October 2013.

A.J. Lohn, P.R. Mickel, and M.J. Marinella, "Mechanism of Electrical Shorting Failure Mode in Resistive Switching," *Journal of Applied Physics*, vol. 116, p. 034506, 2014.

A.J. Lohn, P.R. Mickel, J.B. Aimone, and M.J. Marinella, "Memristors as Synapses in Artificial Neural Networks: Biomimicry Beyond Weight Change," *Cybersecurity Systems for Human Cognition Augmentation*, vol. 61, pp. 135-150, September 2014.

A.J. Lohn, J.E. Stevens, P.R. Mickel, D.R. Hughart, and M.J. Marinella, "A CMOS Compatible, Forming Free TaO_x ReRAM," *ECS Transactions*, vol. 58, pp. 59-65, October 2013.

A Thin Hypervisor for Dynamic Analysis and Security Assessment of ARM-Based Embedded Systems

158742
Year 3 of 3
Principal Investigator: B. K. Eames

Project Purpose:

The center of personal computing is gradually shifting toward commercial mobile devices like smart phones and tablets that act as a window to large-scale networked services. Separately, networked embedded control devices are often deployed to sense and manage distributed critical infrastructure. Together, these mobile and embedded devices have tremendous security relevance as they are increasingly used for personal, commercial, and government business. Mobile systems and networked embedded systems have a key similarity. An overwhelming majority of mobile devices and a significant fraction of power-sensitive embedded systems that require high performance are based on the Advanced RISC Machines, Ltd. ® (ARM) CPU (central processing unit) architecture. To understand and counter the threats posed to such devices, one must be able to observe and influence their runtime behavior. The task is not straightforward due to obscurity, limited standards, and intentional removal of debugging and analysis features by manufacturers. This project seeks to build a virtualization-based dynamic analysis platform for ARM-based mobile devices to facilitate security assessment and to serve as the basis for host-based monitoring and intrusion prevention research on mobile and embedded devices. A robust ARM-based dynamic security and analysis platform directly supports Sandia's role in driving innovation in cybersecurity, particularly considering the emerging ubiquity of mobile computing.

Summary of Accomplishments:

This project has developed dynamic analysis tools to support security research on mobile devices. Santeria represents two separate but related development efforts. The first is an effort at creating a capability for debugging and introspecting system-level software on Android devices that resides within and as part of the platform operating system. We refer to this effort as the "In-Kernel Debugger" (IKD). The second is an effort to develop hypervisor-based debugging technology for mobile devices.

The IKD supports debugging of the operating system kernel running on an Android device. It allows breakpoints to be set and fired, as well as examination and manipulation of memory contents. It facilitates programmed-in reactions to debugging events, and supports multiprocessor synchronization using a master slave locking approach borrowed from the GNU Kernel Debugger. The IKD supports compiled-in user-specified code to react to breakpoints. We have demonstrated the IKD on several mobile devices.

The hypervisor-based debugger is an effort to fundamentally separate the debugging introspection from the system being debugged. It causes the operating system to be transitioned to execute as a virtual machine, monitored by a hypervisor installed as part of the debugging software. The hypervisor has the ability to react to events occurring within the guest operating system and can communicate with the host computer. The current implementation of the hypervisor, while not complete, demonstrates the concepts of virtualization-based debugging.

Significance:

The security research community relies on dynamic analysis tools to understand security measures that have been put in place by system developers, as well as to understand the behavior of malware that attempts to exploit vulnerabilities that may exist in those systems. Currently, available analysis techniques, including JTAG (joint test action group) and existing kernel debuggers, are either too invasive or cannot be applied to production mobile devices without significant low-level modifications. The Santeria debugging software will allow fine-grained analysis on production mobile platforms to support a variety of projects and missions, from malware analysis to security assessments of mobile platforms.

Encryption using Electrochemical Keys (EEK)

158743
Year 3 of 3
Principal Investigator: D. R. Wheeler

Project Purpose:

The goal of this project was to investigate the feasibility of using microelectrochemical cells for data storage. In order to achieve this goal, we needed to understand the nature of the interface between electrodes, ionic liquids, which were used as the electrolyte in the microelectrochemical cells. The organization of the cation and ions as a function of electrode bias and molecular functionalization was investigated by both experimental means and theoretical methods.

Summary of Accomplishments:

We discovered a new method to rapidly interrogate the electronic structure of interfaces using Fourier transform electrochemical impedance spectroscopy. We demonstrated three different types of electrochemical memory based on three different approaches. We built a memory that behaved as a read-only memory. We demonstrated a write-once, read-once memory. And finally, we demonstrated a memory based on electrochemical stripping that generated a flash-like memory with tri-state logic.

Significance:

Our new methods to store data enhance security by providing new methods to store data and may not have the shortcomings of some current type memory devices. We increased the understanding and dynamics of charged interfaces in ionic liquids.

Refereed Communications:

L.J. Small and D.R. Wheeler, "Influence of Analysis Method on the Experimentally Observed Capacitance at the Gold-Ionic Liquid Interface," *Journal of the Electrochemical Society*, vol. 161, pp. H260-H263, 2014.

A.L. Frischknecht, O.H. Deaglan, and M.L. Parks, "Electrical Double Layers and Differential Capacitance in Molten Salts from Density Functional Theory," *The Journal of Chemical Physics*, vol. 141, p. 054708, 2014.

Frequency Translation to Demonstrate a “Hybrid” Quantum Architecture

158782
Year 3 of 3
Principal Investigator: D. L. Stick

Project Purpose:

Modern encryption relies on the computational complexity of factoring large numbers with a classical computer. In 1994, Peter Shor developed a factoring algorithm for a quantum computer, one governed by quantum mechanics, which factors numbers more efficiently and threatens to compromise modern encryption. Most experimental work in quantum computing has focused on systems of identical quantum bits. However, a large-scale quantum computer will likely be composed of several types of qubits, with each qubit selected to exploit its advantages for the overall system. Photons are a natural choice for coupling different qubits due to their ability to travel and interface with different systems.

Due to energy structure differences, one qubit type cannot be directly coupled to another of a different type. Instead, one needs a quantum interface to convert the energy (frequency) without destroying the quantum information that the photon is carrying. Using nonlinear optics (NLO) and quantum frequency conversion (QFC), we plan to make photons emitted from one ytterbium ion indistinguishable from those emitted by a calcium ion. This will be the world’s first photonic coupling of different species of ion qubits, laying the foundation for coupling drastically different types of qubits, such as ions and quantum dots. If successful, this technology will enable new quantum hybrid architectures.

Converting the frequency of the photon to higher wavelengths also makes it compatible with low loss transmission via telecom fibers. This is an important regime, as the long-lived qubit states of the trapped ion plus the frequency-converted photons constitute a quantum repeater. The absence of a quantum repeater has restricted current commercial quantum communication networks that rely on fibers to 10’s of km, limiting their usefulness. A viable quantum repeater would remove this restriction and would be a very important outcome for this work.

Summary of Accomplishments:

In this project, we demonstrated a single photon source by performing a g2 measurement on photons from a calcium ion, which showed the telltale correlation dip. The experiment was performed in a Sandia microfabricated trap, and the ion fluorescence was coupled into a single mode fiber to enforce a single spatial mode on the photon source, in addition to the single frequency mode that is guaranteed by virtue of the atomic structure. In parallel, we worked with two companies to make a nonlinear periodically poled crystal for converting the ion wavelength (397 nm) to an intermediate wavelength (702 nm) using a build-up cavity. We designed and demonstrated build-up in the cavity (Q~200), but were not successful at generating the intermediate wavelength light. We also designed a photonic crystal capable of converting the intermediate light (702 nm) to a telecom wavelength (1273 nm).

Based on our troubles with nonlinear conversion, we learned that the greatest challenge in achieving the program goals of hybrid entanglement (with trapped ions) is successfully converting UV light.

Significance:

Our results have informed the national security mission by investigating one of the most promising techniques for generating entanglement between two different quantum systems. This work is also informative to the quantum communication community. Relevant for both cases, we learned from that the technical issues inherent in UV wavelength conversion pose a major obstacle, which will have to be overcome before work in this topic can succeed.

Cross-Domain Situational Awareness in Computing Networks

158783
Year 3 of 3
Principal Investigator: S. A. Mulder

Project Purpose:

There exists a large theoretical gap in our ability to understand the code executing on our computers and what, in practice, is actually understood. This may be illustrated by the fact that manual reverse engineering can, in practice, unravel almost all programs and characterize their functionality given enough time. Automated defensive processes, however, rely on static signatures and very simplistic feature characterization to identify malicious software. In reality, context is critical to determining whether executable code should exist in a given system and whether its presence indicates malicious intent. In theory, we should have access to information about what capability is present on our information systems, including what code exists in storage (hard disk, flash), and what is executing in memory. Previous work in this area has provided us with rich feature extraction of both stored and executing programs. Two notably missing elements are closely related. Scalable program understanding that leverages the analysis of millions of programs to characterize individual programs, and a cross-domain analysis that provides both host and network context. We will construct a system that allows us to perform experiments combining automated program understanding and context analysis.

Full program understanding is a fundamentally hard problem as it builds on at least one problem that can be proved to be undecidedly hard (correct disassembly). The best that is generally achievable is a series of approximations of increasing semantic meaning and probability. Approaches that examine individual programs without context are limited to relatively simple heuristics. Combining high-speed analysis and characterization heuristics with a scalable architecture that allows us to leverage prior analysis of millions of files should allow us to gain a deeper insight into the structure of the functionality on the network than has ever been achieved.

Summary of Accomplishments:

We developed new techniques for assigning semantic labels to executable code, including a rich layered approach that builds up semantic labels from the instruction level, through functional assignment, and ultimately applies high-level labels to entire programs. We analyzed the value of a large range of features, including developing several new examples, in assigning these labels. We designed and tested new features using machine-learning techniques, including a novel evolutionary algorithm approach, and demonstrated that our feature set was sufficient to assign meaningful semantic categorization given enough data. We developed novel visualizations of new features such as code collocations to provide an interface for a human-in-the-loop categorization.

Significance:

Our work provides the basis for a capability in reducing the gap between theory and practice in automated reverse engineering. The suite of feature extractors, visualization tools, and semantic feature layers directly extends our capability in ways that have been transitioned to customer problems.

Refereed Communications:

H. Jasenko, D.R. Tauritz, and S.A. Mulder, “Evolving Decision Trees for the Categorization of Software,” in *Proceedings of the 38th IEEE Annual Computers, Software and Applications Conference Workshops (COMPSACW ’14)*, Vasteras, Sweden, 2014.

An Empirical Assessment of the Factors underlying Phishing

164764
Year 3 of 3
Principal Investigator: M. C. Kimura

Project Purpose:

High-profile phishing attacks on Oak Ridge National Laboratory and Lockheed Martin have underscored the need for research on the human dimension of cybersecurity. Phishing generally refers to the use of electronic communication (typically email) by an adversary to pose as a trusted source for which a person is willing to provide information or perform actions.

While it is widely recognized that phishing attacks are a major problem and a commensurate amount of effort is being put towards developing solutions, some major gaps still exist. Most published research on phishing focuses on technical mitigations or managerial policy, which ignores the end-user. Others rely on user-reported data or responses from artificial role-playing scenarios to draw conclusions, despite studies indicating that these sources of information are unreliable. Our survey of anti-phishing programs found that those in use today focus almost exclusively on knowledge, despite anecdotal evidence which makes it very clear that a lack of knowledge is not the only reason why people fall for phish. The current state of the art in anti-phishing training is to run phishing exercises on the organization. While this is a large step forward, vital metrics are still missing.

None of these approaches provide metrics that cyber defenders can use to measure the defensive strength of their organization, effectively determine where to concentrate their efforts, and identify the underlying problem. In this project, we developed and deployed an experiment to test hypotheses regarding what factors may correlate with susceptibility to phishing in order to begin addressing these issues.

Summary of Accomplishments:

This project generated a number of steps forward in understanding phishing. We developed a way to think about the problem from a cultural- and psychological-based perspective. We learned about anti-phishing solutions available today, and the pros and cons of each. We identified various factors that may be relevant to why people fall for phish, and then designed and executed an experiment to test our hypotheses regarding those factors. We also developed an online software application for conducting part of our experiment, which was successfully deployed. Perhaps most importantly, we learned how to approach the issue of phishing from a holistic perspective that encompasses policy, technology, and the different roles of people who need to work together to reduce the risk from phishing.

Significance:

Susceptibility to phishing attacks is a major security vulnerability at any organization. The better we can understand that vulnerability, the better we will be able to address it. This work supports the development of that understanding and is a step forward towards finding effective solutions.

Flexible and Scalable Data Fusion using Proactive, Schemaless Information Services

164869
Year 3 of 3
Principal Investigator: P. Widener

Project Purpose:

Exascale data environments are fast approaching, driven by diverse sources such as system and application telemetry streams, open-source information capture, and on-demand simulation output. Storage costs having plummeted, the question is now one of converting vast stores of data to actionable information. The prevailing data management environment in most government agencies is still one of high manual effort, low degrees of awareness across domain boundaries about what related data may exist, and write-once-read-never (data generation/collection rates outpacing data analysis and integration rates). Increasingly, technologists and researchers need to correlate previously unrelated data sources and artifacts to produce fused data objects serving domain-specific purposes. New tools and approaches for creating actionable knowledge from vast amounts of data are vitally important to maintaining research and operational momentum.

We intend to research and develop tools and services to assist in the fusion and analysis of different types of data, allowing users to flexibly create scalable, tailored information streams and objects. A central design principle is specifically not to follow the "build a big fused database of everything" approach by providing a general index over all data. Instead, we wish to make possible a distributed "forest" of loosely connected user-defined index structures (flexible multi-indexing) and provide a mechanism (data proactivity) by which those structures can advertise not only changes in data state (new data collected), but also changes in the state of the information service (new data type exists). In so doing, we hope to encourage discovery and reuse of already-computed indexes and metadata. We envision a decentralized, component-like toolset that allows fine-grained control and is easily customized and/or extended for integration into applications. This research has the potential both to dramatically accelerate individual and cooperative data analysis and management tasks and to assist in transition to a data environment that will scale with the critical data demands of 21st century national security research.

Summary of Accomplishments:

We report the following accomplishments:

1) We designed and implemented a software service for data fusion called Drift. Drift implements the design goals laid out in the project — namely, a scalable service that allows manipulation of fused data types, which are indexed by user-specified analytical index mechanisms.
2) We verified the feasibility of using a graph database such as Neo4J to represent fused data entities.
3) We conducted localized scalability testing for proactive notifications of changes to the service, establishing that service overhead grows linearly with the number of service clients.
4) We developed use cases based on realistic scenarios encountered by information systems staff.
5) We implemented, using the Drift service, solutions to the use cases developed above.
6) We implemented an extension to Drift, which makes its capabilities available through an industry-standard service oriented architecture concept enterprise service bus (ESB).
7) As part of the ESB implementation, we developed several extensions to an open-source ESB software that encapsulate Sandia services such as SAPLE and third-party software used by Drift such as the graph database Neo4j.

8) We developed a user-facing programmatic application-programming interface (API) for Drift.
9) We explored how Drift, or a service like it, might be integrated with other data science tools.

Significance:

Our results demonstrate the utility of a service such as Drift in management/integration of ever-growing data volumes generated by enterprise applications, research projects, and sensing platforms — an important consideration in the data-centric future of DOE, DoD, NSA, NNSA, and DTRA, among many others. We have shown that tools that enable users to deal with data in abstract, fused forms can greatly assist in the curation and analysis of heterogeneous data, a set of tasks whose urgency is underscored not only by increasing data volumes but by the need to retain and expose institutional knowledge as the workforce changes over time.

Refereed Communications:

P.M. Widener, "Data Fusion as an Enterprise Service," in *Proceedings of the 2014 IEEE Conference on Services Computing (IEEE 10th World Congress on Services)*, Anchorage, AK, 2014.

Composing Formally Verified Modules to Analyze Security and Reliability Properties of Large-Scale High-Consequence Systems

165537
Year 2 of 3
Principal Investigator: G. C. Hulette

Project Purpose:

The purpose of this project is to move towards enabling modular formal verification of digital designs. While formal methods and related tools provide a significant advantage over testing (even directed and assertion-based testing), current formal methods do not allow for the divide-and-conquer composition-based design approach that is routine in nuclear weapons (NW) practice. Recognizing that NW digital designers program in a modular fashion, we will research and develop a methodology that permits formal analyses of sub-modules to be composed into a system that preserves formal guarantees. NW designers currently analyze sub-modules separately and surmise the impact on the global system in an ad hoc fashion. Current commercial and open-source tools require that the formal analysis be conducted on a digital design in isolation and provide no systematic or even rule-of-thumb approach for synthesizing separately proven modules into a larger proven composition. To support the needed modularity, we will extend previous research on formal abstractions, in effect coupling each modular component through an interface that is a conservative over-approximation of its peers' behavior. In this way, any proof of correctness that accommodates this superset of peer behaviors will accommodate the actual behaviors, thus preserving formal properties under composition with peers.

New insights arising from our work have led us to a theoretical mechanism for a divide-and-conquer approach to formal methods employing ideas of abstraction and over-approximation, which may enable applying formal verification to components and still retaining guarantees regarding the verification of the composed system as a whole. The results of this work could potentially be incorporated into the Rodin framework for the analysis of NW digital designs.

Cyber Graph Queries for Geographically Distributed Data Centers

165541
Year 2 of 2
Principal Investigator: C. A. Phillips

Project Purpose:

Graph algorithms and analytics are central to a wide variety of cyber-related research and operational activities. Almost without exception, such algorithms assume the availability of a fully constructed graph over which the analysis is performed. In this classic model, all the necessary data is co-located and available, even if large, noisy, or laden with constraints. From this data, a graph is constructed and any of a number of analysis algorithms can be performed.

"Big Data" computing and storage trends are driving a new model, in which raw data is not centrally co-located or available for transformation into a single, global graph for analysis. A global perspective of the data is needed, but the data (and the resulting graph) is instead realized physically as a set of independently collected, overlapping subgraphs that cannot be fully combined. We have seen this model emerging in mission-centric spaces. Data owners recognize the problem, but the technology does not exist to address it.

This project focuses on performing the algorithmic research necessary to adapt and/or recreate classic cyber graph analysis algorithms to this new graph model. Cyber-related graph algorithms (and general graph algorithms as well) have not been designed to function under the constraints of this model. Further, the nature of the model itself does not lead to a straightforward translation of existing algorithms, new algorithms, or at least algorithm kernels, will need to be invented.

Recently, we performed an initial assessment of this model using Connectivity as a motivating example. The team has concluded — and demonstrated — that Connectivity algorithms can be designed that satisfies the constraints of the model. At the same time, we recognized that extending other cyber graph algorithms to this model is a nontrivial research effort, requiring different computational and communication structures than are classically employed.

Summary of Accomplishments:

We developed a new formal model for graph computations for distributed cooperating autonomous data centers. Our previous model limits information sharing to a polylogarithmic portion of the combined graphs. The new one is secure multi-party computation, where each party learns only the answer, revealing nothing to an honest-but-curious data center. We developed an algorithm to determine if two given nodes are connected. Our low-trust algorithm does not make cryptographic assumptions and is more efficient that general circuit-based algorithms.

We proposed a new topological property for human social networks based on social literature. This property concerns the number of triangles a node forms with its neighbors as a function of its number of connections. We conjecture that technological social networks like Facebook or Twitter are the union of a human network and an automated (bot) network. We developed methods for finding some automated nodes in these networks. We developed a human/bot classifier for Twitter accounts based on topological and Twitter properties. We are refining the classifier and using it to validate network-separation methods.

We developed a provably efficient algorithm for finding a planted clique in a social network in the limited-sharing model, assuming our topological property. We must find an artificially added, fully connected sub-network that is larger than those found natively in this type of graph. In our problem, the nodes are selected randomly, but an adversary assigns edges to the data centers. To test such an algorithm on standard social network data sets, we must extract the human network.

Our contributions are the model — which captures realistic constraints on cooperating autonomous data centers, steps to more rigorously analyze social networks, and a start at better understanding the interplay between human and non-human behavior in social media.

Significance:

Autonomous cooperating data centers naturally model any entities that want to, or must, combine information to answer important questions from social networks, but do not wish to actively combine the data. The data could be expensive/commercially valuable or sensitive. This work shows it is possible to solve algorithms requiring global information in the worst case, with limited information sharing.

Our conjecture for a human network topology property, well supported by social literature, implies that some established properties of social networks are strongly influenced by non-human elements. This could have substantial impact on the current active area of social network analysis.

Refereed Communications:

J.W. Berry, A. Kearns, C.A. Phillips, and J. Saia, "Finding a Planted Clique in a Distributed Social Network," presented at the *SIAM Workshop on Network Science*, Chicago, IL, 2014.

