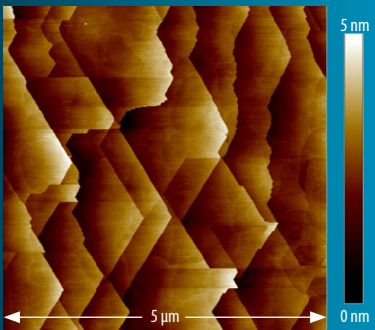# SANDIA NATIONAL LABORATORIES

Exceptional service in the national interest

LABORATORY DIRECTED RESEARCH AND DEVELOPMENT

2018 ANNUAL REPORT

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Sandia National Laboratories

LDRD LABORATORY DIRECTED RESEARCH & DEVELOPMENT
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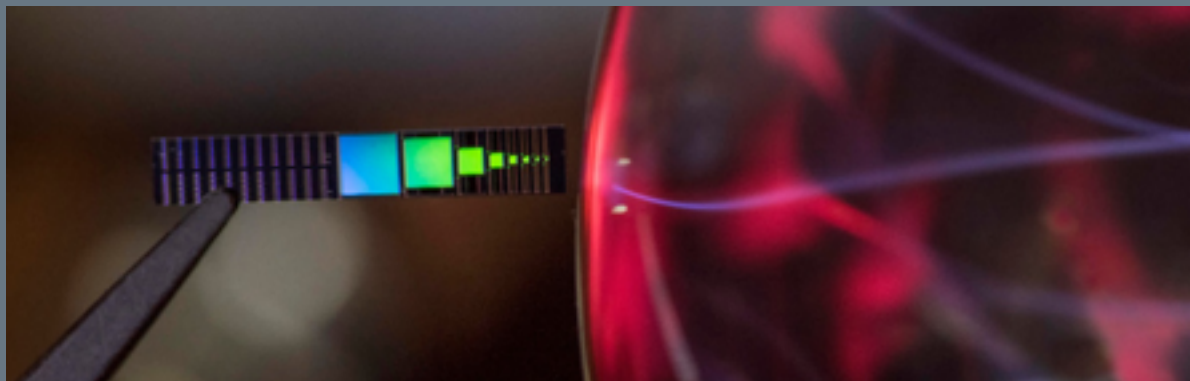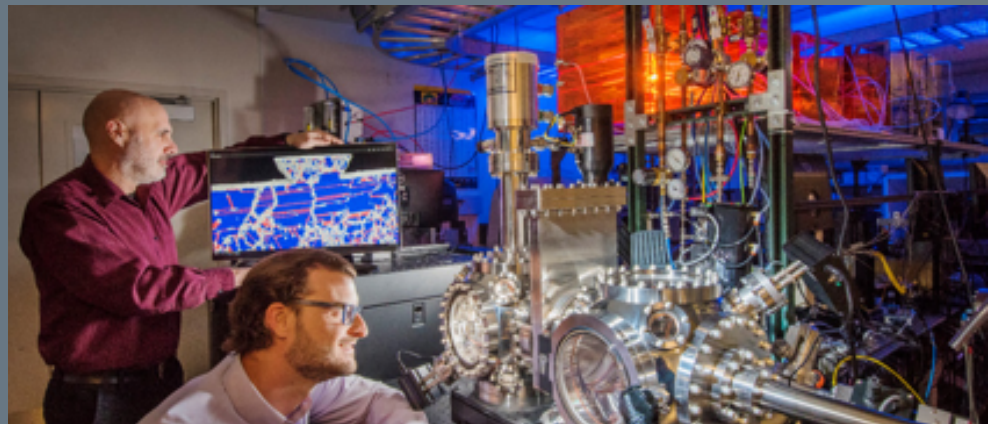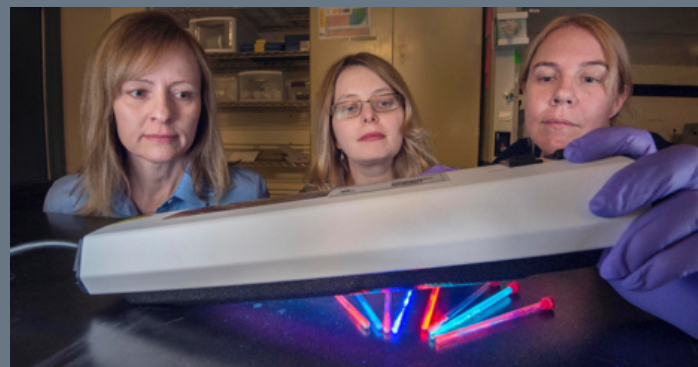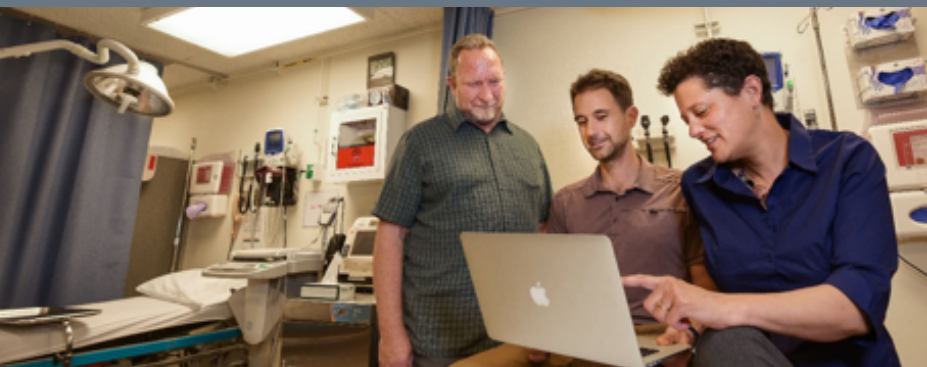
LABORATORY DIRECTED RESEARCH AND DEVELOPMENT

2018 ANNUAL REPORT

March, 2019

Laboratory Directed

Research and Development

From the Chief Research Officer

Every year, Sandia's LDRD program supports innovations that benefit national security. LDRD-funded projects develop advanced technology, engineering, and science that can contribute to the future of the US nuclear deterrent. The LDRD program also funds projects that have made enormous strides on energy security and reliability, nonproliferation, counterterrorism, and other topics essential to the security of the United States and its citizens.

The LDRD program is essential to one of Sandia's top strategic priorities: deploying outstanding engineering, science, and technology to our missions. Sandia's LDRD funding ensures that Sandia can advance the frontiers of knowledge in areas relevant to Sandia missions; supports Sandia researchers developing innovative solutions and novel tools; and helps Sandia attract, develop, and retain a world-class technical workforce. This funding also supports Sandia efforts to deploy technology to the commercial market: the 2018 R&D 100 awards again recognized four Sandia projects with LDRD roots as being among the year's most creative and important innovations to reach the commercialization stage.

Every year, Sandia considers proposals from across the labs, following NNSA and internal processes to select creative projects that align with Sandia strategy and national security requirements, demonstrate technical merit and feasibility, and lead to transformative R&D. Funded projects are rigorously managed to maximize their potential impact.

The LDRD program is the lifeblood of innovation at Sandia. It sustains our core science and engineering capabilities and unleashes the technical creativity of our staff to anticipate and address evolving national security threats.

This report overviews our LDRD program and highlights recent accomplishments of Sandia's talented R&D staff.

Susan Seestrom

Chief Research Officer
Associate Laboratories Director
Advanced Science and Technology

2018

On the Cover

Top Left: Pat Finley, left; Drew Levin, center; and University of New Mexico Professor Melanie Moses have taken inspiration from the immune system to improve how the US detects emerging outbreaks. (Photo by Randy Montoya)

Top Right: Lauren Rohwer, left; Dorina Sava Gallis, center; and Kim Butler are members of a Sandia team that has designed and synthesized metal-organic framework nanoparticles that glow red or near infrared for at least two days in cells. (Photo by Randy Montoya)

Middle Left: Forrest Gittleson, left, and Farid El Gabaly investigate the nanoscale chemistry of solid state batteries, focusing on the region where electrodes and electrolytes make contact. (Photo by Dino Vournas)

Middle Right: Michael Chandross, left, and Nic Argibay show a computer simulation used to predict the unprecedented wear resistance of their platinum-gold alloy, and an environmental tribometer used to demonstrate it. (Photo by Randy Montoya)

Bottom Left: 5x5 μm atomic force microscopy scan of Scandium Aluminum Nitride film annealed at 1800° C for 1 hour, exhibiting clear step bunching along crystallographic planes.

Bottom Right: This tiny silicon-based device developed at Sandia can catch and convert waste heat into electrical power. The rectenna, short for rectifying antenna, is made of common aluminum, silicon, and silicon dioxide using standard processes from the integrated circuit industry. (Photo by Randy Montoya)

Sandia's Laboratory Directed Research and Development Program

As a federally funded research and development center (FFRDC), Sandia National Laboratories **develops advanced technologies to ensure global peace**. We apply advanced science and engineering to help our nation and allies detect, repel, defeat, or mitigate national security threats. Our national security mission has grown from responding to the threat of the Cold War to countering a range of threats—some nuclear, others involving chemical and biological weapons of mass destruction and other acts of terrorism.

A strong science, technology, and engineering foundation enables Sandia's mission through a capable research staff working at the forefront of innovation, collaborative research with universities and companies, and discretionary research projects with significant potential impact. As Sandia's sole discretionary research and development (R&D) program, Laboratory Directed Research and Development (LDRD) funds foundational, leading-edge R&D that nurtures and enhances core science and engineering capabilities. Sandia's LDRD program is an essential element of the Laboratories' purpose to provide "exceptional service in the national interest."

Enduring LDRD Program Goals

The goal of the LDRD program at Sandia National Laboratories is to enable **current and future national security missions** by:

- advancing the frontiers of knowledge in areas relevant to the Labs' missions
- developing innovative solutions and novel tools, and
- attracting, developing, and retaining a world-class technical workforce

Per Congressional intent (P.L. 101-510) and DOE guidance (DOE Order 413.2C, Chg 1), Sandia's LDRD program is crucial to maintaining the Labs' scientific and technical vitality and enhancing its ability to address current and future national security missions.

LDRD plays an essential role in maintaining Sandia's world-class R&D workforce. The program is a vehicle for the Labs' technical staff to express their most creative and innovative contributions at all stages of their careers. LDRD enables staff to develop technical expertise and build new laboratory capabilities, fostering a research environment replete with opportunities to grow professionally and to contribute beyond the constraints of direct program funding. LDRD is a magnet to attract new science, technology, and engineering talent to the Laboratories, either as postdoctoral employees or as new hires.