J.W. Berry, L.K. Fostvedt, D.J. Nordman, C.A. Phillips, C. Seshadhri, and A.G. Wilson, "Why Do Simple Algorithms for Triangle Enumeration Work in the Real World?" presented at the *5th Innovations in Theoretical Computer Science*, Princeton, NJ, 2014.

Applying Cognitively Inspired Computing Systems to Create a Robust Cyber Protection Architecture

165542
Year 2 of 2
Principal Investigator: J. H. Naegle

Project Purpose:

Current technologies protecting from cyber attacks have many significant limitations including:

1) Computational Horsepower: use of commodity processors is a horrific fit for security rule sets that are embarrassingly parallel, typically byte aligned, and require large randomly accessed memory images.
2) Cost: the cost of security is increasing as a percentage of the overall cost of computing. The emerging cloud exacerbates this problem.
3) Vulnerability to Direct Attack: co-resident security software can be compromised by malicious code.
4) Management Complexity: improper management of distributed, diverse software packages can compromise their functionality .

Typical cyber problems can be broken into two categories: threat detection and high-speed matching (or filtering). We propose to address the latter category because it is typically ill suited for von Neumann architectures and can be used to build more advanced detection mechanisms.

A new approach that provides orders of magnitude more compute capability and isolates the security function from systems would improve the dynamics of cyber protection. Several missions are running into computational efficiency problems. The cyber Work for Others (WFO) programs are producing analytics that are beyond the capabilities of current compute systems. It is critically important for our mission partners to create an affordable, distributed security infrastructure to solve problems like security in cloud computing. New streaming compute architectures that promise orders of magnitude improvement in processing and memory performance in a small form factor with less power could be a major advantage. Other domains with streaming compute problems, such as space computing and remote/mobile sensors, would also greatly benefit from a breakthrough in the processing of streaming data. Sandia and Blue I Systems are collaborating on a very simple, cognitive inspired data processing unit based on a cortex model. The design utilizes massively parallel, simplistic compute elements coupled to a uniquely configured, very high bandwidth memory.

Summary of Accomplishments:

We were able to demonstrate that the temporal version of the database processing unit (DPU) architecture could deliver orders of magnitude performance improvement specifically in two cases of interest.

The first application was for a reinforcement-learning agent named BECCA. We developed a cycle accurate software emulator for the DPU to perform the most computationally intensive part of BECCA, the model comparator for determining the best fit of the current state to many previous states. We were able to demonstrate that a field-programmable gate array (FPGA) implementation of the DPU would provide three orders of magnitude performance improvement over the current implementation on a modern Intel processor and that an application-specific integrated circuit (ASIC) would provide five orders of magnitude performance improvement. Even greater improvements would result for power, space, and cost comparisons.

The second application we investigated was the implementation of signature detection in cybersecurity data. The detection of Perl Compatible Regular Expressions (PCRE) rules is a fundamental function for many cybersecurity tools. The SNORT cyber tool is the best example. We determined some of the most difficult and most effective PCRE rules to implement. We developed the required capabilities to allow the DPU to implement those PCRE rules. We compared the performance using the DPU emulator and the existing Intel based SNORT platforms. We measured a performance improvement of 100 times for an FPGA and 3000 times for an ASIC.

We developed and demonstrated pre-attentive visual processing capabilities with the spatial-temporal (st) version of the DPU. We utilized advanced hippocampal models and state storage techniques to implement a predictive tracking system with the st-DPU. While performance was not measured, the ability to perform important problems in this new architecture was a major accomplishment.

Significance:

Many important malware events can be detected by applying PCRE filters with SNORT Internet traffic and alerting on matches. With these performance gains, the SNORT functionality would be much more effective. The low cost of implementation could enable intelligent sensors and provide data for internal threat analysis.

The data delivered from this project provided assurance that brain inspired architectures can be effective at mitigating cyber-attack problems.

Nested Narratives

165543
Year 2 of 2
Principal Investigator: A. T. Wilson

Project Purpose:

There is a great deal of research and development around vulnerability assessment and anomaly detection in a network. Far less focuses on effective communication of these anomalies. Almost none concerns the path from data to insight and decision support. A list of 125 widely used cybersecurity tools include 60 for vulnerability assessment, 17 for monitoring, and 10 for forensics — only six of which are meant specifically for cybersecurity. Moreover, all six of those focus on fine-grained detail and leave analysts to construct the bigger picture without further assistance. Only one tool provides any support for modeling scenarios instead of data.

We will bridge this gap by addressing the following research challenges:

- Attribute traffic on a testbed network to the processes and user actions that caused it
- Help analysts construct stories from that data that tell what is happening and why
- Preserve those stories in multi-layered artifacts that can be used to tell the story at any level from strategic intent down to actual data

We will create algorithms and tools that enable flexible narratives of "how" and "what" backed by original data captured from a network. We will measure success by the richness of the scenarios we can capture as well as by quantifiable benefits to cybersecurity analysts.

Success will narrow the gap between data and understanding, and between an event and situational awareness. It will allow richer communication by bringing data and story closer together and give analysts powerful new building blocks for what they do best.

The idea of narrative has received close attention recently as an accessible representation of complex information. Our innovation stems from embodying narrative in the cyber domain by combining Sandia's unique cyber capabilities and cognitive science and analysis expertise. These capabilities position us uniquely to make this leap.

Summary of Accomplishments:

We demonstrated that providing tools that support the formation of narratives makes a major difference in how well users can perform forensic tasks such as assembling sequences of actions and actors from scattered clues. While we were unable to construct the cyber narrative templates that we had originally planned, the results of this user study strongly support our original hypothesis that framing forensic tasks as narrative formation leads to better performance.

We tested our approach to detection and attribution of computer and network events by instrumenting the operating system to record logs of activity at all levels. We found that this approach alone does not lead to high-confidence causal relationships between different computers.

Significance:

Training incident response teams for cybersecurity is of critical importance. Right now it takes place through an ad hoc apprenticeship where it is entirely incumbent upon the student to learn the tricks of the trade. Our work demonstrates that narrative structure leads to significantly better performance on forensics tasks by inexperienced subjects – exactly the situation we're trying to improve.

Active Learning for Alert Triage

165544
Year 2 of 2
Principal Investigator: J. E. Doak

Project Purpose:

In cybersecurity systems, data from multiple sources are typically logged to a centralized database. When certain conditions in the data are met, an alert is generated in an alert management system. Analysts inspect these alerts to decide if any deserve promotion to an event requiring further scrutiny. This triage process is manual, time-consuming, and detracts from the in-depth investigation of events. Our goal is to develop an automated alert ranking system that is fully integrated into the current analysts' workflow. We will conduct this research by leveraging access to authentic security system data, because we feel this is a superior alternative to theoretical or synthetic data.

We propose the use of active learning to selectively query the analysts for labels on alerts. Empirical and theoretical evidence indicates that active learning can outperform passive learning (i.e., randomly selecting instances for labeling) on a variety of learning tasks. In addition, our literature review indicates that the field of active learning is well established in terms of its theoretical underpinnings, but the application of active learning to real-world problems is in its infancy. Thus, the primary research challenges associated with this project will be how to map active learning theory onto our particular problem and how to address the various practical concerns that will undoubtedly arise.

There are many unknowns in the application of active learning to a cybersecurity problem. For example, which active learning scenarios and query strategies are most appropriate for the problem? What practical, unanticipated considerations will we need to address? Despite the risks, the need is great as cyber analysts are struggling to effectively triage the ever-increasing flow of alerts. This project has the potential to greatly assist analysts by providing a prioritized list of alerts so that only the most important alerts need to be inspected.

Summary of Accomplishments:

We solved the problem of ranking cybersecurity alerts by developing a pipeline that consisted of feature extraction, feature importance/selection, model building, alert ranking, active learning, and evaluation. Our most significant accomplishments were in the areas of features extraction, active learning, and evaluation.

We extracted features for the prediction models using three different techniques. First, we extracted features directly from the alert. An example of this feature type is the time at which the alert was generated. Second, we used other data sources besides the alert dataset itself to enhance our feature set. For instance, we extracted entities from the text of alerts, and then used other data sources to determine our interest in these entities. Third, we deployed cascading models (i.e., using models to generate additional features). Latent Dirichlet allocation is one model we deployed in this fashion and the features it creates are the fractional membership in various topics as determined by the alert text.

We deployed active learning to identify the alerts that, if we obtained labels for them, would most improve the predictions of the learned model. We implemented two active learning strategies: uncertainty sampling and query by committee. Both of these techniques clearly outperformed passive learning (i.e., randomly selecting alerts for labeling) on two alert datasets. We also demonstrated the superior performance of active learning vs.

passive learning on malware and Windows Registry datasets to demonstrate the promise of this technique for other applications.

Our work in evaluation focused on three different areas: cross-validation to evaluate models, evaluation of active learning strategies, and evaluation in the context of recommender systems. Of these, we feel we made our strongest contributions in the area of active learning evaluation by creating a novel strategy for plotting the effectiveness of active learning vs. passive learning.

Significance:

We took the idea of applying active learning to alert triage from conception to production. Thus, we not only performed significant R&D, but we also worked with cyber incident response personnel to integrate our ranking and active learning algorithms into a production alert management system. We made significant R&D contributions in feature extraction, active learning, and active learning evaluation. We also feel that deployment of the alert triage framework to an active production alert management system may significantly aid cyber analysts in their processing of alerts and thus improve cybersecurity posture.

Refereed Communications:

J.E. Doak, J. Ingram, J. Shelburg, J. Johnson, and B.R. Rohrer, "Active Learning for Alert Triage," in *Proceedings of Machine Learning and Applications (ICMLA), 2013 12th International Conference*, pp. 34-39, Miami, FL, 2013.

Quantum Graph Analysis: Engineering and Experiment

165577
Year 2 of 3
Principal Investigator: P. L. Maunz

Project Purpose:

In recent years, advanced network analytics have become increasingly important to national security with applications ranging from cybersecurity to detection/disruption of terrorist networks. While classical computing solutions have received considerable investment, the development of quantum algorithms to address problems, such as data mining of attributed relational graphs, is a largely unexplored space. Recent theoretical work has shown that quantum algorithms for graph analysis can be more efficient than their classical counterparts. Specifically, an adiabatic quantum version of Google's quantum PageRank (QPR) algorithm could offer polynomial speedup in the time required to identify the most important nodes on a graph. We plan a combined theoretical/experimental effort to implement QPR in a system of trapped-ion quantum bits (qubits). Furthermore, we will identify classical graph analysis methods most relevant to national security and seek to develop more computationally efficient quantum alternatives.

Implementing a quantum algorithm is extremely difficult because qubits must be precisely controlled and well shielded from environmental decoherence. The few existing academic groups with quantum algorithm capabilities typically focus on demonstrating elements of universal quantum computing or simulating physical systems. In contrast, we will develop quantum capabilities that target national security concerns, such as quantum graph analysis (QGA). QGA theory is in its infancy and no QGA algorithm has been experimentally implemented.

Over the past decade, Sandia has become a world leader in microfabricated surface ion-trap technology. We have developed the hardware and software infrastructure required for qubit control and quantum algorithm implementation. This infrastructure will be used to implement ion-ion interactions required for a QGA demonstration. We will also continue to advance QGA theory by developing additional QGA algorithms. Our coordinated efforts will establish a strong quantum information processing partnership well positioned to execute future programs relevant to national security.

Highly Efficient Entangled Photon Source for High-Speed Secure Quantum Communication Network

166151
Year 2 of 2
Principal Investigator: D. B. Soh

Project Purpose:

Highly efficient entangled photon sources are key components in high-speed unconditionally secure quantum-communication networks (QCNs), as well as other quantum technologies (e.g., optical quantum computers and quantum sensors). However, current photon-generation technologies do not meet the demands for practical high-speed networks. All published field-tested QCNs employ brute-force attenuated lasers, which have a critical security vulnerability to photon-number-splitting attacks. Additionally, true single-photon sources with nonlinearly converted entangled photons have a prohibitively slow generation rate, resulting in only kHz communication speeds at distances of over 100 km. Considering photon losses through non-ideal detector efficiencies, as well as subsequent error-correction and privacy amplification processes, highly efficient sources of entangled photons are crucial for practical high-speed secure QCNs.

So far, two methods have been used widely to produce entangled photons: spontaneous parametric down conversion (SPDC) in bulk materials and spontaneous four-wave mixing (SFWM) in optical fibers. Besides its intrinsic low efficiency, SPDC suffers a significant loss when coupled into optical fiber, due to the poor beam quality of photons. Although orders of magnitude more efficient, SFWM suffers from photon contamination, which substantially undermines the QCN's security. The lack of high-quality sources of entangled photons significantly impedes the development of practical large scale QCNs.

We intend to develop a highly efficient entangled photon source based on a recent Sandia invention: fiber-based asymmetrically pumped SFWM entangled-photon generation. This pioneering technology addresses the persistent problem of photon contamination. The key idea is to produce and employ two-tone pump photons at desired widely separated wavelengths. Our method creates entangled photons at any desired wavelength (especially at telecom 1.5 micron) when combined with dispersion-engineered photonic crystal fibers (PCFs). This photon source will be a game changer enabling truly uncompromised and practical QCNs. Without photon contamination, one can increase the pump power further to generate high-order entangled photons efficiently. This breakthrough can find important applications in optical quantum computing and quantum sensing.

Summary of Accomplishments:

We developed novel photon sources for the discrete-variable quantum key distribution (DV-QKD) and the continuous-variable quantum key distribution (CV-QKD).

For DV-QKD, we invented a novel fiber four-wave mixing heralded single photon source that utilizes photonic crystal fibers. The developed photon source accomplished a heralded single photon source: twin photons are created through rigorous physical principles, resulting in identical photon number at two modes (polarization modes in our case). Monitoring the number of photons in one mode controls the output gate of the other mode, in order to provide purely single photon source. Unlike the conventional parametric down converted photons, which exhibit Poissonian statistics, the developed single photon rigorously controls the number of output photons, truly generating only single photon events. We also derived detailed fiber four-wave mixing quantum model, resolving the temporal and spectral evolution of the non-degenerate strong pump pulses. Such rigorous treatment of the Helmholtz equation, which governs the evolutions of both the classical wave field (pump lasers) and the quantum wave fields (idler and signal), is necessary in order to optimize the performance of single photon generation in a very detailed manner. We established, for the first time, a rigorous evolution model of quantum fields, incorporating waveguide dispersions and temporal effects.

For CV-QKD, we developed novel squeezed light source utilizing coherent quantum feedback control technique. The coherent feedback not only improves the degree of squeezing, but also creates new dynamics, providing new functionalities with novel spectral characteristics. The developed squeezed source relies on a new dynamic, which is created only through a feedback control network among multiple quantum systems. In order to treat the coherent evolution of quantum systems in the network, we employed the recently developed SLH models of quantum input-output relations and quantum device connections. We successfully demonstrated 2 dB squeezing through the system.

Significance:

Developing single photon sources could impact many national security missions: quantum communication and optical quantum computations utilize the single photons as an information carrier. Quantum enhanced sensing provides unconventional detecting capabilities. Avoiding multiphoton events are important in security of communication and computation since an eavesdropper can practice the photon-number splitting attack. Developing squeezed light as well as understanding the quantum feedback network has even more impact in future computational and communication devices, which will no doubt employ the quantum enhanced features. Overall, the results of this project will be used for future quantum optical systems.

Model Reduction for Quantum Technologies

170973
Year 2 of 3
Principal Investigator: M. Sarovar

Project Purpose:

Precisely controlled, engineered quantum systems will be critical to next-generation measurement, computing, and communication technologies. However, as we attempt to design and construct larger and more complex quantum devices, we quickly approach a difficult impasse. Namely, the task of modeling and simulating such large-to-medium scale quantum mechanical devices becomes computationally challenging since the size of modeling state-space increases exponentially with the number of degrees of freedom. This difficulty severely limits our ability to perform predictive simulation of quantum technology devices.

In this project, we will take a systems-level approach to this problem and develop techniques for reducing the modeling complexity of a broad class of potential quantum devices. The primary thrust of the research will be to extend rigorous model reduction techniques from mathematical engineering (e.g., proper orthogonal decomposition, unsupervised manifold learning) to the quantum realm. Properties such as non-commutative structure preservation will be incorporated into these classical model reduction techniques in order to make them suitable for quantum systems. The successful formulation of such quantum model reduction methods will enable rigorous performance analysis of quantum devices, including application of methods for uncertainty quantification (UQ) and verification and validation (V&V). This, in turn, will enable more rapid development of near-term quantum technologies for tasks such as precision measurement and secure communication.

The proposed research is highly interdisciplinary and develops methods that bridge engineering, physics, and computer science. It has the potential to have broad impact on the quantum information sciences by generating new insights into the modeling and simulation of quantum mechanical systems. The research explores a new interdisciplinary domain and builds unique capabilities in an emergent field.

Using Trusted Execution Environments to Provide Monitoring and Protection of Mobile Operating Systems

173034
Year 1 of 2
Principal Investigator: T. G. Fine

Project Purpose:

The purpose of this project is to understand the TrustZone technology available in Advanced RISC Machines, Ltd. ® (ARM) processors and demonstrate its use in addressing mobile security concerns relevant to US Government organizations. TrustZone separates an ARM-based system into two virtual systems called "Secure World" and "Non-Secure World." The intent is to run a traditional operating system such as Android in Non-Secure World and to run minimal code in Secure World providing desired security functionality. While some components of the TrustZone architecture are mandatory, much of the architecture is optional and can be custom to a specific vendor. While TrustZone provides an air of security, realizing the promised security requires understanding the proper way to use the various TrustZone components.

When developing software to run in Secure World, the code can be entirely custom or can build upon a minimal operating system. A number of such operating systems are available for use as a base, but their security is questionable. Some commercial products utilizing TrustZone have already been compromised due to errors in the code running in Secure World. Some of the operating system options are open source but others are proprietary.

After selecting an approach for writing the software, this effort will develop a prototype implementation of a security feature running in Secure World. This prototype will be used as a vehicle for researching the extent to which TrustZone can enable high-grade security mechanisms.

Using Linkographies of Cyber Attack Patterns to Inform Honeytoken Placement

173035
Year 1 of 3
Principal Investigator: J. C. Jarocki

Project Purpose:

Several research and development projects have deployed honeypots, honeynets, and honeytokens to confuse, slow, and detect cyber adversaries. However, the placement of these resources is typically agnostic of the behavior patterns and goals of the adversaries. This project focuses on learning adversarial patterns during cyber attacks so that the placement of false flags can be chosen to minimize attacker goals while maximizing defensive objectives. By acquiring data on cyber attack steps from real incidents, we can construct similar representations for normal patterns of adversarial understanding, behavior, and activity through a target network. Armed with this information, defenders can reduce the intelligibility of the target network and maximize the effort an adversary must apply to complete the mission.

This project will advance our understanding of cyber-attacker behavior. While effort has been spent characterizing the malware used in cyber attacks, there remains a gap in our understanding of the operators behind these constructs. Although work has been done to gauge the capabilities of cyber attackers, significant opportunities remain in using data from attacks to model cyber behavior. By leveraging techniques from other domains to analyze data, develop models, and create experiments, this research will open the door for future analysis and cognitive modeling of cyber attacks.

Measuring Human Performance within Computer Security Incident Response Teams

173036
Year 1 of 3
Principal Investigator: J. T. McClain

Project Purpose:

Computer Security Incident Response (IR) teams are key to our nation's strategy for addressing cyber threats. IR team training typically focuses on software tool skill sets with less effort devoted to understanding cognitive skills that distinguish experts from novices and promote effective team performance.

Expertise has been defined by Ericsson et al. (1993) as the "extended process of skill acquisition mediated by adequate daily amounts of deliberate practice" and is measured through performance (Dror, 2011). This definition is insufficient for IR training; analysts must quickly become experts, working in teams and identifying novel threats. To achieve efficient progress towards expertise, we argue that tool training is insufficient. Identifying the cognitive processes involved with cyber expertise, such as the acquisition of intuition (Chen & Holyoak, 2010) and acquiring varying perspectives (Chi, 2011) which guides problem solving by pruning strategies, is essential to the development of expertise and will enhance training.

This project seeks to quantify novice/expert differences through empirical testing. We will instrument the Research and Engineering for Cyber Operations Intelligence Laboratory (RECOIL) with validated measures to quantify cognitive/behavioral processes (e.g., electroencephalography [EEG]).

We will test the hypothesis that we can differentiate effective/ineffective individuals/teams by utilizing cognitive measures such as EEG and eye tracking. The integration of technical capabilities to develop a human performance measurement system for IR teams will offer a cornerstone for cybersecurity training programs. This work will be relevant to multiple national security customers.

Using Machine Learning in Adversarial Environments

173037
Year 1 of 3
Principal Investigator: W. L. Davis, IV

Project Purpose:

Intrusion/anomaly detection systems are among the first lines of cyber defense. Commonly, they either use signatures or machine learning (ML) to identify threats, but fail to account for sophisticated attackers trying to circumvent them. We intend to embed machine learning within a game theoretic framework that performs adversarial modeling, develops methods for optimizing operational response based on ML, and integrates the resulting optimization codebase into an existing ML infrastructure developed previously. Our approach addresses three key shortcomings of ML in adversarial settings: 1) resulting classifiers are typically deterministic and, therefore, easy to reverse engineer; 2) ML approaches only address the prediction problem, but do not prescribe how one should operationalize predictions, nor account for operational costs and constraints; and 3) ML approaches do not model attackers' response and can be circumvented by sophisticated adversaries. The principal novelty of our approach is to construct an optimization framework that blends ML, operational considerations, and a model predicting attackers reaction, with the goal of computing optimal moving target defense. One important challenge is to construct a realistic model of an adversary that is tractable, yet realistic. We aim to advance the science of attacker modeling by considering game-theoretic methods, and by engaging experimental subjects with red teaming experience in trying to actively circumvent an intrusion detection system (IDS), and learning a predictive model of such circumvention activities. As a part of this effort, we will generate metrics to test that a particular model of an adversary is consistent with available data. In contrast to other research efforts such as the Counter Adversarial Data Analytics (CADA) project, we will focus on adversarial modeling and response rather than the machine learning algorithms themselves. The two approaches are quite complementary, and will synergistically enhance our ability to provide robust and dynamic defenses for our computational systems.

Threat Relevant, Context-Based, Internal Situational Awareness

173038
Year 1 of 1
Principal Investigator: T. R. Devries

Project Purpose:

The purpose of the project is to develop methods for efficient and scalable analysis of network traffic and integration of business context information with network alerts.

Summary of Accomplishments:

We demonstrated technical methods for efficient and scalable network packet analysis and evaluated several methods to integrate and utilize business context information in alert evaluation.

Significance:

This exploratory research has developed network packet analysis techniques that will be useful to enhance national security and also informs future directions for further research in internal monitoring and business context. A methodology for detecting threat intrusions accurately and reducing the duration and impact of those events would greatly improve national security.

GRAND CHALLENGES

Grand Challenges are bold, game-changing ideas with the potential for enormous impact to the security of the nation through significant advances in science and engineering. Grand Challenge projects are expected to drive the future of Sandia by providing new directions, capabilities, and solutions and to provide long-term impact to multiple programs. These projects result in a long-term ST&E legacy for Sandia from breakthrough scientific discoveries through development of unique and differentiating technical capabilities. These projects are multimillion dollars in size and utilize multidisciplinary teams, often including external collaborators.

A diagram showing three months of civilian air traffic over the US and Canada comprising 440 million data points and over 4.5 million flights. Brighter areas indicate regions of denser traffic, especially around airports and major travel corridors. Trajectory databases such as this one afford the opportunity to develop novel methods to cluster flights based on their behavior and shape, predict where newly detected aircraft may be going, and identify anomalies at scales from a single aircraft to large groups detouring around severe weather. Similar algorithms apply to sea-going traffic, auto traffic and even gaze tracking. (Project 165535)

GRAND CHALLENGES

Science-Enabled Next-Generation Photovoltaics for Disruptive Advances in Solar Power and Global Energy Safety and Security

159257
Year 3 of 3
Principal Investigator: G. N. Nielson

Project Purpose:

With the development of a decentralized electricity grid, the emerging electrification of personal transportation, growing dependence on mobile devices, natural disasters that take centralized power plants offline, and persistent concerns about atmospheric emissions from fossil fuels, there is an urgent need for clean, convenient, and decentralized ways to generate electricity. However, there are no suitable energy harvesting technologies that have the ability to produce electricity from a variety of light sources, the scalability for gigawatt electricity generation, and the versatility to be incorporated directly into devices that need power. While solar energy can meet global energy consumption with orders of magnitude to spare, the collection and conversion of light to electricity remains two to three times more expensive than fossil fuel electricity generation. Unless and until this cost barrier is broken, new energy storage and smart grid technologies will not have an enabling, mainstream role.

Our team has conceived a photovoltaic system design that consists of microsystems enabled photovoltaic (PV) cells in an independently wired configuration, a microlens concentrator array, optics that allows coarse sun tracking, and massively parallel assembly to produce low cost, packaged PV energy systems. Together, these design elements decrease the need for high cost PV materials by three orders of magnitude, increase conversion efficiency per gram of utilized PV material by a factor of 30, and reduce overall system cost by a factor of two to three. These components, combined with our new manufacturing and installation concepts, have never been put together into a complete PV system, but have the potential for solving all key elements of this problem. It is the high cumulative risk along with the prospect of achieving the elusive cost breakthrough that has brought our team together to design, prototype, and test a complete microsystems enabled PV (MEPV) system with the capability to disrupt current fossil fuel and renewable energy generation paradigms.

Summary of Accomplishments:

During the course of this project, we developed key technologies that advance the state of the art in many areas of solar power.

We developed a new cell architecture based on a unique ability to transfer III-V solar cells (InGaP, GaAs, InGaAsP, and InGaAs) to silicon to create the potential for a five-junction, six-terminal multi-junction microscale PV cell that is not constrained by lattice matching, current matching, or spectrum matching. We demonstrated a 29.5% efficient InGaP/GaAs dual-junction cell transferred to silicon, a 3% efficient InGaAs cell transferred to silicon, and created an active silicon junction (solar cell) in the silicon itself. These results provide a direct path to a five-junction cell with a potential efficiency greater than 50%.

We developed new microlens arrays for concentration of light onto sparse arrays of microscale solar cells. These optics provide a very short focal length (~4 mm), 5-10X improvements in acceptance angles relative to current concentrated PV systems, and very high optical transmission (~90% demonstrated, 94% possible). These characteristics enable new concepts for concentrated PV that increase performance and reduce costs compared to all other PV technologies currently available.

We have demonstrated functional prototype modules based on these microscale cells and optics. These modules are 1 cm thick, have an acceptance angle compatible with current flat plate silicon trackers, and are very low cost. Our cost models indicate that this technology provides a clear and viable pathway to $1.00 per watt total installed system costs. This price level would make solar power the lowest cost energy source available.

In developing the microscale cells and demonstrating massive parallel assembly of microscale cells, we demonstrated a new highly flexible, highly efficient PV technology. This technology would allow solar cells to be integrated into the skin of almost any system.

Significance:

The technologies we developed provide new and unique energy harvesting capabilities. The flexible PV technology provides the ability to generate power anywhere there is light with a module that is robust to damage, highly flexible, has an extremely high specific power (~500 W/kg, 10X over current flexible PV technologies), and is inexpensive. Furthermore, the high efficiency cell and low-profile concentrator module technologies allows for very high-energy generation per area and per volume.

Refereed Communications:

B.H. Jared, M P. Saavedra, B.J. Anderson, W.C. Sweatt, G.N. Nielson, and M. Okandan, "Micro-Optic Fabrication for Microsystems-Enabled Photovoltaics," presented at the *ASPE Annual Meeting*, St. Paul, MN, 2013.

G N. Nielson, "Solar Photovoltaic Cell, Module, and System Performance and Functionality Enhancement through MEMS Technologies," presented at the *2013 MRS Fall Meeting and Exhibit*, Boston, MA, 2013.

G.N. Nielson, "Innovative CPV Approaches to Reduce Balance of System Costs," presented at the *5th Concentrated Photovoltaic Summit*, San Jose, CA, 2013.

B.B. Yang, J.L. Cruz-Campa, G.S. Haase, E.I. Cole, Jr., P. Tangyunyong, P.J. Resnick, M. Okandan, and G.N. Nielson, "Failure Analysis Techniques for Microsystems-Enabled Photovoltaics," *IEEE Journal of Photovoltaics*, vol. 4, pp. 470-476, January 2014.

B. Yang, J.L. Cruz-Campa, G.S. Haase, P. Tangyunyong, M. Okandan, and G. N. Nielson, "Stress Factor Assessment for Microsystems-Enabled Photovoltaics," presented at the *IEEE Photovoltaic Specialists Conference*, Denver, CO, June 8-14, 2014.

B.B. Yang, J.L. Cruz-Campa, G.S. Haase, E.I. Cole, Jr., P. Tangyunyong, M. Okandan, and G.N. Nielson, "Comparison of Beam-Based Failure Analysis Techniques for Microsystems-Enabled Photovoltaics," presented at the *International Symposium for Testing and Failure Analysis*, San Jose, CA, 2013.

J.L. Cruz-Campa, G.S. Haase, P. Tangyunyong, M. Okandan, and G.N. Nielson, "Reliability Model Development for Microsystems-Enabled Photovoltaics," presented at the *IEEE Photovoltaic Specialists Conference*, Denver, CO, 2014.

J.L. Cruz-Campa, G. N. Nielson, D. Riley, M. Okandan, A.L. Lentine, W.C. Sweatt, B.H. Jared, P.J. Resnick, J.A. Kratochvil, B. Kim, B.J. Anderson, V.P. Gupta, A. Tauke-Pedretti, J.G. Cederberg, T. Gu, M.W. Haney, S.M. Paap, C.A. Sanchez, C. Nordquist, M.P. Saavedra, M.H. Ballance, J. Nguyen, C. Alford, and J.S. Nelson, "Flat Plate Concentrators with Large Acceptance Angle Enabled by Micro Cells and Mini Lenses: Performance Evaluation," presented at the *28th EuPVSEC*, Paris, France, 2013.

B.H. Jared, M.P. Saavedra, B.J. Anderson, W.C. Sweatt, R.S. Goeke, G.N. Nielson, M. Okandan, B. Elisberg, D. Snively, and J. Duncan, "Micro-Concentrators for a Microsystems-Enabled Photovoltaic System," presented at the *Optics for Solar Energy*, Tucson, AZ, 2013.

G.N. Nielson, "Exploiting Scale Effects in Photovoltaic Cells, Modules, and Systems," presented at the *ARPA-E Microscale Photovoltaic Workshop*, Arlington, VA, 2014.

G.N. Nielson, "New Tech for Resilient Distributed Generation," presented at the *EPRI International Technology Innovation Summit*, New York, NY, 2013.

J.L. Cruz-Campa, J.G. Cederberg, J.S. Nelson, G.N. Nielson, C. Alford, C.A. Sanchez, and I. Luna, "Bonded InGaAs Cells for Microsystems Enabled Photovoltaics," presented at the *Photovoltaic Specialists Conference*, Denver, CO, 2014.

S.M. Paap, V.P. Gupta, A. Tauke-Pedretti, P.J. Resnick, C.A. Sanchez, G.N. Nielson, J.L. Cruz-Campa, B.H. Jared, J.S. Nelson, M. Okandan, and W.C. Sweatt, "Cost Analysis of Flat-Plate Concentrators Employing Microscale Photovoltaic Cells for High Energy Per Unit Area Applications," presented at the *40th IEEE Photovoltaic Specialists Conference*, Denver, CO, 2014.

A.L. Lentine, G.N. Nelson, M. Okandan, J.L. Cruz-Campa, and A. Tauke-Pedretti, "Voltage Matching and Optimal Cell Compositions for Microsystems Enabled Photovoltaic Modules, to be published in the *IEEE Journal of Photovoltaics*.

M.P. Saavedra, W.C. Sweatt, G.N. Nielson, M. Okandan, B. Elisberg, B. Anderson, B.K. Miller, and B.H. Jared, "Efficient Micro-Concentrator for Microsystems-Enabled Photovoltaics," presented at the *American Society for Precision Engineering*, Boston, MA, 2014.

A. Tauke-Pedretti, J.G. Cederberg, C.A. Sanchez, G.R. Girard, C. Alford, B.A. Aguirre, I.E. Luna, M. Okandan, J.S. Nelson, and G.N. Nielson, "Power Maximization in III-V Sub-Millimeter, Radial Front Contacted Cells for Thin Micro-Concentrators," presented at the *40th IEEE Photovoltaic Specialists Conference*, Denver, CO, 2014.

Extreme Scale Computing Grand Challenge

159258
Year 3 of 3
Principal Investigator: K. S. Hemmert

Project Purpose:

Leadership in computing has been a critical factor in national security for the last seven decades. This is particularly true for intelligence, nuclear weapons stewardship, the design and employment of military systems, and the scientific advances that underpin them. Over the last two decades, scientific computing has relied on commodity technologies that have provided ever increasing single thread performance to maintain an impressive rate of performance increases. Data applications have benefited from special purpose architectures designed with latency tolerant mechanisms. Technology trends towards energy constrained computing have made it infeasible to continue increasing single thread performance and have led to the exploitation of on-node parallelism in the form of large vectors and multiple lower performing processing cores. Vendors are still in the process of determining the best way to optimize within these new constraints, providing an ideal opportunity to define the architectural innovations that enable a single set of computing components to support both science and data applications. We intend to develop key architecture concepts that enable a unified physics/data analytics computing platform, or determine what gaps prevent it.

Data transport energy will dwarf compute energy. Fixing this requires rethinking solutions, including finding the most efficient implementation devices, integrating them in a system, and developing new computational models that allow deep insights and new solution methods. Computational science must shift from minimizing run time to minimizing the entire energy-delay product of an application.

Sandia is uniquely qualified to examine new approaches to creating a unified architecture. It alone has the expertise in microelectronic technologies, computer architecture, systems software, and applications that allow it to pursue the comprehensive atoms-to-applications research needed to overcome the energy challenge posed by data movement in such systems. In addition, market forces are directing major computer companies towards hand-held devices and large-scale “cloud” servers, and away from the large-scale tightly integrated systems required for high performance computing (HPC).

Summary of Accomplishments:

We continued work on multiple mini-applications in both the scientific computing and data analytics spaces. Work on miniGhost showed that task parallel decomposition is a promising approach to more efficiently using multi-core processors. We also studied the differences and similarities in execution characteristics between these miniapps using hardware performance counters. This information will be used to determine the feasibility of creating a common set of components to support both the informatics and computational sciences application areas.

We developed simulation models to analyze the effectiveness of processing in memory using traditional applications and also a novel-sorting algorithm that takes advantage of multiple levels of user-level memory. Additionally, we developed simulation models to study the effects of the system level network capabilities on communication patterns representative of two miniapps.

We have demonstrated that co-design between the various levels of the hardware architecture and software can enable efficiency gains at the system level.

The photonics thrust accomplishments were: calculations showing energies of 100 femtojoules/bit at 30 Gbps for silicon photonics interconnects; thermal crosstalk measurements versus modulator/filter separation; closed loop control of the resonant wavelength of a modulator using balanced homodyne detection over 55 degrees with no error rate degradation; and an integrated circuit (IC) design to demonstrate integrated resonant wavelength control. We invented and demonstrated an external heater-modulator, and constructed an automated test set for evaluating yield and wavelength uniformity of devices at the wafer scale.

Significance:

We demonstrated the value of co-design for HPC. It has also created significant capabilities in studying tradeoffs for future HPC systems, most of which are open source and/or freely available. These capabilities will contribute to the national conversation surrounding extreme scale computing and its use in national security missions.

Refereed Communications:

A. Rodrigues, D. Stark, S. Hammond, and J. Laros, "Sandia Advanced Architecture R&D: Simulation and Testbeds," presented (invited) at the *SOS14 Workshop,* St. Moritz, Switzerland, 2014.

A. Rodrigues, S. Hemmert, S. Hammond, and B. Moore, "The Structural Simulation Toolkit: Uses and Roles," presented at *Modeling and Simulation of Systems and Applications*, Seattle, WA, 2014.

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J.A. Cox, A.L. Lentine, D.J. Savignon, R.D. Miller, D.C. Trotter, and A.L. Starbuck, "Very Large Scale Integrated Optical Interconnects: Coherent Optical Control Systems with 3D Integration," presented (invited) at *Integrated Photonics Research, Silicon and Nanophotonics*, San Diego, CA, 2014.

A.L. Lentine, "Silicon Photonics for Software Defined Data Center Networks," presented (invited) at the *OIDA/CIAN Meeting on Software Defined Photonic and Data Center Networks*, San Francisco, CA, 2014.

C.T. DeRose, R. Kekatpure, A. Starbuck, A. Pomerene, and A.L. Lentine, "A CMOS Compatible External Heater-Modulator," in *Proceedings of the IEEE Optical Interconnects Conference*, pp. 17-18, San Diego, CA, 2014.

C.T. DeRose, N.J. Martinez, R.D. Kekatpure, W.A. Zortman, A.L. Starbuck, et al., "Thermal Crosstalk Limits for Silicon Photonic DWDM Interconnects," in *Proceedings of the IEEE Optical Interconnects Conference*, pp.125-126, San Diego, CA, 2014.

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T. Latchu, M. Pochet, N.G. Usechak, C. DeRose, A. Lentine, D.C. Trotter, et al., "Power-Penalty Comparison of Push-Pull and Traveling-Wave Electrode Silicon Mach-Zehnder Modulators," in *Proceedings of the IEEE Optical Interconnects Conference*, pp. 25-26, San Diego, CA, 2014.

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J.A. Cox, A.L. Lentine, D.J. Savignon, D. Trotter, and A.L. Starbuck, "Wavelength Control of Resonant Photonic Modulators with Balanced Homodyne Locking," in *Proceedings of the CLEO: Science and Innovations*, p. STh4M.7, San Jose, CA, 2014.

A. Lentine, R. Grzybowski, and J.M Shalf, "Introduction to the JLT Special Issue on Optical Interconnects," *Journal of Lightwave Technology*, vol. 31, pp. 3905-3906, December 2013.

R.F. Barrett, D.W. Doerfler, S.S. Dosanjh, S.D. Hammond, K.S. Hemmert, M.A. Heroux, P.T. Lin, J.P. Lutjiens, K.T. Pedretti, A.F. Rodrigues, and T.G. Trucano, "Exascale Design Space Exploration and Co-Design," *Future Generation Computer Systems*, special issue on Extreme Scale Parallel Architectures and Systems, vol. 30, pp. 46-58, January 2014.

R.F. Barrett, S. Borkar, S.S. Dosanjh, S.D. Hammond, M.A. Heroux, X.S. Hu, J. Luitjens, S. Parker, J. Shalf, and L. Tang, "On the Role of Co-Design, High Performance Computing," E.H. D'Hollander et al. (Eds.), *IOS Press*, November 2013.

R.E. Grant, S.L. Olivier, J.H. Laros, R. Brightwell, and A.K. Porterfield, "Metrics for Evaluating Energy Saving Techniques for Resilient HPC Systems," in *Proceedings of the 9th IEEE Workshop on High-Performance, Power-Aware Computing*, pp. 790-797, Phoenix, AZ, 2014.

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Pattern ANalytics To Support High-Performance Exploitation and Reasoning (PANTHER)

165535
Year 2 of 3
Principal Investigator: K. R. Czuchlewski

Project Purpose:

PANTHER designs analytic techniques that efficiently detect patterns in high-volume, noisy, remote sensing data. High-consequence, national security decisions rely on timely, comprehensive answers to complex questions, yet critical gaps remain. PANTHER addresses these gaps through fundamental research on:

- Geospatial-temporal feature extraction via image segmentation and classification
- Geospatial-temporal graph algorithms and computational geometry
- Domain-relevant models of human perception and cognition informing the design of analytic systems

Despite advances in remote sensing data collection, national security analysts struggle with complex geospatial-temporal queries. PANTHER is motivated by three classes of challenge problems, which, if solved, could vastly simplify and deepen the analysis of large and growing volumes of geospatial data:

1) Signature Search: PANTHER improves upon simple relational databases. First, we have created a new type of functionality in graph analysis that permits detection of relationships that would otherwise remain obscure. Second, we overcome computational hurdles by encoding only non-constant features. Third, we measure uncertainty in results by addressing error bounds on the underlying data.
2) Motion and Trajectory Analysis: Existing tracking algorithms do not easily represent and store track attributes. PANTHER approaches this problem by representing tracks as ensembles of geometric attributes. One can efficiently search these scalars for patterns and outliers and, thereby, solve the currently intractable problem of track comparison.
3) Practical Applications: Our human analytics research is designing metrics and experiments to test the performance of our algorithms in everyday practice.

Our integrated, mathematically and computationally elegant approach will support human problem solving.

PANTHER's cross-disciplinary R&D approach, and pursuits of the fundamental science and mathematics to understand how to maximize decision systems distinguishes us from industry and academia. Our project is a fundamental rethinking of key aspects of geospatial data analysis, motivated by real national security problems.

Sandia Communications and Authentication Network using Quantum Key Distribution (SECANT QKD)

173103
Year 1 of 3
Principal Investigator: R. Camacho

Project Purpose:

To address the challenge of securing communication networks against increasingly sophisticated cyber attacks, we envision a microsystems-enabled communications and authentication environment with information security based on quantum physics using a radically new approach to quantum key distribution (QKD). This technology, if successful, will dramatically change the landscape of cyber warfare, mitigate technology surprise, and allow for rapid exploration of weaknesses in similar systems adopted by adversaries.