Sandia's research strategy arises from the Labs' strategy: LDRD investments are managed through a strategic and balanced portfolio that is structured around several major types of research, which are further broken down into Investment Areas (IAs). Each IA is focused on discipline- or mission-based research priorities set by Sandia's leadership. The LDRD program structure and the allocation of funds to the associated IAs are designed to align LDRD investments with Sandia strategy and future national security mission needs.

LDRD Investment Area Roles

Research Foundations: Sandia maintains a set of discipline-based Research Foundations that represent the Labs' core science and technology competencies. Research Foundations seek to anticipate and provide for the future ST&E needs of the Laboratories, foster its science base, and maintain and build technical excellence in key areas needed to address the broad set of national security challenges across the Labs' mission space. The seven Research Foundations (**see Figure 1**) focus on stewarding differentiating or unique capabilities in these areas.

Our key technical capabilities have proven their uniqueness and value time and time again, through decades of delivering to DOE/NNSA—our primary sponsor—as well as the Department of Defense, the Department of Homeland Security, and other federal agencies. The LDRD program is a critical investment in the Laboratories' foundation.

LDRD Research Foundations conduct fundamental/discovery research in disciplines germane to and inspired by national security mission needs to advance the frontiers of knowledge, explore innovative solutions, and build/maintain technical capability.
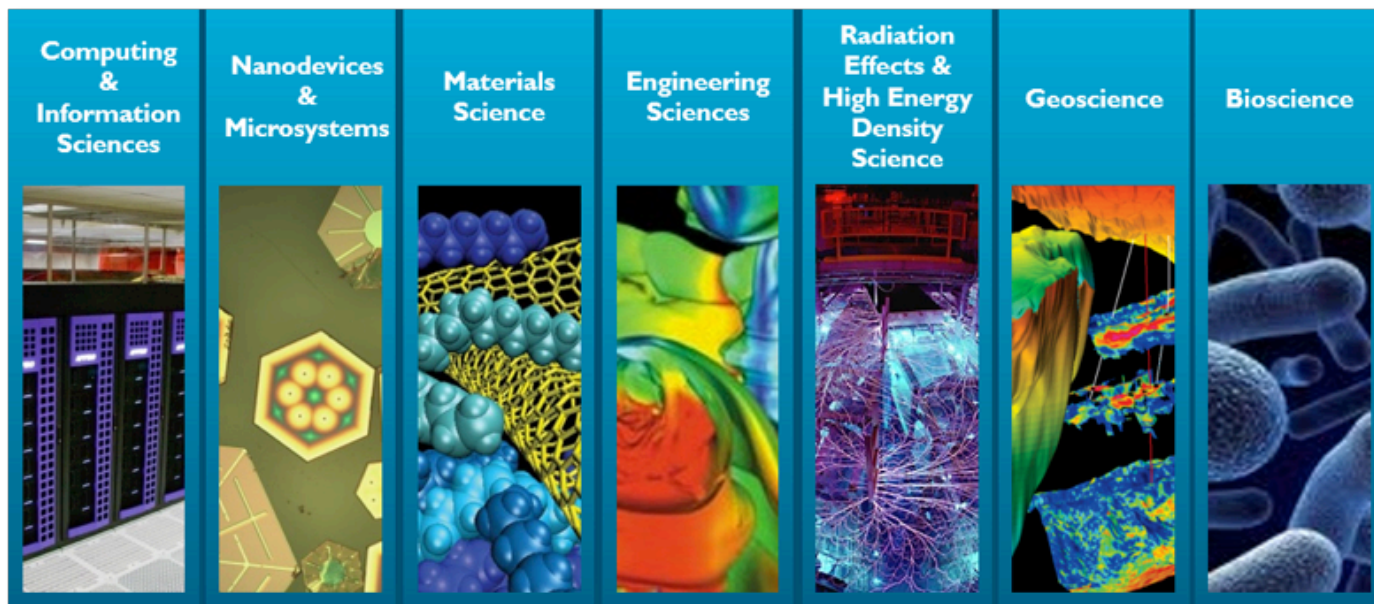
Figure 1. Research Foundations steward disciplines, considered core to the technical base, that enable mission success.

Mission Foundations: Sandia executes its broad national security missions through five major mission portfolios (Program Portfolios: see **Figure 2**). The LDRD program is key to developing capabilities to address our national security mission challenges. LDRD Mission Foundations, aligned to the Program Portfolios, conduct applied research in areas directly relevant to current/anticipated missions to develop and demonstrate new capabilities and prototype new solutions.

Strategic Initiatives address major research challenges requiring large multidisciplinary teams to develop bold solutions to important national security challenges (Grand Challenges projects) or agile, strategic processes to bridge ST&E and mission and move intentionally from idea to impact (Mission Campaign Investment Areas).

Corporate Investments encourage and support strategic academic collaborations (118 LDRD-supported university collaborations in FY2018), the Truman and Jill Hruby Postdoctoral Fellowships, and Exploratory Express, an agile mechanism to rapidly answer key research questions related to novel R&D ideas.
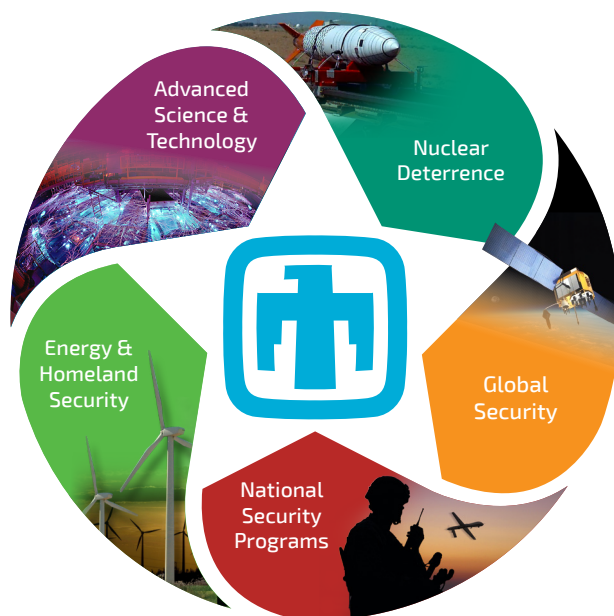

Figure 2. Sandia's LDRD Mission Foundations provide innovative solutions aligned with Sandia's five Program Portfolios.

Enabling Mission Success

Sandia's LDRD program invests in research to enable mission success. As a multidisciplinary laboratory, Sandia brings researchers from all areas of science and engineering. By working together on LDRD projects, researchers develop leading-edge solutions to both current and future challenges. From building foundational science capabilities to applied research to technology development, each LDRD project addresses one or more of the following: DOE/NNSA's missions, as well as the national security missions of the Department of Homeland Security, the Department of Defense, and Other Federal Agencies.
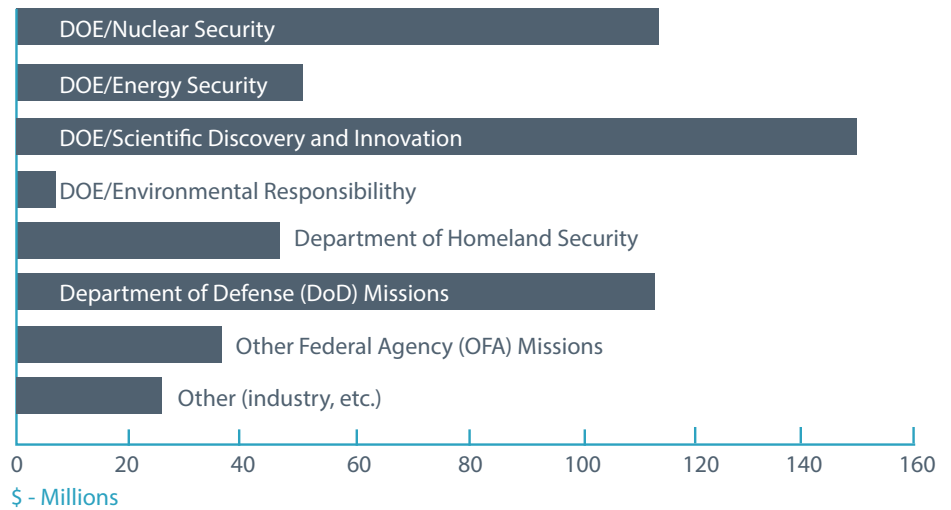

$ - Millions

Figure 3. Each LDRD project addresses one or more of these national security missions. Total FY2018 LDRD R&D costs were $160,249,672.

Project Selection and Oversight

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. Each proposal undergoes a rigorous review process, including peer review by subject-matter experts. The Sandia LDRD program is highly competitive. In the main FY2018 selection process, 749 short idea proposals were submitted; the Investment Area selection committees invited 176 of those to submit full proposals. Of those proposals, 91 new projects were funded. When added to ongoing projects, and to 78 projects started during the year (e.g., those from the Exploratory Express Investment Area), 371 projects were active in FY2018.

FY 2018 LDRD Program Statistics

$162.7M	$341K	371	169
Total Program Cost	**Median Project Size**	**Total LDRD Projects**	**New Projects in 2018**

LDRD Participants
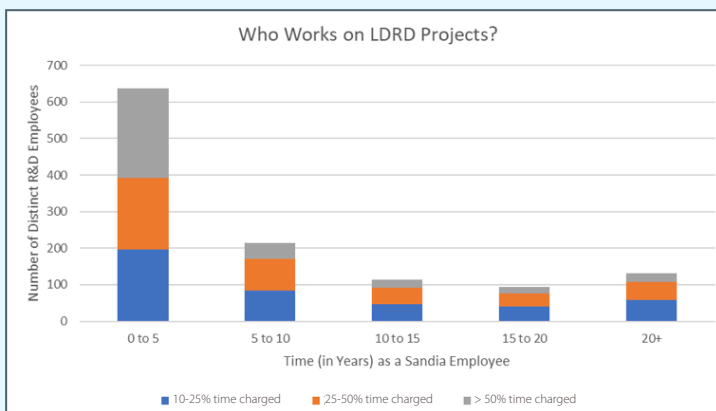
LDRD-Supported Postdocs	**133**	44% of Sandia total
LDRD-Supported Postdoc to Staff Conversions	**25**	47% of Sandia total
Refereed Publications	**293**	23% of Sandia total
Technical Advances	**112**	44% of Sandia total
Patents Issued	**75**	54% of Sandia total
Software Copyrights	**18**	15% of Sandia total
R&D 100 Awards	**4**	80% of Sandia total

ADVANCING THE FRONTIERS OF SCIENCE, ENGINEERING AND KNOWLEDGE IN AREAS RELEVANT TO SANDIA'S NATIONAL SECURITY MISSION

Sandia is a 21st century, broad spectrum national security laboratory. 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. Sandia researchers work across a broad spectrum of disciplines, collaborating to advance the frontiers of science and engineering in areas that are critical to Sandia's national security mission areas.