Currently, communications security relies on widely accepted (though never proven) beliefs in the difficulty of solving certain mathematical problems and is not "future proof." In contrast, our planned SECANT QKD system uses the laws of quantum mechanics to enable a network of authorized parties to establish secret cryptographic keys. All current QKD systems rely on bulky tabletop components limited in speed (<Mbt/s) and distance (<100 km), and require central trusted nodes for network operation. Through this project, we will address major scientific challenges in chip-scale quantum optics to integrate a full QKD system on a chip and demonstrate a novel network architecture allowing direct node-to-node key generation and authentication.

Addressing these challenges requires leveraging leading-edge capabilities across Sandia. For example, developing multiplexed chip-scale single-photon detectors (one of many QKD components) requires several innovations, substantial microfabrication equipment, and years of expertise in materials, semiconductor, and quantum science — all now present for the first time at Sandia. The entire effort will also require state-of-the-art expertise in integrated silicon photonics, fiber lasers, quantum sources, optical communications, and cryptography.

Just as chip-scale transistors displaced vacuum tubes, chip-scale quantum transceivers will displace current QKD systems and transform secure communications. Such advances would dramatically alter the state of the art in QKD and allow for widespread implementation in existing telecommunications infrastructure. If successful, this project will establish a critical intellectual property portfolio for Sandia with major commercial and national security importance, and serve as a national resource for secure communications research.

New Capabilities for Hostile Environments

173104
Year 1 of 3
Principal Investigator: P. J. Griffin

Project Purpose:

The purpose of this project is to develop new physical simulation capabilities in order to support the qualification of non-nuclear weapon components in hostile radiation environments. The project contributes directly to the goals of maintaining a safe, secure, and effective US nuclear stockpile, maintaining strategic deterrence at lower nuclear force levels, extending the life of the nuclear deterrent capability, and to be ready for technological surprise.

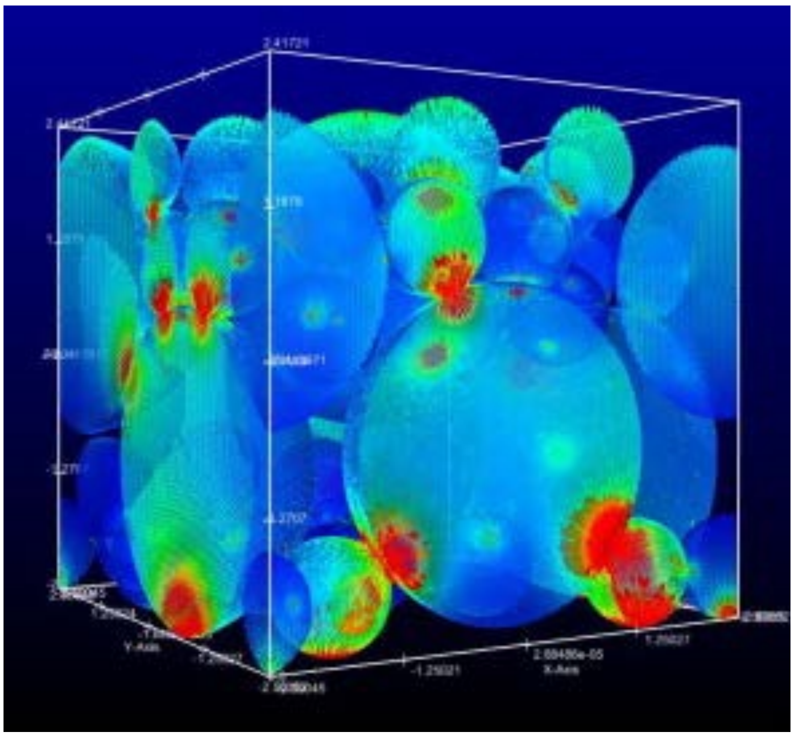
We will develop fast neutron and warm x-ray sources and provide radiation effects testing environments on the Z Pulsed Power Facility that will fill gaps in presently available experimental capabilities at fluences and spectra of interest and over object sizes of interest to stockpile qualification. These new capabilities will enable the stockpile modernization program to take advantage of risk-informed tradeoffs between margin, cost, schedule, and hardness for the design and qualification of advanced technologies.

Our planned technical path leverages the advances made in our understanding of the physics and performance of classified Z-pinch targets over the last six years. Development of the sources will require use of innovative ways to increase the delivery of current to Z-pinches, further advances in the target design of warm x-ray and neutron sources, and in developing an innovative scientific and engineering basis to safely use tritium on the Z Facility. Equally important, we must develop warm x-ray and fast neutron science platforms on Z that allow the fielding and diagnosis of powered and actively probed circuits during Z operation.

This project will utilize a dual-pronged approach to develop experimental platforms and innovative neutron and x-ray sources that will bridge present and forecasted gaps in nuclear weapons mission space. We will significantly enhance our capability through iterative development cycles of theory, simulation and design coupled with experiments on Z to validate innovative source designs, and development and fabrication coupled with experiments on Z to validate experimental configurations and advanced diagnostics.

RESEARCH CHALLENGES

Research Challenges seek to surmount a critical-path technical obstacle to solving a difficult national security problem. They address a complex problem by bringing together a broad cross-section of Sandia capabilities, engaging expertise ranging from fundamental science to technology application.   A Research Challenge is expected to leave a science and engineering legacy that enables Sandia to strongly address future national security missions. Initiated during mid-FY 2013, the Research Challenge/Mission Challenges Investment Area sponsors LDRD projects that align with Sandia's most current and forward-thinking strategic endeavors, preparing Sandia for the future by sponsoring groundbreaking interdisciplinary research challenges that create transformational opportunities in national security.



A modeled simulation of heat flux in a grandular material, showing what appear to be several preferential "channels" for heat flow. (Project 171054)

RESEARCH CHALLENGES

Revisiting the Applied Mechanics Paradigm: Multiscale Modeling of Transport Processes in Complex Materials

171054
Year 2 of 2
Principal Investigator: J. B. Lechman

Project Purpose:

The complex response of inhomogeneous materials to mechanical and thermodynamic loads results from multiple dynamical/stochastic processes, anti-correlated and correlated, occurring over multiple length and time scales leading to significant variability in performance. Current challenges in predicting this behavior include: 1) identifying and characterizing physical and/or chemical processes, and their couplings across multiple length and time scales; 2) modeling information transfer between scales; and, 3) resolving inhomogeneities in order to quantify uncertainty. Overcoming these challenges to create engineered solutions requires multiscale materials theory/modeling and experimental discovery/characterization. Many multiscale modeling efforts employ a hierarchy of governing equations and simulation tools each specific to a particular scale; however, this approach is limited by a priori assumptions of the degree of coupling between scales and a posteriori methods of restoring this coupling. In practice, these so-called hierarchical approaches rely on one-way propagation of information: atoms-up. Moreover, although numerical simulation with concurrent coupling of, say, classical atomistic dynamics and macroscale governing equations is possible, transfer of information can be significantly hampered by scale mismatch, and becomes computationally intractable when a series of mesoscales with associated phenomena are present.

The project goal is to discover and create modeling techniques for predicting the behavior of inhomogeneous materials. Hence, we will develop a novel scale-consistent modeling framework for formulating governing balance equations — coupling spatial and temporal correlations from micro- through meso- to macroscales. Scale-consistent models reduce complications associated with multiscale data transfer and coupling between simulation tools because multiple scales are embedded in the model formulation. However, this requires advancing experimental discovery and characterization tools for complex materials and processes spanning relevant scales. If successful, this project will demonstrate a methodology that provides multiple scale effects in one approach. While demonstrating the approach for thermal properties in pyrotechnic applications, it can be extended to different materials applications.

Summary of Accomplishments:

A concomitant experimental characterization and model development strategy was deployed in this project. We advanced several experimental characterization techniques at various scales to elucidate the multiscale nature of the thermal transport problem in particulate materials. We implemented and demonstrated a flash diffusivity capability for measuring homogeneous thermal conductivity of powders. We demonstrated the use of IR techniques to resolve the thermal field at speeds and scales relevant to engineering parts. We used focused ion beam scanning electron microscopy (FIB-SEM) imaging techniques to visualize pyrotechnic powders. Finally, we applied time-domain thermoreflectance to measure boundary conductance between constituent materials of pyrotechnic powders. In concert with these efforts, several modeling and simulation advancements were made. A new approach to predict contact resistance from first principles simulations was developed. Finally, new mesoscale computational approaches for conduction in particle packs were implemented and demonstrated. These included particle-scale image segmentation and numerical simulation of conduction, implementation of stochastic algorithms for conduction in heterogeneous materials, and analysis of applicability of continuous-time random walk models for scale bridging. As a result, several notable "firsts" associated with advancement of the frontiers of science and engineering were accomplished including: application of applied time-domain thermoreflectance to pyrotechnic material, FIB-SEM particle-scale imaging and visualization of pyrotechnic powders, and demonstration of applicability of continuous-time random walk models to scale-bridging for conductive transport in particulate materials. These led to improved prediction of interface thermal conductance from first principles calculations, the development of workflows for image segmentation and mesoscale simulation of thermal conduction in particle packs, and development of reduced order models for potential use in rapid prototyping or optimization.

Significance:

This multidisciplinary effort is advancing the science technology and engineering competencies that provide the foundation of the NNSA mission. Specific advances made under this project include enhanced characterization of pyrotechnic materials and properties that are impacting engineering development. Follow-on efforts will seek to advance techniques based on flash diffusivity and IR camera. Particle-scale modeling will be applied to additive manufacturing processes. Additionally, follow-on external partnerships seek to quantify material variability across scales, the role of processing and develop workflows for parameterizing new models. This work is aligned with Sandia's Engineering of Materials Reliability Research Challenge, and was an initial step toward developing the multiscale picture of transport in energetic materials.

Refereed Communications:

L.M. Phinney, W.W. Erikson, and J.B. Lechman, "Uncertainty Quantification for Multiscale Thermal Transport Simulations," in *Proceedings of the 11th AIAA/ASME Joint Thermophysics and Heat Transfer Conference*, Atlanta, GA, 2014.

Breaking Antibiotic Resistance: Use of High-Throughput, Multidimensional Data Analyses and Revolutionary Advances in Engineered Nanoparticles to Design and Deliver Antisense RNA

171055
Year 2 of 2
Principal Investigator: E. C. Carnes

Project Purpose:

Antibiotic resistance has become a major public health and national security concern and is now considered by the National Institute of Allergy and Infectious Disease (NIAID), the Department of Homeland Security (DHS), and the Centers for Disease Control and Prevention (CDC) to be a Category C priority. There is, therefore, an urgent need for strategies that reverse resistance and restore the efficacy of widely available, clinically proven antibiotics. Attempts to use antisense strategies for this purpose have failed, however, due to poor RNA design and inherent limitations of many state-of-the-art RNA delivery vehicles. To this end, we propose to use high-throughput bioinformatic approaches to identify genes that contribute to antibiotic resistance and design antisense RNAs that interfere with drug resistance mechanisms. In parallel, we will engineer mesoporous silica nanoparticle-supported lipid bilayers ("protocells") for high capacity delivery of antisense RNA and antibiotics to drug-resistant bacteria. Our proposed effort will result in generic bioinformatic approaches that can be used to rapidly characterize emerging threats and design highly effective RNAs with minimal off-target effects. Furthermore, due to the protocell's enormous cargo capacity, high degree of stability, and exquisite targeting specificity, this work promises to result in a universal delivery vehicle that is capable of both verifying predictive genomic analyses and effectively treating infections caused by the so-called "superbugs," such as multidrug-resistant *Klebsiella pneumoniae* and methicillin-resistant *Staphylococcus aureus*, and by bacterial threats with engineered antibiotic resistance.

Our proposed effort aligns with the Integrative Biological System Analysis and Engineering Research Challenge, and combines two high-risk, high-impact research avenues to address a problem with serious biosafety, biosecurity, biodefense, and public health implications: 1) high-throughput development of predictive models using multi-dimensional data sets and 2) use of engineered nanoparticles to translate predictive model output into actionable knowledge. Our approach should prove effective against the highly antibiotic-resistant "superbugs" and provide the ability to identify links between genomics and function for various microorganisms of importance to biodefense and bioenergy.

Summary of Accomplishments:

In FY2014, we sequenced the *Klebsiella pneumoniae* superbug and published that information in *PLoS ONE*. We developed a rapid test strip for detection of antimicrobial resistance and filed an invention disclosure for that device. We also developed a device to allow rapid identification of antibiotic resistance genes and the ability to use that information to identify the host microbe. An invention disclosure was also filed on that device.

We designed and tested molecules to silence numerous antibiotic resistance genes and tested them *in vitro*. We developed and tested nanoparticles capable of packaging these silencing agents and demonstrated their effectiveness to silence genes within bacteria. Additionally, we demonstrated the ability to enhance the efficacy of traditional antibiotics through nanoparticle packaging and cell-targeted delivery. Finally, we collected preliminary *in vivo* data demonstrating proof of concept in small animals.

Significance:

These results demonstrate, in principle, the ability to mitigate a bioterror attack or public health crisis featuring antibiotic resistant bacteria. Our discovery combines synthetic biology with nanotechnology to render resistant microbes susceptible to common, widely available antibiotics. The new materials and processes developed for this project may also be used in next-generation therapeutics against a plethora of diseases, ranging from cancer and cystic fibrosis to Ebola and HIV.

Refereed Communications:

C.E. Ashley and E.C. Carnes, "In Vivo Delivery Applications of Porous Nanoparticles," presented at the *Pharmaceutical Sciences and Toxicology Seminar Series*, College of Pharmacy, University of New Mexico, Albuquerque, NM, 2013.

C.M. Hudson, Z.W. Bent, R.J. Meagher, and K.P. Williams, "Resistance Determinants and Mobile Genetic Elements of an NDM-1-Encoding *Klebsiella pneumoniae* Strain," *PLoS One*, Volume 9, p. e99209, June 2014.

Flexible, Adaptable, Full-Spectrum Imaging via Nanoantenna Enabled Two-Dimensional Detectors

171056
Year 2 of 2
Principal Investigator: D. W. Peters

Project Purpose:

Improved infrared detector performance is always a demand from end users. Likewise, energy conversion efficiency always needs to be increased. In this effort, we design and fabricate low-loss nanoantennas on a proven infrared detector, integrate nanoantennas with a thermal energy harvesting rectenna, and integrate nanoantennas with a bilayer graphene (BLG) based detector. Nanoantennas are subwavelength structures that offer an enabling technology for visible to terahertz components; here, we focus on the infrared. Nanoantennas offer existing infrared detectors a means to make the detector much thinner and thus lower the dark current and pixel crosstalk and increase performance. Bilayer graphene offers a new tunable detector platform, however, it is only two atomic layers thick. For detection efficiencies over a few percent, it must have a method of light concentration: the nanoantenna is unique in its ability to concentrate light into a small volume and makes BLG detectors possible. Similarly, the rectenna is reliant on the light concentration that the nanoantenna offers to squeeze light into a very thin tunnel diode; past efforts at rectenna fabrication without a nanoantenna yielded 0.1% efficiency.

Nanoantenna fabrication and integration with the disparate materials used in each technology is non-trivial. Initial attempts to fabricate nBn detectors in the geometry required for a nanoantenna has proved extremely challenging. For this reason, this effort will not only improve upon nanoantenna design, but as importantly, examine advanced integration of these novel concepts into actual devices in order to realize improved detector performance. Sandia's MESA (Microsystems and Engineering Sciences Applications) facilities are unique in their capability and flexibility to handle silicon, III-V semiconductors, and silicon carbide substrates and the various other materials then deposited on them. The anticipated rewards from this project are high: high-performance mid-wave infrared (MWIR) detectors, tunable long-wave infrared (LWIR) graphene detectors, and the first demonstration of heat into electrical power with a rectenna.

Summary of Accomplishments:

This project sought to improve infrared detectors and infrared energy harvesting. Each of these goals utilized a nanoantenna: a subwavelength patterning over the surface of the device. The nanoantenna converts incident radiation into tightly bound surface modes. This confinement of the radiation to a thin layer is the mechanism that allows us change the detector architecture to accommodate much thinner active layers of detector material.

We fabricated and characterized two different types of infrared detectors using a nanoantenna architecture. The first utilized indium antimonide as the active layer. This material has been used in infrared detectors for several years, but in much thicker layers. We were able to reduce the active layer thickness by a factor of 20, and observed a drop in dark current by a factor of 4.5 compared to an equivalent thick detector.

We also fabricated a nanoantenna on a layer of graphene. Graphene could make an interesting detector material since it can be made to sense a different band of wavelengths with the application of a voltage, thus allowing a detector's spectral sensitivity to be changed in real time. Unfortunately the atomic thinness of graphene means it absorbs only a small fraction of the incident light. Using the concentration of the nanoantenna, we demonstrated a 10X increase in the light absorption.

Our third thrust used the nanoantenna as the first stage of a device that converts heat into electrical power. We demonstrated a structure that can convert heat of one polarization into a DC electric current with ~3% efficiency. While small, this is an important first step in realizing power from waste heat at low temperature differentials.

All three thrusts have advanced the science of nanoantennas and using that knowledge for applications of interest to the national security community.

Significance:

This project aligned with the Detection at the Limit Research Challenge. Both infrared sensing and conversion of waste heat into power are useful across a large range of national security fields. Infrared sensing is a prime detection mechanism for satellite-based nonproliferation efforts. Terrestrial applications include thermal imaging for the warfighter in operations where "owning the night" is of importance. Heat into power allows unattended sensors a long-term power source. Batteries for warfighter devices could be recharged in the field from any heat source, day or night. Use of waste heat as a power source would also offer a secondary power source for satellites and a corresponding reduction in solar array size.

Comparative Approach for a Physics-Based Understanding of Power Spectrum Analysis Signatures

171057
Year 2 of 2
Principal Investigator: P. Tangyunyong

Project Purpose:

The power spectrum analysis (PSA) technique is an electrical technique developed at Sandia to detect electrical differences in devices. The goal of this project is to develop a fundamental understanding of the physical mechanisms that generate PSA signatures. We propose to develop a physics-based understanding of component level PSA signatures using first principle modeling and simulation.

Summary of Accomplishments:

We have accurately simulated the dynamic operation of simple devices with several theoretical models; the modeling results agree very well with experimental PSA data. The modeling results also provide an insight into the nonlinear processes that generate PSA signatures, as well as a better understanding of the limitation and detection sensitivity of PSA.

We have also successfully simulated the linear dynamic operations of more complex devices. We were able to accurately simulate nonlinear operation in a few devices; the nonlinear operation in most devices was, however, too complex to simulate.

Significance:

The modeling works provide unmatched insight into the dynamics that generate distinct PSA signatures. The modeling also provides unique information that enhances the effectiveness and sensitivity of the PSA technique. This work is aligned with Sandia's Trusted Systems and Communications Research Challenge, and addresses reliable methods to authenticate the integrity of microelectronic devices required by NNSA and DoD.

Counter-Adversarial Data Analytics

171059
Year 2 of 2
Principal Investigator: W. P. Kegelmeyer

Project Purpose:

Sandia makes critical use of data analytics in defense of national security. Our adversaries, therefore, seek to sap, even suborn, those analytics. Through understanding our methods, they seek to produce data which is evolving, incomplete, deceptive, and otherwise custom designed to defeat our analysis. Further, we cannot prevent them from doing so. We live in a changed world, in which we frequently must depend on data over which our adversaries have unprecedented influence.

In this project, we develop and assess novel data analysis methods to counter that adversarial influence. We also generate implementations and at least one prototype deployment in support of a mission challenge.

We thus face paired problems. First, we must perform data 'science', discovering generalizable and quantifiable counter-adversarial principles. Second, our national security mission requires methods that are *relevant*, applicable to analytics that matter, with realistic assumptions, useful uncertainty assessments, and practical implementations.

Being simultaneously scientifically rigorous and practically relevant seems challenge enough. Adding the fact that we are also trying to counter dedicated, agile, intelligent adversaries who will closely observe and learn from our behaviors makes this a high-risk effort indeed.

Yet, if successful, the payoff will be immense. The ability to anticipate and defeat attacks on the data analytics at the heart of, for example, cyber security, stockpile assurance, counter proliferation, and biotechnology for threat detection is critical to a range of Sandia missions.

Further, although the work is high risk, Sandia is positioned for success. We have staff expertise in machine learning, statistics, game theory, and network analysis. We have prior experience in attacking our own algorithms. We have direct access to pertinent national security data. And, we have sufficient existing integration, knowledge and mutual respect among our research and application organizations to have already successfully transitioned ideas from research results to operational changes.

Summary of Accomplishments:

We invented, implemented, and exhaustively analyzed a number of label tampering attacks. One unfortunate resultant discovery is that cross-validation and out-of-bags assessments, standard methods for determining machine learning accuracy, are not only useless but actually deceptive in the context of adversarial tampering.

We also invented and exhaustively tested and established the effectiveness of Ensembles of Outlier Measures (EOM), a method for detecting and remediating tampered data. We demonstrated that EOM has the counterintuitive property of often being able to recover performance without needing to be certain as to exactly which labels were altered.