Most wear-resistant metal alloy in the world engineered at Sandia. Sandia's materials science team has engineered a platinum-gold alloy believed to be the most wear-resistant metal in the world. It is 100 times more durable than high-strength steel, making it the first alloy, or combination of metals, in the same class as diamond and sapphire, nature's most wear-resistant materials. Sandia's team recently reported their findings in *Advanced Materials*. "We showed there's a fundamental change you can make to a material alloy that will impart this tremendous increase in performance over a broad range of real, practical metals," said materials scientist Nic Argibay, an author on the paper. In the short term, the alloy could be added to blade-pitch motors and communication slip rings used in wind turbines, which would not need to be opened and fixed repeatedly. Reduced maintenance costs, along with the longer life of parts, could offset the high cost of the metals. The platinum-gold alloy is in the process of being patented. The research is being used as a springboard to find other wear-resistant alloys cheaper than platinum-gold. The researchers also want to test the effectiveness of platinum-gold coatings down to a few hundred nanometers.
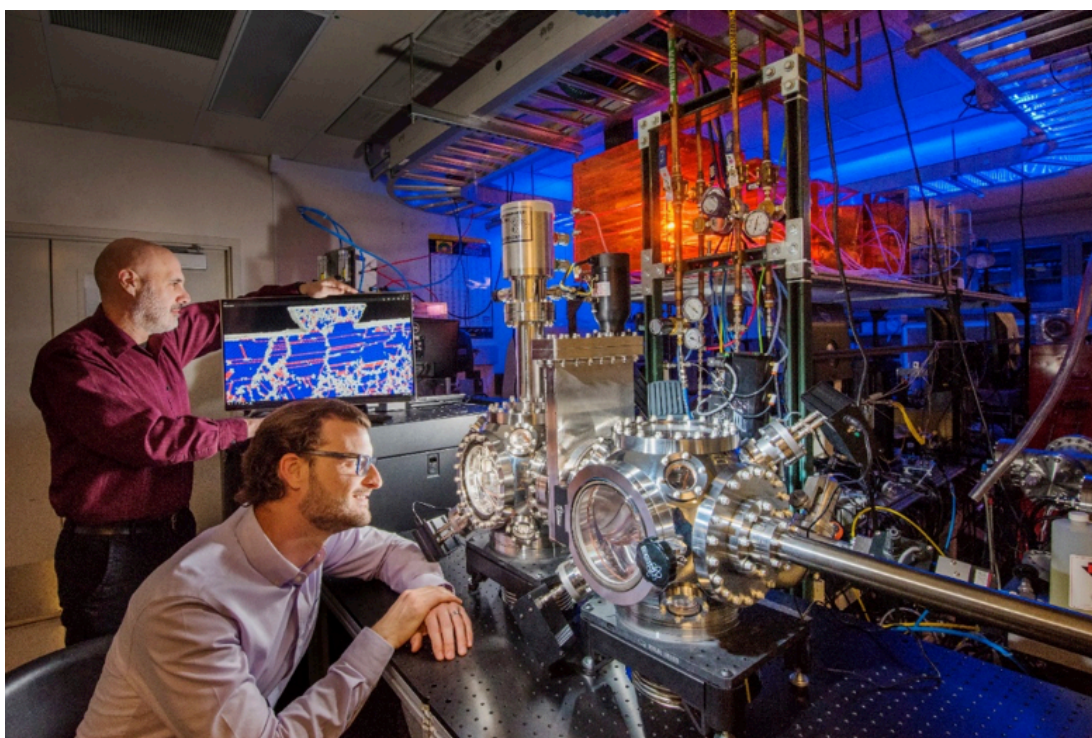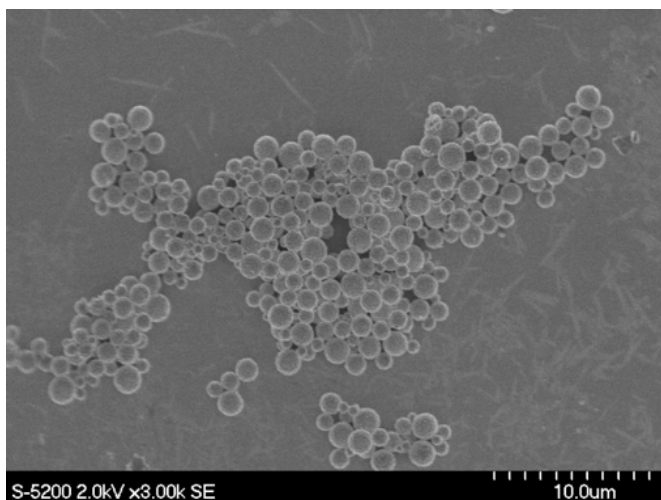

Sandia National Laboratories researchers Michael Chandross, left, and Nic Argibay show a computer simulation used to predict the unprecedented wear resistance of their platinum-gold alloy, and an environmental tribometer used to demonstrate it. (Photo by Randy Montoya)

Nanotechnology experts at Sandia create first terahertz-speed polarization optical switch. A Sandia National Laboratories-led team has, for the first time, used optics rather than electronics to switch a nanometer-thick thin film device from completely dark to completely transparent, or light, at a speed of trillionths of a second. Ultrafast information processing "matters in computing, telecommunications, signal processing, image processing and in chemistry and biology experiments where you want very fast switching," Igal Brener said. "There are some laser-based imaging techniques that will benefit from having fast switching, too." Done in collaboration with North Carolina State University, the work was funded by Sandia's LDRD program and published in *Nature Photonics*.
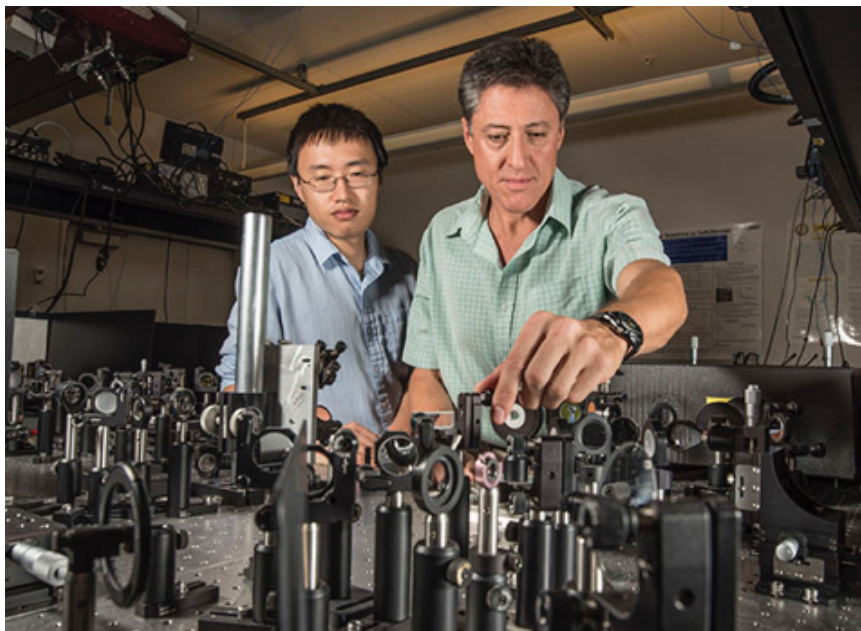
USING OPTICS—Former Sandia researcher Yuanmu Yang, left, and Sandia's Igal Brener set up to do testing in an optical lab. The pair were part of a team that, for the first time, used optics rather than electronics to switch a nanometer-thick thin film device from completely dark to completely transparent in trillionths of a second. (Photo by Randy Montoya)

A splash of detergent makes catalytic compounds more powerful. Sandia researcher Hongyou Fan has produced a uniform powder that outperforms commercial varieties used as catalysts in solar cells and could be used to produce clean-burning hydrogen fuel. Fan is working on optimizing materials for potential applications like energy conversion in solar cells, phototherapy for cancer treatment, and hydrogen production for clean fuel sources by creating well-known particles in brand new shapes. LDRD researcher David Rosenberg is scaling up the technology for application to his explosives work for national security, where unpredictable materials are unacceptable. The technology is the subject of a recent paper in *Nano Letters*.

Under high-power microscopy, a powder made with detergent-based technology at Sandia National Laboratories consists of perfect spheres. Without it, the material would look like coarse gravel. Consistency makes catalytic materials considerably more effective. (Photo courtesy of Hongyou Fan)

The LDRD Grand Challenge NanoCRISPR project has discovered new functionality. CRISPR-Cas9 is a breakthrough technology used as a genome-editing tool to target and modify specific DNA sequences in different organisms. In addition to DNA, researchers discovered that certain Cas9 enzymes also target RNA, the "genetic middleman" between DNA and proteins. This new capability for Cas9 enzymes opens the door for the development of novel RNA targeting therapies, viral countermeasures, cell and nucleic acid diagnostics, and gene regulation tools. This patent-pending research was performed in collaboration with Prof. Jennifer Doudna (UC Berkeley), co-inventor of CRISPR-Cas9 technology. It was published in *eLife* (2018, DOI 10.7554/eLife.32724).

CRISPR-associated protein Cas9 can target and cut DNA, but its ability to efficiently target RNA was unclear. The discovery of RNA targeting by a subset of Cas9 enzymes lays the foundation for programmable RNA targeting applications.
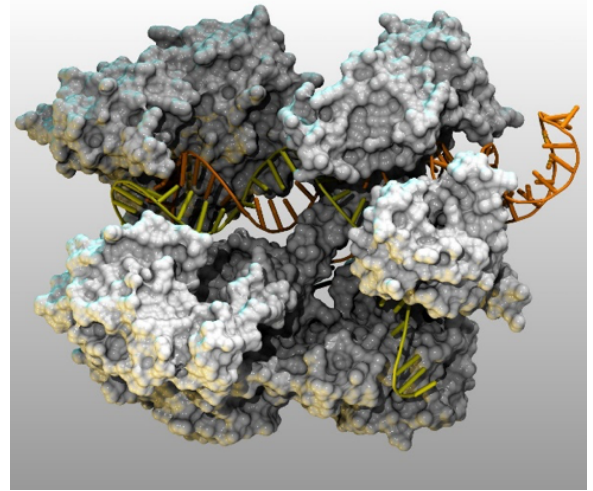
DEVELOPING INNOVATIVE SOLUTIONS AND NOVEL TOOLS TO ENABLE CURRENT AND FUTURE MISSION NEEDS

LDRD projects create and enhance capabilities and products that support national security missions through innovative science, technology, and engineering. LDRD has been, and will continue to be, a key contributor to the development of science and engineering capabilities used to secure our nation now and into the future. The Labs and its strategic partners gain from collaborative research results, and many technological breakthroughs originating from, or improved through the LDRD program, are transferred to industry, commercialized under licensing agreements, and brought to market for the US public good.