We established that that these insights and methods also apply to clustering methods. Specifically, we demonstrated previously unexpected vulnerabilities in a popular and frequently used clustering algorithm, quantified the impact of these vulnerabilities to "sample injection" attacks designed to undermine a plagiarism detector, and, perhaps most importantly, demonstrated that EOMs were general enough to be effective even here.

In addition to assessing or detecting individual tamperings, we addressed the goal of a quantified, statistical assessment of whether a data set was tampered with at all: quantified paranoia. We derived and implemented test based on Raftery's interpretation of pseudo-Bayes factors that has distinguished between untampered data, ineffectively tampered data, effectively tampered data, and stealthily tampered data, all without requiring the specific identification of corrupted data points.

As the field is relatively new, and we were doing novel work, we necessarily created new concepts and attendant terminology ("confidence" vs. "evasion" attacks, "data mines" as an attacker method), new metric methods (degradation curves and the area underneath, oracle or "best guess" remediation curves, overall average tampers and the average matching accuracy drop), and new software for their visualization, resulting in the open source release of the "toyplot" Python plotting package.

Significance:

"Adversarial machine learning" is a nascent field, yet a critical one, as insider threats, network compromise, and the necessary use of observational data all provide motivated adversaries means by which they can identify and then actively suborn national security analysis algorithms. We have advanced science in this domain and simultaneously helped to harden national security analysis through, for instance, quantitatively demonstrating that cross-validation assessment is not only useless, but actually deceptive in context of adversarial tampering, and by inventing Ensembles of Outlier Measures (EOM), an effective and surprisingly general method for detecting and remediating tampered data. This project is aligned with Sandia's Data Science Research Challenge and is expected to benefit the cybersecurity needs of DOE/NNSA, DoD, other government agencies, and commercial enterprise.

Refereed Communications:

P. Kegelmeyer, T. Shead, D. Zage, K. Rodhouse, and J. Crussell, "Machine Learning Detection of Malware in the Presence of Adversarial Tampering," presented at the *Malware Technical Exchange Meeting*, Albuquerque, NM, 2014.

D. Zage, K. Rodhouse, P. Kegelmeyer, R. Colbaugh, and K. Glass, "Identifying Abnormal Software via Time Series Data and Machine Learning," presented at the *Malware Technical Exchange Meeting*, Albuquerque, NM, 2014.

R. Colbaugh, K. Glass, and D. Zage, "Increasing Cyber Resilience via Predictability-Based Defense," in *Proceedings of the 6th International Symposium on Resilient Control Systems (ISRCS)*, San Francisco, CA, 2013.

Y. Vorobeychik, "Using Machine Learning for Operational Decisions in Adversarial Environments," in *Proceedings of Autonomous Agents and Multiagent Systems*, Paris, France, 2014.

Beyond Moore's Law Computer Architecture

171060
Year 2 of 2
Principal Investigator: E. Debenedictis

Project Purpose:

The challenge is to extend what is popularly called "Moore's Law" for both national security and economic productivity. To do so will first require identifying or inventing a replacement for computers' underlying device technology that is faster and more power-efficient. In addition, a computer architecture must be created that is both tuned to the new device and to the evolving nature of computer applications.

This is a widely recognized problem, but industry is looking at a solution space dominated by "drop in replacements" for the current devices (complementary metal–oxide–semiconductor or CMOS) in current architectures (multicore microprocessors). In order to address national security needs, this project will look more broadly.

The project will focus on a few device types, looking beyond "drop in replacements" for CMOS as has been done in other projects. The project will also provide a fair, rigorous assessment of a broader range of devices.

The solution will go beyond the common practice of analyzing devices in isolation, developing an entire "technology stack" of circuits, architectures, and software. This will yield a more realistic vision of the end result, as opposed to a thorough analysis of just the first step.

The solution will consider alternatives or enhancements to the preeminent Von Neumann architecture. A requirement of the proposed solution will be execution of today's "legacy" software, yet the solution may be optimized for code that uses non-Von Neumann features such as learning.

Two stretch goals will be considered:
1) Cyber security and supply chain trust are very important. Subject to available resources, this project will consider whether the underlying physical technology and architecture can help address these issues.
2) A "Beyond Moore" physical prototyping capability will be considered. MESA or a new fab at Sandia could be considered for a role analogous to the DARPA-sponsored prototyping service that bootstrapped CMOS.

Summary of Accomplishments:

We have created a new computing concept that has general applicability and physical, architectural, and software scaling paths. This concept exists in several variants.

In one variant, we invented a combined memory and logic architecture and coupled it with a principal in computation called "adiabatic logic." We call the result optimal adiabatic scaling and the processor-in-memory-and-storage (PIMS) architecture. The combination would be capable of executing key popular computation kernels with extraordinarily high levels of energy efficiency. The exemplary kernel comprises sparse matrices. Sparse matrices can be applied to graph algorithms, numerical algorithms (e.g., finite element method), and artificial intelligence (deep learning).

In a second variant, we developed a framework for evaluating the performance of brain-inspired neural systems. This method is based on ultimate theoretical limits and is like an analog, neural-inspired version of Landauer's *kT* energy limit on irreversible logic. This type of performance evaluation allows what-if analyses of devices, architectures, and software, and thereby turns previously ad hoc design choices into questions that can be answered by evaluating an expression.

In a third variant, we developed ideas for superconducting processors consistent with the previous paragraphs. Superconducting electronics are not as mature as room-temperature electronics, so these ideas are somewhat further out. However, we developed ideas on 3D packaging of superconducting processors and compatible memory.

Finally, we interacted with many of the physical science efforts in advanced devices throughout Sandia. This resulted in some existing physical science efforts becoming part of the computer inventions above. For example, memristor technology has become the baseline for PIMS architecture.

Significance:

There is a rapidly growing realization that the US Government and industry must ride Moore's Law to its end while preparing for a shift to new concepts in computing on a decadal timeframe. All of the efforts above are candidates for a new concept in computing as envisioned by Sandia's Beyond Moore's Law Research Challenge, and are relevant to the future computing needs of DOE/NNSA and DoD.

Refereed Communications:

A.A. Talin, A. Centrone, M.E. Foster, V. Stavila, P. Haney, R.A. Kinney, V. Szalai, F. El Gabaly, H.P. Yoon, F. Léonard, and M.D. Allendorf, "Tunable Electrical Conductivity in Metal-Organic Framework Thin-Film Devices," *Science*, vol. 343, pp. 66-69, December 2013.

M.J. Marinella and V.V. Zhirnov, "Emerging Memory Devices: Assessment and Benchmarking," in *Emerging Nanoelectronic Devices*, A. Chen, J. Hutchby, V. Zhirnov, G. Bourianoff, eds. Wiley, 2014.

V.V. Zhirnov and M.J. Marinella, "Memory Technologies: Status and Perspectives," in *Emerging Nanoelectronic Devices*, A. Chen, J. Hutchby, V. Zhirnov, G. Bourianoff, eds. Wiley, 2014.

M.J. Marinella, "Emerging Resistive Switching Memory Technologies: Overview and Current Status," in *Proceedings of IEEE International Symposium on Circuits and Systems*, pp. 830-833, 2014.

V. Stavila, A.A. Talin, and M.D. Allendorf, "MOF-Based Electronic and Optoelectronic Devices," *Chemical Society Reviews*, vol. 43, pp. 5994-6010, May 2014.

A.W. Cummings, J. Varennes, and F. Léonard, "Electrical Contacts to Three-Dimensional Arrays of Carbon Nanotubes," *IEEE Transactions on Nanotechnology*, vol. 12, pp.1166-1172, September 2013.

A.A. Kane, A.C. Ford, A. Nissen, K.L. Krafcik, and F. Léonard, "Etching of Surfactant from Solution-Processed, Type-Separated Carbon Nanotubes and Impact on Device Behavior," *ACS Nano*, vol. 8, pp. 2477-2485, February 2014.

C. Spataru and F. Léonard, "Fermi-Level Pinning, Charge Transfer, and Relaxation of Spin-Momentum Locking at Metal Contacts to Topological Insulators," to be published in *Physical Review B*.

First to High-Yield Fusion

171061
Year 2 of 2
Principal Investigator: S. A. Slutz

Project Purpose:

Achieving controlled fusion ignition, and ultimately high yield (~1 GJ/pulse), using laboratory facilities would be a transformative capability for our country. History shows that it is also an extremely challenging and multidisciplinary problem that will require continued innovation. Sandia has begun evaluating a new magnetized liner inertial fusion (MagLIF) concept [S.A. Slutz, et al., Phys. Plasmas 17, 056303 (2010)] in which the Z pulsed power facility implodes a cylindrical liner filled with deuterium fuel. The fuel is heated during the implosion with the Z-beamlet laser and magnetized with external field coils in order to reduce thermal losses between the hot plasma and cold liner. This concept may reduce the pressure required to achieve fusion to about 5 Gbar, the implosion velocities to 100 km/s, and the fuel convergence ratio to 23 (compared to indirect drive capsule requirements of 400 Gbar, 300 km/s, and 35, respectively).

However, the fuel plasma parameters in MagLIF targets are intermediate between those typical of magnetic and inertial confinement fusion and thus are not well studied. It could be that electron thermal transport across magnetic field lines is worse than predicted, as with Bohm diffusion. It is also unknown whether the use of a laser to preheat the fusion fuel will work as predicted, or if beam filamentation or laser-plasma instabilities will cause problems. Magnetization and preheat may have additional unforeseen effects on the overall target behavior. We propose to investigate alternative target designs to MagLIF that would trade off robustness to some of these issues for higher risk in others.

The MagLIF concept is already a high-risk, high-potential line of research in that it combines new techniques (magnetization and preheating) that may reduce fusion requirements. This project would test more aggressive target designs than the baseline MagLIF approach. Though these designs may fail, we believe they will nonetheless provide insight into magnetization and preheating physics.

Summary of Accomplishments:

High yield using magnetized liner inertial fusion (MagLIF) depends on preheating 4-10 mg/cc of deuterium/tritium (DT) gas with 20-30 kJ of energy prior to the implosion. Lasers, which are a convenient way to provide this fuel preheat, have been used experimentally to demonstrate the basic MagLIF concept on the Z machine. Presently the Z-Beamlet laser provides 4 kJ (insufficient to ignite a high-yield liner), but we have shown analytically and numerically that 20-30 kJ of fuel preheat should be possible with a larger laser. However, there are challenges. An important laser plasma instability is the two phonon decay (TPD), which is active above ¼ critical density or ~4.3 mg/cc for 0.5 µm laser light. We demonstrated numerically that this instability could be avoided by first penetrating the DT with about 3 kJ of 0.25 µm laser light. This laser heating generates a radially expanding blast wave that results in substantially lower gas densities that can be effectively penetrated by 0.5-1.0 µm laser light, without exciting TPD. Simulations indicated that 30 kJ of energy could be deposited in the DT gas over a distance of 1 cm, which is appropriate for a high-yield MagLIF target with a yield in excess of 1 GJ. These simulation results have generated interest in testing laser preheating of fuel at energies relevant to high yield with other lasers such as the Omega and National Ignition Facility (NIF) lasers.

Pulsed power is energy rich and very inexpensive as compared to lasers. We have investigated two novel approaches to provide fuel preheat which use pulsed power directly. We have performed detailed numerical simulations of these approaches, which indicate that > 30 kJ could be deposited. We have executed a series of experiments on Z to test these approaches. The first experiments, which are described in our final report, were very encouraging.

Significance:

Scientists have been working toward fusion in the laboratory for over 50 years. We have investigated three means of providing the fuel preheat needed for high-yield (> 1 GJ) magnetized liner inertial fusion. The achievement of such high fusion yields in the laboratory would be immediately useful for stockpile stewardship and weapon effects experiments, and, in the longer term, would enable serious research toward fusion energy.

Direct Observation of Electrothermal Instability Structures in the Skin Layer of an Intensely Ohmically Heated Conductor

178661
Year 1 of 2
Principal Investigator: T. J. Awe

Project Purpose:

Magnetically driven implosions (MDIs) on the Z Facility assemble high-energy-density plasmas for radiation effects and ICF experiments. MDIs are hampered by the Magneto-Rayleigh-Taylor (MRT) instability, which can grow to large amplitude from a small seed perturbation. Such asymmetries reduce achievable stagnation pressures and temperatures. The metallic liners used in Magnetized Liner Inertial Fusion (MagLIF) experiments contain astonishingly small (~10 nm root mean square[RMS]) initial surface roughness perturbations; nevertheless, unexpectedly large MRT amplitudes are observed in experiments.

A prevailing hypothesis suggests the electrothermal instability (ETI) provides a perturbation which exceeds the initial surface roughness. For a condensed metal, resistivity increases with temperature. Locations of locally higher resistivity undergo increased ohmic heating, resulting in locally higher temperature, and thus still higher resistivity. Such unstable temperature growth produces density perturbations when the locally overheated metal changes phase. These density perturbations seed MRT growth. ETI seeding of MRT on thick conductors (where the metal is thicker than the magnetic skin depth; the regime relevant to MagLIF liners) has thus far only been inferred by evaluating MRT amplitude late in the experiment. A direct observation of ETI is vital to ensure our simulation tools are accurately representing the seed of the deleterious MRT instability. This is an outstanding and important fundamental physics question with far-reaching practical implications.

We propose to directly measure the ETI structure formed on ohmically heated thick conductors using a high resolution, high sensitivity, near-IR/visible framing camera. To our knowledge, this would be a first of its kind measurement. Targets must be extremely smooth and metallic structure must be well characterized in order to differentiate physical mechanisms that may drive ETI (e.g., grain boundaries). Data will fill a gap in understanding concerning the seeding of MRT that has persisted for many decades. This will increase our ability to mitigate MRT, thus enabling increased stability of higher-aspect-ratio, higher-velocity liners.

This project aligns with the First to High-Yield Fusion Research Challenge.

Predicting the Multiscale, Mechanical Response of Additively Manufactured Materials across a Wide Spectrum of Loading Conditions

178667
Year 1 of 2
Principal Investigator: D. P. Adams

Project Purpose:

This project will 1) elucidate how the complex microstructures of additively manufactured materials give rise to mechanistic transitions between quasi-static and inertial strain rates and 2) develop a new understanding of whether homogenization and multiscale theory can predict the dynamic mechanical behaviors of these materials.

We will start by characterizing the microstructure of near-full-density stainless steel 304L test specimens made by Laser Engineered Net Shaping (LENS™) and implement this structure in Sandia's state-of-the-art direct numerical simulation (DNS) technique to predict the grain-scale response of nonuniform microstructures. The results will be compared with those generated by homogenization theory. Recently developed solvers for Sierra/SM implemented in near-exascale architectures will permit the first, efficient solution of this complex problem.

Mechanical testing experiments will then be used to determine the validity of model predictions and drive to answer the question of whether homogenization theory remains useful for simulating the complex, highly anisotropic microstructures produced by additive manufacturing. Mechanical testing covers the range of strain rates covered by simulations, but we also extend to previously untested strain rates associated with high-velocity impacts.

As a final task, we contrast the mechanical behaviors of stainless steel 304L made using LENS™ with that of traditional, ingot-derived material. LENS™-made alloys have a complex solidification microstructure with crystallographic texture and large grain structure, while conventional materials have a relatively simple, equiaxed grain structure.

This project aligns with Sandia's Engineering of Materials' Reliability Research Challenge.

Decision Analytics for Complex Supply Chain Networks

178670
Year 1 of 2
Principal Investigator: G. K. Kao

Project Purpose:

The purpose of this project is to develop decision-support technologies enabling decision makers to perform risk-based cost-benefit prioritization of security investments to manage supply chain integrity and risk. We propose a new systematic approach to examine the lifecycle phases (e.g., design, implementation, testing, deployment, maintenance, retirement) of supply chains by leveraging a new security risk metric based on the degree of difficulty adversaries will encounter to successfully execute the most advantageous attack scenario (Wyss, et al., 2011). The key challenge is that the scale of the end-to-end supply chain lifecycle problem is too large and complex. To manage this complexity, we propose a hierarchical decomposition methodology in modeling the supply chain lifecycle. Our framework consists of 1) hierarchical representation, 2) macro state-of-health assessment, 3) adversary action evaluation, 4) difficulty and consequence evaluation, and 5) optimization. The hierarchical representation modeling enabled us to decompose the supply chain problem into manageable pieces such that risk and state-of-heath evaluation can be performed. High-level metrics will be developed to enable decision makers and analysts to identify critical areas for further deep dives. The macro state-of-health assessment is analogous to measuring vital signs (blood pressure, pulse, respiration, and temperature) before administering any diagnoses. Data analytics techniques will be developed to address data integrity issues. Deep dive analysis will consist of generating adversary scenarios based on functional grammars. Difficulty and consequence metrics will be used to help understand the risk space. These metrics are intended to enable decision makers to overcome complexity of quantifying security risk, and will be suited for cost-benefit optimization. New optimization techniques such as multilevel optimization methods will be explored. By design, the hierarchical and recursive approach will address the supply chain problem comprehensively at various depths. Our methodology will help manage the complexity of the problem such that analysts can understand and gain insights into the end-to-end supply chain to make risk-informed effective decisions.

This project is aligned with Sandia's Trusted Systems and Communications Research Challenge.

Robust Operations and Algorithms for Quantum Information Systems

178675
Year 1 of 2
Principal Investigator: T. S. Metodi

Project Purpose:

Few examples of quantum applications running on quantum hardware exist due to the challenge of creating hardware that is reliable and scalable enough to accommodate the overhead associated with active noise suppression. As a result, quantum information processing (QIP) is widely viewed as a long-term goal, with few near-term applications. Our proposal challenges this conventional wisdom by focusing on few-qubit devices that can run practical applications or serve as building blocks for larger systems. It aims to show that, even if universal QIP is very hard, specialized hardware and algorithms for few-qubit devices may solve important problems in the near term. To that end, the purpose of this project is to develop and accurately characterize robust quantum operations for two technologies at the physical one-qubit and two-qubit gate level and to develop intrinsically robust algorithms at the high-level. The improved physical hardware resulting from these new gates and characterization protocols will ultimately lead to prototype devices enabling experimental tests of robustness in a set of specialized applications. Our overall proposed plan follows two co-dependent themes: robust operations and robust algorithms with the following major milestones addressing each of the two themes:

- Develop a new two-qubit gate within a silicon quantum computing (Si-QC) system, specifically designed to have low decoherence and high robustness

- Develop reliable techniques for characterizing and validating one-qubit and two-qubit quantum gates in trapped ions

- Pursue the development of specialized, small quantum algorithms that solve computationally difficult problems and function reliably without active noise suppression

- Develop algorithms that implement a universal set of topologically protected logic operations that can significantly reduce the overhead of error correction and also exhibit intrinsic noise robustness. Develop optimization techniques for specific types of noise.

Unconventional Approaches to Neutron Generators

178917
Year 1 of 2
Principal Investigator: M. S. Derzon

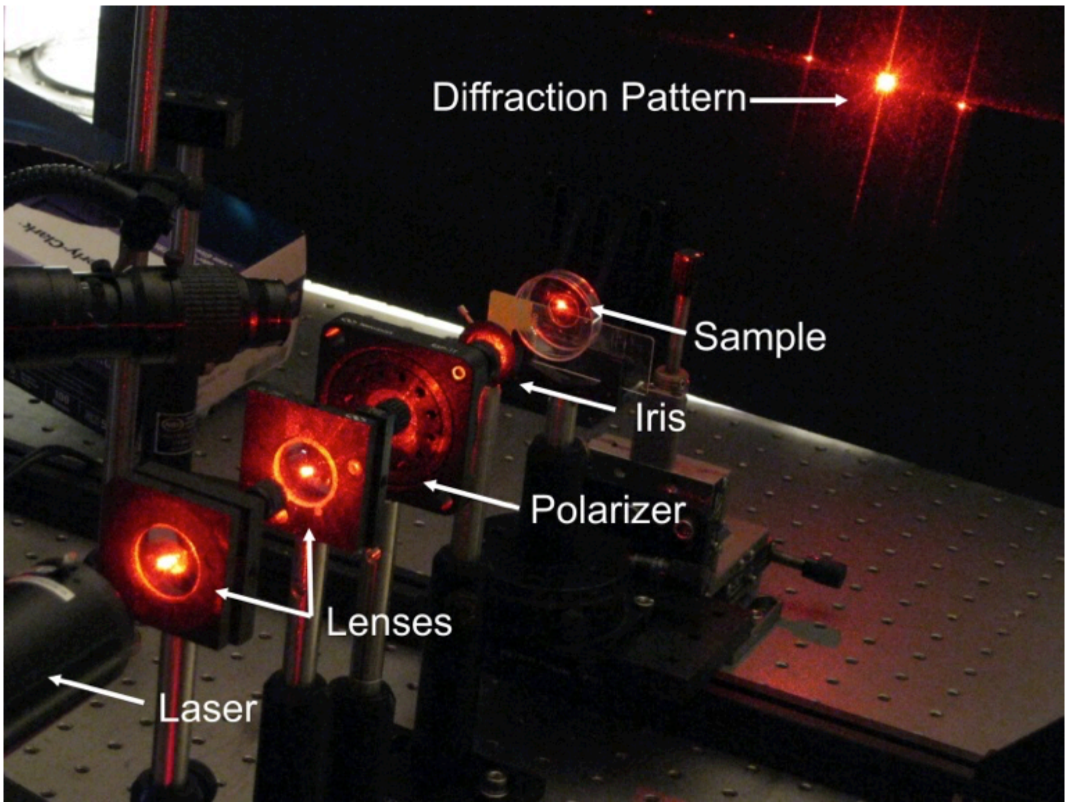
Project Purpose:

The purpose of this project is to demonstrate a new physical basis for the production of neutrons from a compact source. Models suggest that this new method of neutron production is both highly energy efficient and lower voltage relative to existing techniques. These are expected to translate into improved size, weight, power, lifetime, and safety. It should also be capable of giving new temporal and spatial profiles for neutron production. If these attributes can be demonstrated experimentally, a variety of potential applications become viable.

This project is aligned with the Revolutionary Approaches to the Stockpile Research Challenge.

EXPLORATORY EXPRESS

The Exploratory Express Investment Area provides a mechanism for maturation and testing of a novel idea that has potential to become very important for one of Sandia's strategic missions. This Investment Area was initiated to provide a vehicle to explore novel ideas that are generated by researchers spontaneously through the year rather than in response to a specific proposal call. Proposals may be submitted throughout the year with the selection of funded projects occurring approximately monthly. A small amount of funding (≤ $50K) is provided to Exploratory Express projects over a period of no more than a few months to address one critical question as the basis for determining whether the idea is desirable for Sandia to pursue more thoroughly to mature its strategic importance for Sandia's national security missions.



Experimental setup of grating testing showing a projected diffraction pattern of a quality graded index (GRIN) novel optical film material developed using multiphoton lithography. (Project 177860)

EXPLORATORY EXPRESS

Advancing the State of the Art in Brute Force Vulnerability Discovery

173656
Year 1 of 1
Principal Investigator: M. A. King

Project Purpose:

Fuzzing is the state-of-the-art, brute force technique for discovering vulnerabilities in the implementation of an interface or protocol library. Fuzzing works by sending specially crafted packets containing unexpected data, called the "fuzz." The fuzzing system then checks to see if the interface properly handles the malformed data. If the interface performs unexpectedly or the fuzz causes the device to crash, then this may indicate a potential vulnerability.

Fuzzing can be decomposed into two approaches. The first approach treats the protocol as a black box and the fuzzer simply sends random bytes at the interface. This approach is general and scales across protocols, but tends to produce few vulnerabilities. The second approach requires an in-depth understanding of the interface or protocol under test: the fuzzer must understand the protocol being verified to know which fields must be present and which values may be manipulated to expose potential vulnerabilities. This protocol-aware approach is time consuming and requires highly skilled labor, as a detailed protocol specification must be produced for every protocol to be tested. This protocol-aware approach is highly effective at identifying potential vulnerabilities, but does not scale across protocols. In either approach, fuzzing can take a substantial time to reveal vulnerabilities either in running time (in the black-box approach) or in set-up time (in the protocol-aware approach).

Wireshark is an open-source protocol stream analyzer for transmission control protocol/internet protocol (TCP/IP) traffic. It provides the ability to parse protocols at different layers of the TCP/IP stack through the use of protocol packet dissectors.

We plan to create a fuzzer generator that uses Wireshark dissector code to automatically produce protocol-aware fuzzers. This novel approach will automatically decompose protocol structure into a field-selectable, fuzzer-generation prototype. If successful, the new hybrid system will dramatically decrease the time needed to find vulnerabilities in target software and hardware while maintaining the high discovery rates associated with protocol-aware fuzzing systems.

Summary of Accomplishments:

The parser handled the initial case very well; however, after attempting to use Owlet (the fuzzer generator tool we developed) on multiple protocols, it became clear that there were some technical hurdles that needed to be overcome. A lack of standardization makes it much more difficult to write a 'one size fits all' parser. There are many corner cases where the writer of a protocol dissector may develop the dissector in a non-intuitive way. It would be the job of the tool to recognize and handle those cases.

There is currently no facility for handling bit fields in protocols. Currently, those fields are just grouped into bytes and included as static data into the fuzzer protocol block description. Owlet was tested on the following protocols:

- Ethernet: Owlet handled it very well. All fields were broken out properly and typed appropriately in the derived protocol block description.
- TCP: Owlet works for the TCP protocol packets where the packets are transporting information for higher-level protocols.
- HTTP: Owlet has been shown to work well for two different types of HTTP protocol packets; the HTTP CONNECT packet and the HTTP CONNECTION ESTABLISHED packet.
- Modbus: Owlet has been shown to be successful for Modbus.
- GOOSE: Owlet has been shown to be successful for the IEC61850 GOOSE protocol. The tool correctly disassembled the packet fields into fuzzable tokens that were correctly typed.
- CIP (common industrial protocol): Owlet failed to properly derive a protocol block description from the fields of a CIP packet.

Significance:

Overall Owlet was a success. A proof of concept proving the hypothesis (that a protocol block description could be derived from a Wireshark protocol dissector) was developed during the course of this work. As the algorithms are refined, this technique could change the way fuzzing is done in the field of vulnerability discovery.

Ferrite Solutions for Electromagnetic Shock Lines

173659
Year 1 of 1
Principal Investigator: P. D. Coleman

Project Purpose:

The goal of this work is to identify tools and test procedures for identifying ferrites suitable for use in shock line applications.

Electromagnetic shock lines have been used to provide fast rising voltage pulses for many applications. In these applications, a slow rising pulse is injected into the line where currents drive the ferrites into saturation leading to a fast rising output pulse. A shock line's unique capabilities could be applied to new detonator configurations. A properly conditioned voltage pulse is critical for fire set applications.

Traditional circuits use ferrites operating in a linear regime. Shock lines push the ferrites well into the nonlinear regime where very few tools and data currently exist. Ferrite material is key to the operation of these shock lines and tools for identifying suitable ferrites are critical.

Summary of Accomplishments:

A testbed has been constructed that allows characterization of ferrite-based shock lines. A circuit model that includes basic ferrite nonlinearity physics has been used to compare with experimental data. Comparisons between measurements and model predictions show good agreement. Having a model allows quick exploration of different parameters to identify optimal shock line designs.

Significance:

The testbed and modeling conducted in this project will enable optimal designs for future shock line applications. A carefully designed shock line could provide a passive solution to generating a fast rising voltage pulse for fire sets. Another application is in generation of high power microwaves. This project benefits the science and engineering base required in securing the nation's nuclear stockpile.

In Situ Immobilization of Selenium in Sediment

176039
Year 1 of 1
Principal Investigator: R. C. Moore

Project Purpose:

Selenium contamination of groundwater and surface water is a major problem in the US. Major sources of selenium contamination involve US energy, agriculture, and resource production including uranium, phosphate and coal mining, coal ash pile leaching at power plants, agricultural activities (California's central valley), and hydrofracking operations. Currently, there is no inexpensive and highly effective treatment method for selenium-contaminated water. We intend to develop a novel permeable reactive barrier (PRB) for immobilization of selenium in groundwater. The barrier is formed in situ by injecting chemical reagents into the path of the selenium-contaminated groundwater. The chemical reagents form apatite, a mineral know to immobilize selenium.

Summary of Accomplishments:

We discovered that carbonated apatite has a strong sorbent affinity for selenium in the rescued state. Carbonated apatite was synthesized by a precipitation method and characterized. Batch selenium kinetic and equilibrium experiments were performed. The results were reported in the literature.

Significance:

Although selenium is an essential nutrient at very low concentrations, at higher concentrations it is toxic. The use of carbonated apatite in permeable reactive barriers may provide an effective, inexpensive technology to remediate selenium-contaminated sites. The success of this work will lead to the development of a passive, inexpensive treatment technology for selenium contamination with broad applicability to US selenium contamination issues.

Tightly Coupled GPS/INS Flight Test Demonstration

176605
Year 1 of 2
Principal Investigator: J. D. Madsen

Project Purpose:

The purpose of this project is to demonstrate global positioning system (GPS) tracking in ultra-high dynamic acceleration environments. New integrated GPS/inertial navigation system (INS) tracking approaches will be demonstrated in conjunction with a rocket test ride of opportunity at White Sands Missile Range. Once verified in flight, these new approaches will enable GPS receiver signal tracking in significantly more challenging dynamic environments than previously demonstrated. We plan to mature and fully implement the flight software and hardware interfaces required to support the test. The required integration tracking algorithms were completed and verified in limited bench top testing. Telemetry capability was also developed, and the required commands for launch day support were finished. The required flight hardware was identified and integrated. The required cable set was also defined and fabricated. A new hardware-in-the-loop simulation capability was set up and prepared to verify the resulting flight code. Hardware to mount the experiment in the rocket was defined and fabricated. The resulting set of hardware and software is nearing completion to support the flight test. Invaluable data will be gathered during the flight test that will potentially inform the work of high dynamic GPS tracking for many other projects. The actual rocket flight test is scheduled to occur in the fourth quarter of 2014.

Can Nanoporous-Carbon Host Materials Enable Multivalent Ion Electrochemical Energy Storage?

176606
Year 1 of 1
Principal Investigator: M. P. Siegal

Project Purpose:

Lithium-ion chemistry has achieved near-optimal electrochemical energy storage performance, limited by its single electron valence. Developing multivalent (e.g., Mg^{2+}, Ca^{2+}, Al^{3+}) battery chemistries is forward-looking and promising for increasing energy density, driven by the greater number of electrons transferred per metal cation. In principal, these metals could be used directly as anodes to electrodeposit/dissolve from themselves; however, the inevitable solid electrolyte interphase slows cation transmission rates. Intercalation electrode mechanisms eliminate such concerns and have been used in rechargeable lithium batteries. Multivalent ion intercalation is not theoretically limited; the challenges are the energetics of ion delivery into an acceptable carbon host. Nevertheless, negligible progress for multivalent energy storage has been made since existing carbonaceous materials have insufficient interstitial spacing within their crystallographic structures to host the larger sizes of partially solvated multivalent ions. We will determine if nanoporous carbon (NPC), with tunable graphitic interstitial spacing and a plethora of grain boundaries, can be used as an intercalation host for Mg^{2+}. This will be successful if reversible diffusion of Mg^{2+} can be demonstrated into a NPC host with the appropriate physical parameters.

NPC mass density can be controlled from 0.1 - 2.0 g/cc, consisting of randomly oriented domains ~3 - 6 graphene layers thick with only 1 - 4 nm lengths. These graphene sheet fragments are spaced 0.4 - 0.7 nm apart (compared to 0.335 nm for graphite). Finally, nm-scale domain boundaries exist throughout the material. Coupling these boundaries with the expanded interstitial spacings accounts for the high chemical diffusion rates and sorption masses for NPC in chemical sensor devices.

We will use cyclic voltammetry to detect and measure the insertion/extraction of multivalent ions into a NPC host anode, as well as the resulting charge transfer. These experiments will be performed for magnesium (Mg) ions as a function of NPC interstitial/boundary spacings to determine if NPC can be used as an insertion host material for multivalent ions.

Summary of Accomplishments:

We discovered a narrow range for NPC mass density that demonstrates the ability to intercalate Mg^{2+} ions, a critical finding to potentially enable multivalent ion energy storage. Specifically, we identified three distinct electrochemical behaviors for NPC-coated anodes as a function of mass density. Using pulsed-laser deposition, we grew NPC on stainless-steel disk substrates with controlled mass densities ranging from 1.0 g/cc to below 0.1 g/cc and used them as the anode in fabricated coin cell batteries to perform basic electrochemical characterizations. We used an Mg foil as the cathode and a Grignard-based solution as the electrolyte. While not optimal, the use of a constant cathode and electrolyte solution sealed in coin cell configuration enabled the independent testing of NPC for utility as an intercalation host for multivalent ions.

We performed cyclic voltammetry to study the electrochemical behavior of the fabricated coin cells as a function of NPC mass density. Using slow scan rates (100 – 500 μV/sec) to minimize mass transport limitations arising from the non-optimal coin cell arrangement, we identified three distinct electrochemical behaviors as a function of NPC mass density. The density of graphite is ~2.2 g/cc.

For NPC densities >0.5 g/cc, the cyclic voltammograms form relatively symmetrical hysteresis loops typical of classic charge/discharge currents generated from parallel plate capacitors.

For NPC densities 0.2 g/cc, the voltammograms showed both cathodic and anodic peaks with slight asymmetry. Intriguingly, the regions around the peaks represent behavior associated with possible Mg ion intercalation into the NPC anode.

For NPC densities <0.1 g/cc, the asymmetrical voltammograms are analogous to double layer surface charging.

In summary, we determined that there exists a range of NPC mass density that may be appropriate to use in further studies for the development and understanding of multivalent ion energy storage.

Significance:

We identified a narrow range of NPC mass density between 0.1 and 0.5 g/cc that demonstrates the potential to reversibly intercalate Mg ions, a critical finding for the future development of NPC anode materials to enable multivalent ion energy storage. Three distinct patterns of electrochemical behavior are observed for different NPC mass densities. Since the electrolyte, electrode material and mass, cell geometry, and electrochemical test method is held constant, it appears that the tortuous paths during ionic mass transport through the NPC are responsible for the different electrochemical behaviors.

Demonstrating multivalent-ion intercalation into a graphitic network opens the possibility of developing advanced energy-storage concepts. Enabling energy-storage systems that expand chemistry options to span a range of gravimetric/volumetric, energy/power densities and lifetimes can possibly help meet future energy security missions, as well as applying on-chip micropower for remote sensors, autonomous microelectronics, and extreme environments.

Graphene Oxide Desalination Membranes

176607
Year 1 of 1
Principal Investigator: L. Biedermann

Project Purpose:

The overall research goal is to develop low-energy, chlorine-tolerant desalination membranes. Water scarcity in the US and abroad (e.g., Army contingency bases) drives desalination of brackish and saline water and reuse of greywater. Current desalination technologies such as reverse osmosis (RO) are energetically expensive; the 2005 US desalination energy cost was ~4x10^9 kWh. Commercial polyamide RO membranes require dechlorination (<0.1 ppm) of feed water to prevent polymer degradation; chemical and reduced run time costs to ameliorate biofouling add significantly to operating costs. Chlorine (bleach) resistant membranes will prolong system lifetime and enable greywater reuse.

Reducing the energy demands requires a new paradigm in which the intrinsic membrane structure, rather than external pumps, drives desalination. Such low-energy desalination is achievable with graphene oxide (GO) membranes. In laminar GO membranes, oxygen modalities on the GO basal plane act as nanopillars, separating the aromatic graphene regions and holding the intersheet spacing, d, at 0.7 - 1.1 nm. Water flows through this thin-slit geometry as a bilayer of solid ice, between and around the GO sheets [Boukhvalov 2013]. The narrow intersheet spacing energetically discourages permeation of solvated ions. Low-energy water permeation is attributed to the strong adsorption of water in the aromatic regions, which drives an enhanced capillary pressure of 10^3-10^4 bar, 10^7 greater than the vapor pressure across the membranes, resulting in permeation of water vapor at 0.25 L $m^{-2}h^{-1}$ [Nair 2012]. Prior work has not demonstrated commercially viable durability and performance.

We investigated if covalently bonding the laminar GO to the porous polymer support improved ion rejection and membrane durability. Preliminary tests of GO/polymer membranes had shown that the dominant failure mechanism was GO delamination from the polymer support. Proven organic adhesives functionalized the polymer support and provided a covalent linkage to the laminar GO. Membrane performance, organic adhesive effectiveness, and chlorine tolerance are evaluated via permeance and ion rejection measurements and optical spectroscopy.

Summary of Accomplishments:

We demonstrated that covalent cross linking functional groups increased the mechanical robustness of the laminar GO structures, minimizing inter-membrane fracture and allowing for ion (sulfate) rejections of >80 %. Our primary goal of increasing GO membrane robustness was achieved. Scanning electron microscopy (SEM) analysis of the filtration area of a membrane sample showed no defects or fractures following deionized water (DI) water permeance measurements at driving pressures up to 5 bar. This robust binding of the GO to the polymeric support is in sharp contrast to the delamination and fracture previously noted for GO membranes sans covalent cross linkage.

Raman spectroscopy showed that the GO nanosheets are stable following extended exposure to 1 ppm free chlorine (>650 ppm-hour). Extended exposure to 100 ppm free chlorine (>65,000 ppm-hour) did degrade the nanosheets, as evidenced by the increased D peak and diminished 2D peak in the Raman spectra. From a practical point of view, a 1 ppm level of free chlorine in the feed water would significantly diminish biofouling, decreasing the operating costs of membrane-based desalination.

Permeances of the functionalized GO membranes are comparable to that of commercial polyamide reverse osmosis membranes, comparable to the 0.5 L $m^{-2}h^{-1}$ bar^{-1} and 2 L $m^{-2}h^{-1}$ bar^{-1} permeances of the GO membranes operated at the much lower driving pressures of 3 bar.

Significance:

Reliable, affordable access to water is critical to national security. Our work demonstrates that supported graphene oxide membranes may be capable of reaching the goal of chlorine-tolerant, low-energy desalination membranes, thus benefiting military and energy customers. The US Army Corp of Engineers requires chlorine-resistant membranes to reduce the water demands of contingency operating bases by enabling greywater reuse. Such desalination membranes would conceivably aid the Army's goal of Net Zero water use at six installations by 2020. Energy-efficient membranes would enable closed-loop cooling for thermal power plants, decreasing their water needs and thus reducing their vulnerability in water stress conditions.

Optimizing Enzymatic Depolymerization of Lignin: Surface Analysis of Chemical Effects is Key

176729
Year 1 of 1
Principal Investigator: M. S. Kent

Project Purpose:

Lignin represents the largest renewable source of aromatic compounds on our planet. Lignin is a complex 3D polymer made up of three monolignols that combine randomly. In nature, lignin is broken down by complex microbial communities that secrete oxidative enzymes and small molecule mediators. To date, attempts to break down lignin with individual purified microbial oxidative enzymes have failed, likely because the necessary complexity in terms of multiplicity of enzymes and mediators has not been achieved. Enzyme mixtures have not been studied because there is currently no assay that can examine large numbers of samples. Furthermore, while a small number of oxidative enzymes from ligninolytic fungi and bacteria have been well characterized, large-scale efforts are under way to discover new ligninolytic enzymes from various ecological niches. However, the current lack of an assay that can handle a large number of enzymes will severely limit the value of this effort. In order to benefit from the discovery of new enzymes, and to understand how to optimize mixtures of oxidative enzymes and their mediators, an assay method is needed that can be multiplexed to handle large numbers of samples. In this work, we will develop a new assay for lignin degradation based on lignin films. The loss of mass from the lignin films is assayed by measuring changes in film thickness using ellipsometry. This method has the advantage of being highly sensitive and quantitative, as thickness can be measured to within +/- 10 Å from a 1000 Å film with ellipsometry. The familiar multi-well plate format can be achieved using a silicone mold that is clamped against the lignin-coated silicon wafer. We will develop this concept and apply it to assay a large-scale experiment of 20-50 simultaneous test conditions to demonstrate proof of principle.

Summary of Accomplishments:

We have developed a new methodology for detecting and quantifying lignin depolymerization. The assay is based on casting films of lignin on silicon wafers and measuring loss of mass through decrease in thickness. A silicone mold in the form of a standard 96-well plate is pressed against the silicon wafer to create a highly multiplexed format. The assay is highly sensitive, quantitative, and compatible with standard 96-well plate robotic fluid handling systems. This assay will enable assessment of the ligninolytic potential of a large number of catalytic chemistries, ligninolytic enzymes, reaction conditions, and rapid identification of ligninolytic organisms and microbial communities. The multiplexed device was constructed, refined through several stages, and then several trials were performed involving the Fenton reaction. The Fenton reaction, in which highly potent hydroxyl ion is generated by reaction of hydrogen peroxide and ferrous salt, is used to treat industrial waste and organic contaminants in groundwater and has been employed in biomass pretreatment strategies. The trials demonstrated that up to 80 different reaction conditions can be assayed simultaneously. The results revealed a highly nonlinear dependence of release of soluble fragments on the concentration of ferrous salt. This is very likely due to competing factors involving the physical chemistry of the oxidative reactions and the competition between depolymerization and repolymerization. An invention disclosure has been filed on the device and the assay concept. We plan to use this device to optimize catalytic and enzymatic processes for maximum rate of breakdown and to generate the most favorable product distribution.