SHIELD Technology Transferred to Raytheon. Sandia transferred its SHIELD Physical Unclonable Function (PUF) technology platform to Raytheon Space and Airborne Systems in El Segundo, California for testing and evaluation. The SHIELD PUF platform provides microprocessors with an inherently unique and random cryptographic key that is used in an on-board Advance Encryption Standard (AES) encryption engine to provide secure identification and communication to authorized queries. PUFs are based on physical variations that occur naturally during semiconductor manufacturing that make it possible to differentiate between otherwise identical semiconductors. Sandia researchers developed and integrated both the PUF and a passive temperature sensor into the SHIELD dielet, representing two of the five core technologies for SHIELD. The Sandia PUF used in the SHIELD dielet is an outgrowth of a 2014 LDRD Reliable PUFs for Supply Chain Assurance. PUF technology will benefit integrated circuits susceptible to cryptographic attacks, as well as nuclear deterrence and national security program technologies exposed to supply chain risks for microelectronics.
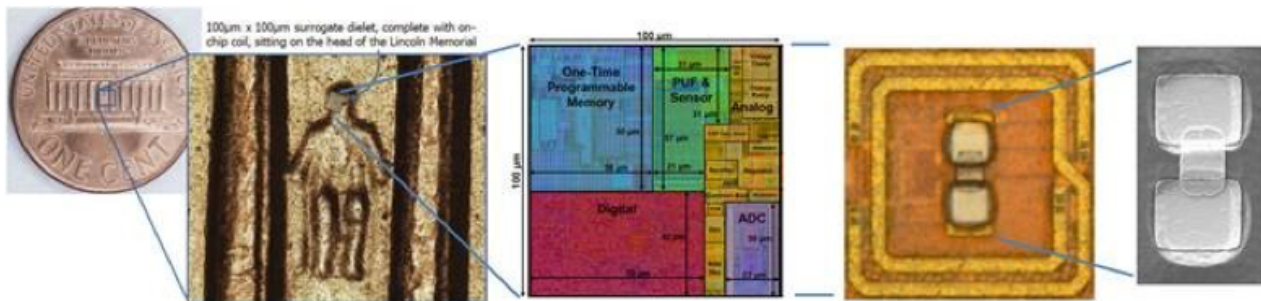
SHIELD dielet is smaller than Lincoln's head on the back of a penny, consists of Sandia National Laboratories developed physical unclonable function and passive thermal sensor.

Sandia's robotic work cell conducts high-throughput testing 'in an instant'. Sandia National Laboratories has designed and built a six-sided work cell, similar to a circular desk, with a commercial robot at its center that conducts high-throughput testing to quickly determine the performance and properties of the part. This flexible, modular and scalable system is called Alinstante, Spanish for "in an instant." The goal of Alinstante is to speed up the testing of 3D-printed parts and materials science research. Industry partners are being sought to help expand or discover more uses for the new robotic testing system. The technology to speed up qualification and testing was the result of Sandia materials scientist Brad Boyce's work in the spring of 2015. He was working on Sandia's Born Qualified Grand Challenge, an LDRD-funded project to improve the qualification of custom 3D-printed parts.
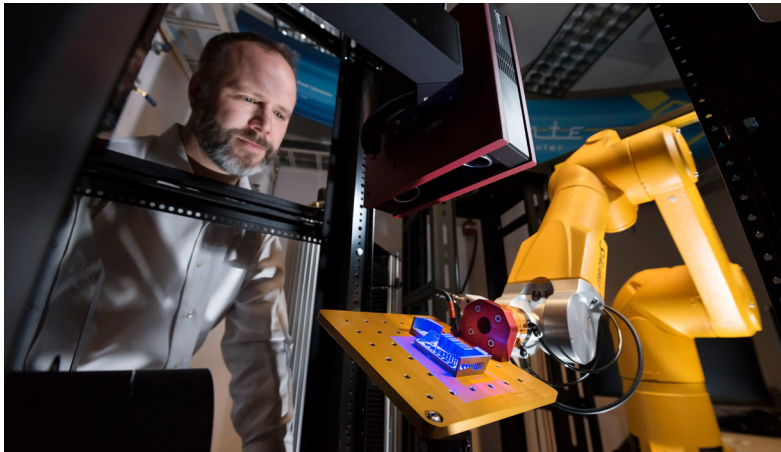
Sandia National Laboratories materials scientist Brad Boyce watches as the Alinstante robotic work cell scans a 3D-printed part to compare what was made to the original design. This test part was devised to push the limits of 3D printing technology. The goal of Alinstante is to speed up the testing of 3D-printed parts and materials science research. (Photo by Randy Montoya)

Stopping anthrax in its tracks using charged liquid droplets to attract and pull spores out of the air. Sandia researchers have tested a new spray knockdown system partly developed with LDRD funds and refined by Sandia technologist Charles Brusseau. Using a very fine mist of charged liquid droplets (dilute decontamination foam or even plain water) they can attract and pull anthrax spores out of the air. This system could prevent people from breathing in anthrax and might even help stop its spread at a standalone facility such as an airbase.