Significance:

The valorization of lignin is currently one of the greatest challenges in developing renewable transportation fuels based on lignocellulosic biomass. Developing efficient routes to break lignin into aromatic monomers or other valuable small molecules is an intense area of current research. There is currently no simple, rapid, and sensitive method for assaying the degradation of lignin. We developed a new assay for degradation of high molecular weight insoluble lignin. This assay will enable assessment of the ligninolytic potential of a large number of catalytic chemistries, ligninolytic enzymes, reaction conditions, and rapid identification of ligninolytic organisms and microbial communities. It is likely that companies involved with lignocellulose biomass, such as the emerging biofuels industry, pulp and paper industry, and agricultural companies, will be interested in the capability for high throughout assays of lignin depolymerization.

Two-Fluid Hydrodynamic Printing for Electronic Components

176752
Year 1 of 1
Principal Investigator: D. M. Keicher

Project Purpose:

Printing technologies are changing how electronic components are produced. Screen printing is widely accepted for production applications, and gravure, ink jet (IJ) and aerosol jet (AJ) printing technologies are finding application in the production of electronics. A shortcoming of these technologies remains in their ability to consistently produce features less than approximately 50 µm with properties sufficient for low volume and high performance applications.

Current research in microfluidics has shown that hydrodynamic focusing can be used to form conductive nanowires as small as 400 nm in diameter. The purpose of this effort is to demonstrate that hydrodynamic focusing can be used to create a printing technology for very fine conductive features. This capability would overcome many of the limitations imposed by IJ, AJ, and extrusion technologies used for printed electronics applications. To enable deposition of a single material using hydrodynamic focusing, it will be necessary to remove the majority of the coaxial sheath fluid after focusing has been performed to allow the focused core fluid stream to be impacted onto a print substrate. Superheating is a proposed method to allow the sheath material to be selectively evaporated upon exiting the print head enabling the single material print capability. The focus of this effort will explore the feasibility of this approach. There is a risk that vaporizing the sheath fluid will affect other aspects of printing and so it is important to understand any issues associated with selective vaporization. Addition of features within the microfluidic flow cell to recycle most of the sheath fluid could provide an alternative solution/enhancement to aid in separation of the sheath and core fluids. Developing a print technology to produce high quality, conductive micron/submicron features would impact the ability to print high performance transistors and provide a cost effective alternative to wire bonding and traditional lithographic processes for low volume, high mix applications.

Summary of Accomplishments:

We demonstrated the feasibility to use hydrodynamic focusing of two fluid steams to create a novel microprinting technology for electronics and other high performance applications. Initial efforts focused solely on selective evaporation of the sheath fluid from print stream provided insight in developing a unique print head geometry allowing excess sheath fluid to be separated from the print flow stream for recycling/reuse. Fluid flow models suggest that >81% of the sheath fluid can be removed without affecting the print stream. Further development and optimization is required to demonstrate this capability in operation. Print results using two-fluid hydrodynamic focusing yielded a 30 µm wide by 0.5 µm tall line that suggests that the cross section of the printed feature from the print head was approximately 2 µm in diameter. Printing results also demonstrated that complete removal of the sheath fluid is not necessary for all material systems. The two-fluid printing technology could enable printing of insulated conductors and clad optical interconnects. Further development of this concept should be pursued.

Significance:

Maintaining a leadership position in Additive Manufacturing (AM) is critical to the security of the nation. The two-fluid hydrodynamic printing technology demonstrates a new printing capability for advancing AM in the area of printed electronics and multi-material structures. This technology also opens up the opportunity to expand AM into areas such as printed optical interconnects. Innovations discovered through the course of this project demonstrate the ability of Sandia to provide a leadership role in advancing the AM technologies for next-generation opportunities.

Validating Host-Directed Therapeutics Targeting Wnt Signaling for Treatment of Emerging Infectious Disease

177858
Year 1 of 1
Principal Investigator: O. Negrete

Project Purpose:

Biodefense and emerging infectious disease (BEID) pathogens represent a critical threat to national security as most of these agents lack countermeasures. The most significant agents of biodefense concern are those listed as Category A priority pathogens. Rift Valley Fever virus (RVFV), a Category A pathogen, is a mosquito-borne virus that is endemic to Africa, but has the potential of being introduced into the US and becoming established in the mosquito population, very much like what happened in the case of West Nile virus. RVFV causes serious morbidity and mortality in humans and livestock, has a potential for bio- and agro-terrorism, and no treatments exist for RVF disease. The combination of functional genomic approaches, comprehensive computational pathway analysis, and literature mining have identified the cellular Wnt signaling pathway as an important host pathway regulating RVFV infection. Perturbations in Wnt expression, signaling, and the battery of Wnt-regulated genes (collectively the canonical Wnt pathway) are known to manifest in a variety of clinically relevant disease states, including cancer and cardiovascular disease. Cancer therapeutic companies are actively engaged in identifying Wnt inhibitors as treatments for a variety of cancers. Using the significant progress made in Wnt/cancer field, we will seek to identify a potent inhibitor of the Wnt pathway that blocks RVFV infection, identify the mechanism of Wnt activation by RVFV infection, and test inhibitor treatments with attenuated RVFV strains (e.g., MP12) and related viruses. Targeting host responses to invading viruses has been the focus of recent antiviral research. Targeting the host is an attractive antiviral approach since drug resistance can occur less frequently as compared to direct viral protein inhibitors. The ultimate goal of these studies is to find suitable Wnt signaling host target, which would minimally affect cell function but greatly impact the virus viability. An ideal candidate would also be capable of inhibiting more than one virus, thus demonstrating broad-spectrum utility.

Summary of Accomplishments:

To aid in countermeasure development for RVFV, we previously employed high-throughput RNA interference (RNAi) screening as a functional genomic approach for comprehensive virus-host interaction analysis and host-directed therapeutic target identification. In the screen, HeLa cells were reverse transfected with siRNAs in a 384 well format then infected with the recombinant vaccine strain RVFV MP12 encoding green fluorescence protein (GFP) in place of the nonstructural protein NSs. Genome-wide RNAi screening identified 381 cellular genes whose knockdown reduced viral infection as indicated by reduced GFP fluorescence. These 381 genes were classified into canonical pathways and the Wnt/Beta-catenin signaling pathway was among the most represented. Further analysis indicated that RVFV-GFP infection increased Wnt signaling in a beta-catenin reporter assay, inhibitors of Wnt signaling decreased RVFV-GFP infection, and RVFV-GFP infection was enhanced when Wnt signaling was pre-activated. Similar results were found using authentic (non-recombinant) RVFV-MP12. As control experiments, similar Wnt signaling experiments were performed with two other viruses, vesicular stomatitis virus (VSV) and vaccinia virus (VacV). VSV and VacV did not activate the Wnt pathway — they also did not increase infection in cells pre-activated with Wnt ligands, nor were blocked by Wnt inhibitors. While viruses RVFV, VSV and VacV each replicate in host cell cytoplasm, each use different replication mechanisms. The subtle differences in their replication strategies might explain their differential requirement for Wnt signaling during infection.

Significance:

RVFV is classified as a HHS/USDA overlap select agent due to its bio- and agro-terrorism potential. A growing concern over these particular types of human/agriculture pathogens has prompted funding agencies such as the Department of Homeland Security to fund “new, cost-effective, biological-based countermeasures for foreign animal disease and zoonotic pathogens affecting major domestic livestock species” research. The ultimate goal of our studies is to find suitable Wnt signaling inhibitor, which would minimally affect cell function but greatly impact the virus viability, ideally with broad-spectrum utility. Countermeasure development for bioterrorism agents is of major national security interest. We anticipate this new understanding of the fundamental mechanisms of RVFV infection combined with the development of Wnt inhibitors for cancer treatments will aid in the design of efficacious host-directed anti-RVFV therapeutics.

High-Density, Reactive Films with Nanometric 2-D Periodicity by Atomic Layer Deposition

177859
Year 1 of 1
Principal Investigator: R. V. Reeves

Project Purpose:

Exothermic thin films produce high temperature reactions without gas production, making them attractive as heat sources for joining and other applications. However, sputter deposition, the current state of the art for producing exothermic films, has weaknesses that limit the films' utility. First, the produced material is brittle. Cracks can prevent reaction propagation, reducing component performance or causing component failure. Also, production is limited by the sputter rate, so scaling production is only possible by increasing the size or number of sputter guns, both of which are expensive options. The orientation of the periodicity in the sputtered material also inhibits direct viewing of the interface between reactants, preventing in situ study of reaction kinetics.

We will create exothermic composite films with increased flexibility through easily scalable means. Using a flexible, porous, device silicon substrate, we will deposit platinum through atomic layer deposition (ALD) to create 2D periodic reactive composites that retain the flexibility of the substrate, have comparable reaction behavior to current materials, and allow direct monitoring of the reactive interfaces. The deposition will be characterized by microscopy and the reaction behavior of the material will be characterized and compared to traditional, sputter-deposited reactive films.

There is a need for flexible reactive materials and a scalable method for producing them. Our use of flexible substrates as a reactant and deposition base is an innovative idea for producing reactive materials. The use of ALD, an easily scalable production method, to create reactive composites is also a novel method.

Summary of Accomplishments:

The main achievement is the development of a process to create high density, 2D periodic reactive materials using a novel process that provides nanometric spatial control. The original process was modified during the duration of the project in order to compensate for weaknesses in the base materials and produce viable reactive material. The generated material exhibited the spatial control necessary to access the type of high performance reactions associated with nanometrically periodic reactive materials. The structure of these materials could also provide advantages over the current method for producing thin film reactive materials. From a research standpoint, the orientation of the reactant periodicity allows for direct monitoring of reactive interfaces, which was not previously accessible. This could allow for in situ visualization of fast reaction kinetics in solid state reactive materials. From a practical view, the scalable processes utilized could provide cost and productivity benefits.

Significance:

These results, the production process, and the new materials created in this research advance science by allowing new methods of directly monitoring hard to study chemical processes. Previous research in this area has relied on inference of behavior from monitoring bulk scale events. The new materials could allow for direct monitoring of events at length scales pertinent to the chemical processes. The knowledge gained from these studies could affect national security applications that utilize similar materials. National security missions can also benefit from the improved scalability of this process over current methods for producing thin film reactive materials.

Graded Index Materials for Advanced Optical Concepts

177860
Year 1 of 1
Principal Investigator: D. Scrymgeour

Project Purpose:

The purpose of the project is to demonstrate the creation of graded index (GRIN) materials, which are dielectrics that have a non-uniform spatial variation of refractive index n with position, using multiphoton lithography (MPL). MPL is an intrinsic 3D direct-write technique where a pulsed laser beam is focused within chemical precursors to drive photochemical reactions (e.g., photopolymerization) only at the focus point. This technique is ideally suited to creating GRIN materials, as written voxels can be restricted to 100 nm^3 — below the threshold to create low scatter optical materials even at visible wavelengths. This work will focus on creating index gradients through variations in density in polymeric materials known to be compatible with MPL. We seek to specifically quantify index gradient, achievable index change (dn) and spatial variation (dn/dz), an important metric to inform the future design of GRIN devices. We also want to demonstrate the replacement, exchange, and infiltration of these scaffolds with other materials (i.e., silica) using established chemistries to create higher index contrast and/or better mechanical properties. Fabrication of GRIN materials with user-defined profiles would provide a revolutionary advance in optics and create a new class of optical materials with enhanced properties currently unrealizable.

Summary of Accomplishments:

We successfully demonstrated the writing of graded index structures using MPL. We fabricated, using direct writing methods, grating structures in hydrogel materials comprised of bovine serum albumin (BSA) protein and then quantified the index change of the written grating structures via optical techniques. We were able to successfully demonstrate index changes of up to 10^{-2}, which is similar to laser densified glass and other polymer systems. Finally, we demonstrated the conversion of BSA-written density variation structures directly to silica (SiO_2), opening up the possibility of transforming MPL written density structures to other relevant material systems.

Significance:

This direct-write approach to creating GRIN materials significantly reduces development costs, allows rapid prototyping, and most importantly enables 3D arbitrary index distributions, which is lacking in current GRIN fabrication approaches. This arbitrary index capability is key to realizing advanced GRIN concepts such as radically simplifying optical designs and enabling perfect lensing and cloaking technologies. Advances in fabrication of GRIN materials will advance fabrication of functionally graded materials, where the material properties vary spatially in two or three dimensions according to functional requirements and are important to tailoring a range of phenomena including mechanical, thermal, and transport properties.

At a fundamental level, this project is an example of basic energy science and research in advanced manufacturing and nanoscience, including scientifically tailored materials where we are advancing the state of science for the benefit of DOE/NNSA. This work has potential impacts in future optical materials, systems, and designs that have nuclear security, defense, and nonproliferation implications.

Exploring Charge Transport in Guest Molecule Infiltrated $Cu_3(BTC)_2$ Metal Organic Framework

177861
Year 1 of 1
Principal Investigator: A. A. Talin

Project Purpose:

The goal of this project was to expand the understanding of the physical properties of our recently discovered class of materials consisting of metal-organic frameworks (MOF) with electroactive 'guest' molecules that together form an electrically conducting charge-transfer complex, described here as " molecule@MOF". Thin films of a MOF composed of binuclear copper ions bridged by carboxylate groups, known as $Cu_3(BTC)_2$, were grown on fused silica using solution step-by-step growth and were infiltrated with the molecule tetracyanoquinodimethane (TCNQ). The infiltrated MOF films were extensively characterized using optical microscopy, scanning electron microscopy, Raman spectroscopy, electrical conductivity, and thermoelectric properties. Thermopower measurements on TCNQ@$Cu_3(BTC)_2$ revealed a positive Seebeck coefficient of ~400 μV/K, indicating that holes are the primary carriers in this material. The high value of the Seebeck coefficient and the expected low thermal conductivity suggest that molecule@MOF materials may be attractive for thermoelectric power conversion applications requiring low cost, solution-processable and nontoxic active materials.

Summary of Accomplishments:

We discovered that a metal-organic framework material, $Cu_3(BTC)_2$, infiltrated with the molecule TCNQ is a p-type semi-metallic conductor with a high Seebeck coefficient. This result is supported by our first principles calculations which indicate that the Fermi level in this material should lie very close to the valence band maximum.

Significance:

Our discovery of a hybrid organic/inorganic material with high thermopower coefficient is promising for energy conversion applications involving waste heat recovery. The fact that the material is made up of earth abundant elements, is nontoxic, and can be deposited from solution over complex shapes makes it attractive for integration in a variety of applications where current inorganic thermoelectric materials are impractical due to high cost, toxicity, and difficulty in processing.

Investment in novel electronic materials is essential to advanced electronics, with a range of applications where electronic transport is either essential or highly desirable including novel computing devices, detectors, and chem/bio-sensors for the defense and national security communities.

Refereed Communications:

V. Stavila, A.A. Talin, and M.D. Allendorf, "MOF-Based Electronic and Optoelectronic Devices", *Chemical Society Reviews*, vol. 43, pp. 5994-6010, May 2014.

Engineering Intrinsically Stable Nanocrystalline Alloys

177963
Year 1 of 1
Principal Investigator: B. Clark

Project Purpose:

Traditional metallurgical pathways to stabilize metallic grains are through either solute drag or pinning at second phase particles. However, drag and pinning approaches merely delay the kinetics of degradation by slowing the mobility of grain boundaries. While these strategies work to some extent, their applicability to nanostructured metals is limited due to the extremely high energetic driving force associated with boundary energy: the internal boundary energy of a nanocrystalline metal is 10^9 times higher than that of a conventional microcrystalline material.

Recently, a paradigm shift has emerged wherein the driving force for grain boundary migration is eliminated, rather than simply limited by kinetics. This is accomplished by modifying the local thermodynamics of the grain boundary, similar to the role of a surfactant in stabilizing the interfacial area of a microemulsion. Preliminary results from the Schuh group at MIT indicate that this can be achieved in specific binary nanocrystalline systems, where there is greater driving force for solute segregation than solute mixing in these interface-dense materials. However, the single experimentally demonstrated system published to date, a nanocrystalline tungsten-titanium (W-Ti) alloy, was produced via a ball milling process which may have introduced impurities into the grain boundaries or resulted in formation of oxides. These uncertainties make it difficult to assess if the segregated solute or other factors are the crux of their observation of exceptional thermal stability. The goal of this work was to better understand the influence of microstructure and processing on the thermal stability of nanocrystalline W-Ti alloys.

Summary of Accomplishments:

We deposited W-20 atomic % Ti nanocrystalline films using pulsed laser deposition and assessed their thermal stability for comparison with previously reported (by Schuh et al.) grain size stability of ball milled nanocrystalline powders held at 1100 ºC for one week. We discovered a correlation between film thickness and final microstructure following anneal. Thin films were prone to dewetting, wherein the Ti agglomerated around small nano islands of W. This is in contrast to the final microstructure reported in the literature, wherein 10 micron powders with 10 nm grain size had a thickness to grain size ratio that was 100 times greater than in our 100 nm thick films. Thus, the role of surface effects in W-Ti in determining final microstructure, which was previously unexplored, has been elucidated through this work.

To mitigate the effects of the surface-driven annealing processes described above, we deposited thicker, 400 nm thick films and again performed anneals at 1100 ºC. These anneals were performed under both vacuum and reducing environments. The reducing environment was chosen to avoid the formation of oxide during anneal, in order to assess whether suppressing the formation of TiO_2 in the segregated solute regions would impact the final annealed microstructure. Results showed similar microstructures with nanocrystalline grain size following anneals in both the vacuum and reducing environments, indicating that the role of oxide is not the controlling factor in determining thermal stability in nanocrystalline W-20 atomic % Ti. Our findings support the theory that segregated Ti solute, and not oxide at the grain boundaries introduced during processing, controls the thermal stability of nanocrystalline W metal.

Significance:

Work conducted through this project provided insight into the role of processing in controlling solute segregation in nanocrystalline alloys and laid the foundation for further work. Fundamental insight into stabilization of grain boundaries could lead to development of inherently thermomechanically stable nanocrystalline alloys, which would be widely applicable to multiple applications, including for example electrical contacts, microsprings, and hard coatings. Optimization of such materials could potentially impact long-term predictability and performance of a wide range of nuclear weapon components in both normal and abnormal environments, directly impacting the DOE's nuclear security goal.

Control of Surface State Transport in a Topological Insulator using Corbino p-n Junction

177968
Year 1 of 1
Principal Investigator: P. A. Sharma

Project Purpose:

Topological insulators (TI) are bulk semiconductors expected to have dissipationless spin polarized surface states. We intend to fabricate a novel Corbino p-n junction device structure designed to simultaneously resolve two outstanding science questions in the field of TI materials physics. First, existing transport evidence for spin polarized surface state transport is tenuous and limited to low temperatures due to the inability to control doping in TI materials, which results in a strong coupling between bulk and surface electronic states. Second, spin polarization is naively expected to occur on opposite surfaces of a semi-infinite bulk topological insulator. However, real transport experiments are of finite size and thus far only planar Hall bar geometries have been used to investigate surface transport. In a Hall-bar geometry, current flow occurs over all surfaces and, therefore, mapping a specific surface to a specific spin polarization is not well defined. We plan to solve the first problem by using inhomogeneous doping, leading to a space charge region that will null bulk conduction and leave surface states intact. We plan to solve the second problem by using a Corbino geometry, where a current can be made to flow on one surface only. Current S&T approaches use homogeneous materials, limiting progress.

Summary of Accomplishments:

We demonstrated the formation of p-n junctions in topological insulator Bi_2Se_3 and developed a process flow for device structures useful for separating surface and bulk currents.

Significance:

The device structures we have developed are primarily useful for solving a set of outstanding science questions in the field of topological insulators. An invention disclosure has been submitted on the technology we have developed. The main result presented here should also be a stepping stone to more complex structures useful for new devices based on the transport of topological insulator surface states. This project developed proof of concept for a device relevant to advanced sensing applications.

Microscopic Understanding of Fischer-Tropsch Synthesis on Ruthenium

179990
Year 1 of 1
Principal Investigator: P. J. Feibelman

Project Purpose:

To make solar power viable at large scale, we need an economical way to store the captured energy, optimally in a liquid fuel. Sandia's Sunshine to Petrol Grand Challenge project is aimed at a first step, developing cyclic reactors that use solar energy to generate syngas ($CO + H_2$) from CO_2 and H_2O. Much is known about the final step, the Fischer-Tropsch (F-T) process, combining carbon monoxide (CO) and hydrogen (H_2) over a catalyst to make liquid hydrocarbons. But new, atomic scale images of CO and hydrogen co-adsorbed on the most efficient of F-T catalyst materials, elemental Ruthenium (Ru), promise deeper understanding of the catalytic pathway, perhaps a more efficient F-T process. New images remarkably suggest that adsorbed CO and hydrogen intermix on the ruthenium surface rather than segregating into pure CO and pure adsorbed hydrogen islands, as typically happens. Are the new images credible evidence for a mixed surface phase on ruthenium? If so, what is its nature? Does it help explain the superior catalytic F-T activity of ruthenium? The S&T problem is that the scanning tunneling microscope (STM) images electron density, not atomic positions. Thus, an interpretation based on first-principles computational modeling is needed. Density functional theory (DFT) calculations will be conducted for this purpose, producing binding energies vs. surface atom arrangement, simulated STM images, adsorbate vibration frequencies, and adsorbate-induced core-level shifts. The results generated should help to decipher the nature of key intermediates in F-T synthesis.

Summary of Accomplishments:

Several ideas were developed that point toward a successful interpretation of molecular-scale images of an intermixed structure of hydrogen atoms (H) and CO on the close-packed surface of ruthenium. One is that structures containing less hydrogen are energetically more favorable. A second is that the only way to explain the STM images is with a symmetry-breaking ad-molecule arrangement. Specifically, the H-atom populations of every other triangle of CO molecules must be different. The third is that the Tersoff-Hamann approximation is inadequate to the task of simulating the observed images. It does not yield a dark spot where a H-atom lies. Contact has, therefore, been initiated with Jorge Cerdá (Madrid) who has implemented a more sophisticated computational approach to image simulation, based on electron scattering theory, and including the nature of the probe tip. A collaborative effort with him should resolve the problem of H atoms not corresponding to dark image spots, and thereby make it possible to explore H + CO structures by comparing simulated to experimental images, and not just by attempting to minimize system energy. This may be important if energy barriers prevent the system from finding its lowest energy state.

Significance:

Intermediate states in catalytic processes are notoriously difficult to isolate and identify. Progress made in the course of this effort suggests that the mixed H + CO structures seen in scanning probe images will soon be understood and provide an important clue toward explaining why ruthenium is the best Fischer-Tropsch catalyst. This should yield the insight into developing a cheaper substitute for very costly ruthenium metal, and thus help make "Sunshine to Petrol" an economically competitive source of sustainable fuel.

Non-Resonant Nanoscale Extreme Light Confinement

179991
Year 1 of 1
Principal Investigator: G. S. Subramania

Project Purpose:

The goal of this project is to obtain preliminary experimental verification of the broadband optical transmission in a non-resonant "double-groove" structure due to quasistatic electronic response. A wide spectrum of photonics activities Sandia is engaged in such as solid state lighting, photovoltaics, infrared imaging and sensing, and quantum sources, rely on nanoscale or ultra-subwavelength light-matter interactions (LMI). The fundamental understanding in confining electromagnetic power and enhancing electric fields into ever-smaller volumes is key to creating next generation devices for these programs. The prevailing view is that a resonant interaction (e.g., in microcavities or surface-plasmon polaritons) is necessary to achieve the necessary light confinement for absorption or emission enhancement. We propose a new paradigm that is non-resonant, and therefore broadband, and can achieve light confinement and field enhancement in extremely small areas [$\sim(\text{lambda}/500)^2$]. The project is based on a theoretical work [G. Subramania et.al., Phys. Rev. Lett. 107, 163902 (2011)] previously performed at Sandia. The paradigm structure consists of a periodic arrangement of connected small and large rectangular slits etched into a metal film named double-groove (DG) structure. The degree of electric field enhancement and power confinement can be controlled by the geometry of the structure. The key operational principle is attributed to quasistatic response of the metal electrons to the incoming electromagnetic field that enables non-resonant broadband response. Experimental verification of this phenomenon is a key first step to designing in the future more complex structures that can be incorporated into detectors and sensors. This non-resonant approach can not only offer new physical insights like broadband Purcell enhancement but also have significant advantages over its resonant counterpart by potentially enabling devices with large operational bandwidth, faster response, and robustness.

Summary of Accomplishments:

We developed a process to fabricate DG structure using electron beam lithography patterning and metal deposition and lift-off. Using this process, we fabricated several DG devices on 50 nm thin gold film with a lattice constant of 800 nm and ~1mm X 1mm in size. These devices had narrow sub-wavelength gap regions between 80-150 nm, where theoretically one expects broadband electric field enhancement of > 5X in the mid-infrared wavelength region. This is an important technical accomplishment in process development that lays the foundation for achieving more challenging designs with considerably smaller lattice constants (<300 nm) and sub-wavelength gap widths (<50 nm) in the future as required for pump-robe spectroscopy experiment. This riskier aspect of the project was, therefore, scaled back to demonstrate broadband transmission response. Several fabrication runs were performed to obtain the nanofabrication processing parameters to achieve these structures on mid-infrared transparent substrates. We discovered that it was considerably more challenging to fabricate these structures on BaF_2 substrates than CaF_2, although BaF_2 is more desirable due to its broader optical transparency region. We used computational simulations (finite difference time domain) to guide the design of the structures and to predict the optical response. We performed preliminary optical transmission measurements on devices that were fabricated on CaF_2 substrates using Fourier transform infrared spectroscopy. It is encouraging that the optical response demonstrated broadband transmission with features similar in behavior to that predicted by theory. Our work will enable, for the first time, the ability to observe broadband sub-wavelength electric field enhancement and power confinement.

Significance:

This work demonstrates experimental fabrication of the double-groove structure to explore non-resonant, broadband ultra-subwavelength light confinement. Results obtained have brought us a step closer to understanding non-resonant field concentration. This research can directly impact a broad range of application areas in sensing and imaging key to Sandia's national security missions, for example remote infrared (IR) imagers and chem/bio detectors, by making them broadband, fast, and robust. This work also directly relates to DOE's mission of "strengthening connection between fundamental science and advanced technology."

Time Series Feature Engineering via Evolution

179992
Year 1 of 1
Principal Investigator: A. J. Scholand

Project Purpose:

The purpose of the project is to address the problem of classifying high dimensional time series sensor data using a combination of unconstrained but goal-directed optimization with feature-based supervised machine learning. Existing approaches to high dimensional classification suffer from either of two challenges. Classifying in the parameter space of the raw data is difficult because the high dimensionality of the data disperses the training exemplars widely so that new data can be expected to occur far from known types of their classes. Reducing the data down to a lower dimensional representation by extracting features from the data reduces this distance problem but discards information. The information lost may be critical to discriminating between classes, degrading classification performance on the extracted features. Ideally, we need features where the information loss in projecting to feature space is orthogonal to the information distinguishing each class. Unfortunately, the current state of the art for feature ideation and evaluation is a manual process, meaning that the vast majority of possible features possible via transformations of the raw data are left unexplored. This project addressed this gap by exploring the use of guided search in the feature transformation space on representative high dimensional sensor data from optical sensors.

Summary of Accomplishments:

We performed fundamental exploration of combinatoric arrangements of well-studied data transformations, gaining insight into the performance/computation cost tradeoffs of signal processing arrangements of varying degrees of complexity. We also examined the interactions between types of classifier (linear support vector machine (SVM), random forest, gradient boosting) and feature processing. We constructed a computational 'lab bench' which enabled this research and can be easily and simply extended to explore more exotic data transformations or more sophisticated classifiers. We discovered a wide range of approximately 100 different approaches that demonstrated exceptional utility against 'first observed' signals of interest and modified/distorted signatures without debilitating false positive rates.

Significance:

The research findings have applications to sensor and signal processing technologies that may benefit DOE's mission to enhance nuclear security through nonproliferation efforts. The research increased the operational skills of the technical workforce in state-of-the-art machine learning.

Magnetic Nitride Films for Superconducting Memory Devices

180623
Year 1 of 1
Principal Investigator: N. A. Missert

Project Purpose:

Superconducting electronics (SCE) is one of the leading technology candidates for high performance, ultra-low power computation needed to address our society's needs. Although high-speed, digital superconducting circuits has been demonstrated, the promise of extending these devices to high performance computing has been severely hindered by the lack of a fast, low-energy, high capacity, integrated memory cell and scalable 3D architecture. Recently, ideas for manipulating the critical current of Josephson junctions (JJ) using magnetic interlayers have been proposed. The magnetization of a ferromagnetic layer can be set to control the magnitude of the junction critical current, resulting in two distinct states representing a "O" or "1." Such cells could then be used as a fully integrated, energy-efficient, scalable, non-volatile RAM. Identifying and demonstrating a ferromagnetic layer that can be switched at high speeds with low power is critical for this technology. This work investigates magnetic nitride thin films to address this issue. Although chromium-doped aluminum nitride (AlN) and gallium nitride films have promising ferromagnetic properties, their incorporation into a switchable memory device has never been attempted.

Summary of Accomplishments:

This work investigated pulsed laser deposition of Cr-doped AlN thin films for use as ferromagnetic layers in memory cells for superconducting electronics. We used pulsed laser deposition to fabricate these films under conditions and at temperatures compatible with incorporation into superconducting electronic structures and measured their surface morphology, crystalline structure, and magnetic properties in order to assess their performance for future memory cells. The film morphology, crystalline structure and magnetization were investigated as a function of laser fluence on the target and background N_2 pressure during deposition. Higher laser fluence resulted in films composed of a smooth under layer with a high density of poorly adhered, rough crystallites at the surface. Lower laser fluence reduced the density of surface crystallites significantly. X-ray diffraction showed that films grown at high laser fluence show crystalline peaks associated with AlN. Both types of films showed hysteretic magnetization curves consistent with films grown by other deposition techniques.

Significance:

This work shows that ferromagnetic Cr:AlN films can be grown by pulsed laser deposition. The clear difference between low and high laser fluence for film surface morphology and x-ray diffraction spectra suggests that for this porous, fragile Cr:AlN target, high laser fluence produces large crystallite ejecta in addition to congruent ablation of the target species. The similarity in the magnetization for both low and high laser fluence indicates that the smooth background film comprises Cr:AlN, as AlN is not ferromagnetic. The morphology of the smooth background films is exactly what is needed for the ferromagnetic layers in multilayer superconducting memory cells.

This project contributes to DOE's mission to enhance US security and economic growth through transformative science, technology innovation, and market solutions to meet our energy and environmental challenges by providing a technological path to enable energy-efficient high performance computation. It also benefits other federal agencies (such as DHS and NSA) with needs for low power, energy efficient, high performance computing to ensure national security.

Electrochemical Solution Growth of Magnetic Nitrides

180788
Year 1 of 1
Principal Investigator: T. Monson

Project Purpose:

Magnetic nitrides, if manufactured in bulk form, would provide designers of transformers and inductors with a new class of better performing and affordable soft magnetic materials. According to experimental results from thin films and/or theoretical calculations, magnetic nitrides would have magnetic moments well in excess of current state of the art soft magnets. Furthermore, magnetic nitrides would have higher resistivities than current transformer core materials, and therefore, not require the use of laminates of inactive material to limit eddy current losses. However, almost all of the magnetic nitrides have been elusive except in difficult to reproduce thin films or as inclusions in another material. Now, through its ability to reduce atmospheric nitrogen, the electrochemical solution growth (ESG) technique can bring highly sought after (and previously inaccessible) new magnetic nitrides into existence in bulk form. This method utilizes a molten salt as a solvent to solubilize metal cations and nitrogen ions produced electrochemically to form nitrogen compounds. Unlike other growth methods, the scalable ESG process can sustain high growth rates (~mm/hour) even under reasonable operating conditions (atmospheric pressure and 500 °C). Ultimately, this translates into a high throughput, low cost, manufacturing process. The ESG process has already been used successfully to grow high quality gallium nitride, GaN.

Summary of Accomplishments:

The initial part of our effort focused on building our experimental setup. Due to the hygroscopic nature of the LiCl/KCl eutectic salt and potential reactivity of iron cations, all experiments were carried out in a nitrogen-purged glove box. A total of four experiments were conducted using lithium nitride (Li_3N) as a nitrogen source. One final experiment was run, replacing Li_3N with flowing nitrogen gas as the nitrogen source. After each experiment, our product (either an electroplated wire or a powder removed via filtration) was collected and analyzed using x-ray diffraction (XRD). The product trapped in a Ni mesh filter after the flowing N_2 gas experiment was thoroughly washed by soaking in dried and distilled dimethyl sulfoxide (DMSO). The substantial amount of black crystallites formed in just one hour of electrochemical growth is very encouraging. This powder had one potential Fe_2N peak but will require additional microprobe characterization to confirm the presence of iron nitride. The electroplated wire did not have any iron nitride peaks when examined by XRD. However, a substantial amount of the iron nitride formed could be in the amorphous state and may require annealing to crystallize so that it can be detected using XRD.

Significance:

The synthesis of iron nitrides using ESG will create a new opportunity to fabricate affordable and commercially viable high saturation magnetization and low loss inductor/transformer core materials while also addressing current magnetic core shortfalls. These new materials could enable technological advancements such as better hybrid and electric vehicles, the integration of more renewable energy generation, and higher capability forward deployed military installations. Furthermore, the ability to synthesize and study a new class of magnetic materials in bulk form would have enormous implications in the basic research and understanding of magnetic materials.

Unpublished Summaries

For information on the following FY 2014 LDRD projects, please contact the LDRD Office:

Laboratory Directed Research & Development
Sandia National Laboratories
Albuquerque, NM 87185-0359

Project Number	Title
158755	Advanced Imaging Optics Utilizing Wavefront Coding
158757	Applying Discrimination Methods to Collected and Synthetically Modeled Explosive Signatures
158759	Remote Optical Sensing of Ionizing Radiation
158781	Breaking the Language Barrier
158850	Miniature Tritium Free Neutron Generator
158859	New Radiation-Resistant Materials
165549	Precise and Persistent RF Detection, Tracking, and Location
165550	Hardware Solution to Flash Memory Accessibility Problems
165559	Board and System Level Spectral Analysis
165566	Electromagnetic-Wave Probing of Electrical Circuits
165578	Distributed Receiver Approach to Robust Satellite Signal Reception
173039	Novel, Semi-Destructive FA Technique for Stacked Die
173040	Novel Memory Analysis
173042	Data Provenance for Automotive CAN Networks
173044	New Methods for Characterizing Hardware Protocols
173046	Novel Technology Development
173049	Advanced Target Phenomenology for Emergent Threat Detection
173154	Radiation Hardness of MEMS Capacitive and Electromagnetic Accelerometers
173182	Nonlinear Transmission Line Based Technology
176115	Advanced Deprocessing Techniques to Investigate White Light LVP and Other Imaging

Appendix A: FY 2014 Awards and Recognition

Award Description	LDRD Contribution
R&D 100 Award, *R&D Magazine:* The BaDx (Bacillus anthracis diagnostics): Melissa Finley	Project 158813, "Development of a Sustainable Anthrax Diagnostic Test for Countering the Biological Threat"
R&D 100 Award, *R&D Magazine:* Goma 6.0: Randall Schunk	Project 150123, "Stochastic Study of Microparticle Adhesion due to Capillary Condensation," and others
R&D 100 Award, *R&D Magazine:* Triplet-Harvesting Plastic Scintillators (THPS): Patrick Feng	Project 141681, "Use of Metal Organic Fluors for Spectral Discrimination of Neutrons and Gammas," and others
Asian American Engineer of the Year: Yifeng Wang	Project 173102, "Fundamental Study of Disposition and Release of Methane in a Shale Gas Reservoir"
Most Promising Scientist or Engineer-Advanced Degree, Ph.D., by Great Minds in STEM, HEAAC: Edward Jimenez	Project 158182, "High Performance Graphics Processor-Based Computed Tomography Reconstruction Algorithms for Nuclear and Other Large Scale Applications"
Federal Laboratory Consortium: Far West/Mid-Continent Region awarded notable technology development: C. Jeff Brinker and Susan Rempe	Project 165609, "The Engineering and Understanding of Nanoparticle/Cellular Interactions"
Federal Laboratory Consortium: Far West/Mid-Continent Region awarded notable technology development for Spin DX	Project 158820, "Rapid Affinity Reagent Development for Emerging Pathogen Detection"
Federal Laboratory Consortium: Far West/Mid-Continent Region awarded notable technology development for Sandia Cooler	Project 151304, "Tier 2 Development of Sandia's Air Bearing Heat Exchanger Technology"
Federal Laboratory Consortium: Far West/Mid-Continent Region awarded Outstanding Regional Partnership to UNM Health Sciences Center and Sandia	Project 171055, "Breaking Antibiotic Resistance: Use of High-Throughput, Multi-Dimensional Data Analyses and Revolutionary Advances in Engineered Nanoparticles to Design and Deliver Antisense RNA," and others
Fellow of the American Society of Mechanical Engineers (ASME): Earl Reedy, Jr.	Project 165649, "A Process and Environment Aware Sierra/SM Cohesive Zone Modeling Capability for Polymer/Solid Interfaces"
Fellow of the American Physical Society (APS): Kevin McCarty	Project 165698, "Predicting Growth of Graphene Nanostructures Using High-Fidelity Atomistic Simulations"
Fellow of the Institute of Electrical and Electronics Engineers (IEEE): Igal Brener	Project 158826, "Electrically Tunable Metamaterials for Agile Filtering in the Infrared," and others
Fellow of the Institute of Electrical and Electronics Engineers (IEEE): Michael Cuneo	Project 154060, "New Strategies for Pulsed Power Transmission Lines: From Repetitive to Replaceable to Recyclable"
IEEE Nuclear and Plasma Sciences Society (NPSS) Early Achievement Award: David Ampleford	Project 165733, "Z-Pinch X-Ray Sources for 15-60keV"
IEEE Young Engineer Award Recipient for the New Mexico Chapter: Jose Luis Cruz-Campa	Project 159257, "Science-Enabled Next Generation Photovoltaics for Disruptive Advances in Solar Power and Global Energy Safety and Security"

Award Description	LDRD Contribution
IEEE Plasma Science and Applications Award: Mike Desjarlais	Project 151365, “Dynamic Temperature Measurements with Embedded Optical Sensors,” and others
IEEE Nuclear and Plasma Sciences Society Merit Award: Jim Schwank	Project 173134, “A Space-Like Low-Energy Proton Test Environment to Rapidly Qualify Advanced Microelectronics for Flight Readiness”
DOE Office of Science Early Career Research Program Award: Stephanie Hansen	Project 165733, “Z-Pinch X-Ray Sources for 15-60keV”
DOE Hydrogen and Fuel Cells Program Award: Brian Somerday	Project 173116, “Multi-Resolution Characterization and Prediction of Environmentally Assisted Intergranular Fracture”
Fusion Power Associates' 2014 Excellence in Fusion Engineering Award: Dan Sinars	Project 141537, “Stability of Fusion Target Concepts on Z”
Best Paper of the Year: International Journal of Solids and Structures 2014: Benjamin Reedlunn	Project 165574, “Large Motion High Cycle High Speed Optical Fibers for Space-Based Applications”
Best Paper Award: IEEE Nuclear and Space Radiation Effects Conference: Nathaniel Dodds	Project 173134, “A Space-Like Low-Energy Proton Test Environment to Rapidly Qualify Advanced Microelectronics for Flight Readiness”
Best Poster Award: 36th Symposium on Applied Surface Analysis: Eric Romero and Ping Lu	Project 158822, “In Situ Study of Dynamic Phenomena at Metal Nanosolder Interfaces using Aberration-Corrected Scanning Transmission Electron Microscopy”
Best Poster Award: Materials Research Society Spring 2014 Meeting: Carlee Ashley	Project 173493, “Metal Organic Frameworks for Targeted, Triggered, Sustained, and Systemic Delivery of Antibiotics,” and others
Best Poster Award: 32nd International Conference of the System Dynamics Society: Peter Kobos, et al.	Project 165631, “Natural Gas Value-Chain and Network Assessments”
Best Poster Award: Atom Probe Tomography and Microscopy (International Field Emission Society): R. Karnesky, et al.	Project 173116, “Multi-Resolution Characterization and Prediction of Environmentally Assisted Intergranular Fracture”
Best Poster Award: Sanibel Symposium: Marie V. Parkes, et al.	Project 165632, “Novel Metal-Organic Frameworks for Efficient Stationary Energy Sources via Oxyfuel Combustion”
Best Student Paper: IEEE Summer Topicals Meeting Series: David Borlaug	Project 173490, “Plasmonic-Based Optical Modulators and Switches”
Best Oral Presentation: 2013 MRS Fall Meeting: Christina Ting	Project 165824, “Crossing the Membrane Barrier: Implications for Developing Medical Therapeutics”

Award Description	LDRD Contribution
Best Student Oral Presentation: 25th Annual Rio Grande Symposium on Advanced Materials: Julian A. Vigil	Project 165636, "Developing Next Generation Graphene-Based Catalysts
Best Presentation Award: MRS Spring 2014 Meeting. Symposium Y: Biomaterials for Biomolecule Delivery and Understanding Cell-Niche Interactions: Caroline Bouvie, et al.	Project 171055, "Breaking Antibiotic Resistance: Use of High-Throughput, Multi-Dimensional Data Analyses and Revolutionary Advances in Engineered Nanoparticles to Design and Deliver Antisense RNA," and others
Outstanding Talk Award: Composites at Lake Louise: Erik Spoerke, et al.	Project 158825, "Crystalline Nanoporous Frameworks: a Nanolaboratory for Probing Excitonic Device Concepts"
Forum Award Winner: 2014 International Parallel and Distributed Processing Symposium: Mehmet Deveci	Project 158793, "Architecture- and Resource-Aware Partitioning and Mapping for Dynamic Applications"