Sandia engineer Mark Tucker holds a sample of decontamination foam modified to stick to the walls and ceilings of subway tunnels. Mark has spent much of the past twenty years thinking about ways to clean up chemical or biological warfare agents. (Photo by Randy Montoya)

New fractal-like concentrating solar power receivers are better at absorbing sunlight. Sandia engineers have developed new fractal-like, concentrating solar power receivers for small- to medium-scale use that are up to 20 percent more effective at absorbing sunlight than current technology. The receivers were designed and studied as part of a LDRD project and are being applied to Sandia's work for the Solar Energy Research Institute for India and the United States (SERIIUS). Sandia engineer Cliff Ho says, "The goal of concentrating solar power and SERIIUS is to develop efficient, cost-effective solar-driven electricity production with energy storage. The use of a solarized supercritical carbon-dioxide Brayton cycle would increase efficiencies, reduce space requirements, and reduce costs associated with current large-scale concentrating solar power systems."

NEW SOLAR RECEIVERS. Year-round Sandia intern Jesus Ortega inspects one of the new bladed receivers at the National Solar Thermal Testing Facility. (Photo by Randy Montoya)
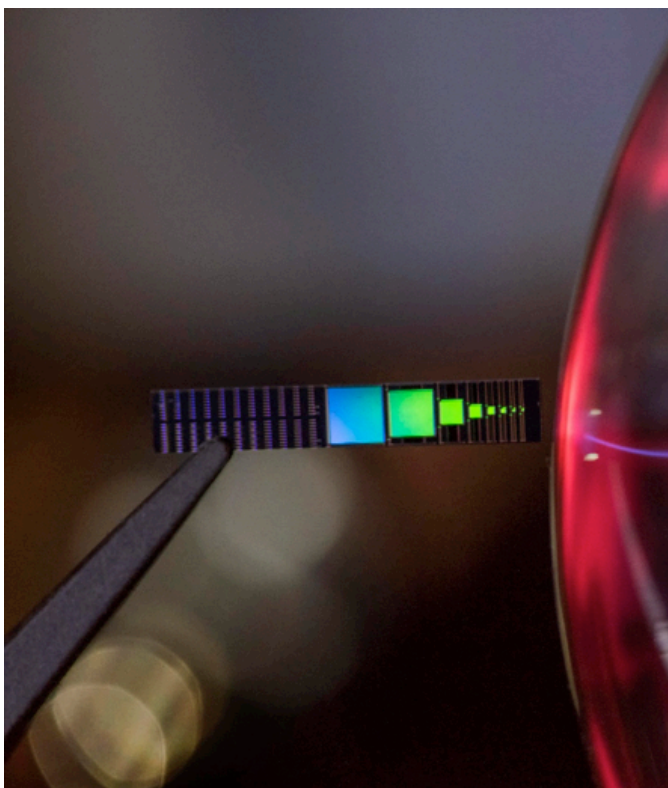
New Sandia solid-state silicon device may one day power space missions. Sandia researchers have developed a tiny silicon-based device that can harness what previously was called waste heat and turn it into DC power. Their advance, called an infrared rectenna, was published recently in *Physical Review Applied*. The research was funded by Sandia's LDRD program.

This tiny silicon-based device developed at Sandia can catch and convert waste heat into electrical power. The rectenna, short for rectifying antenna, is made of common aluminum, silicon and silicon dioxide using standard processes from the integrated circuit industry. (Photo by Randy Montoya)

Smarter, safer bridges with Sandia sensors. Sandia worked with Structural Monitoring Systems PLC, a UK-based manufacturer of structural health monitoring sensors, to outfit a US bridge with a network of eight real-time sensors able to alert maintenance engineers when they detect a crack or when a crack reaches a length that requires repair. Sandia Senior Scientist Dennis Roach presented his team's work at the ninth International Conference on Bridge Maintenance, Safety and Management. The team's work on smart infrastructure began in 2005 through a Sandia-sponsored LDRD project. The project explored using mounted sensors and wireless data transfer to continuously monitor a wide array of civil structures ranging from heavy mining equipment to railway systems and bridges. These sensors can monitor the health of structures and mechanical devices by detecting the presence of corrosion and cracks and even the condition of critical moving parts.

Sandia mechanical engineer Stephen Neidigk positions a Comparative Vacuum Monitoring sensor on a bridge. In his other hand is the control system that periodically checks the sensor and a wireless transmitting device to autonomously alert the maintenance engineers if it detects a crack. (Photo by Randy Montoya)

Biologically inspired membrane purges coal-fired smoke of greenhouse gases. Sandia and University of New Mexico researchers have jointly developed an inexpensive memzyme capable of ridding coal smoke of carbon dioxide, the most prevalent greenhouse gas. The patented work, reported recently in Nature Communications, has interested power and energy companies that significantly and inexpensively want to reduce emissions of carbon dioxide. Initial work was supported by Sandia's LDRD program.

Enzymatic liquid-membrane design and mechanism of CO_2 capture and separation. The Sandia/UNM membrane is fabricated by formation of approximately 1-micron-deep arrays of 8-nanometer diameter cylindrical silica mesopores. Using atomic layer deposition and oxygen plasma processing, the silica mesopores are engineered to be hydrophobic except for an 18-nm-deep region at the pore surface which is hydrophilic. Through capillary condensation, carbonic anhydrase enzymes and water spontaneously fill the hydrophilic mesopores to form an array of nanostabilized enzymes with an effective concentration greater than 10 times of that achievable in solution. These catalyze the capture and dissolution of carbon dioxide at the upstream surface and regeneration of carbon dioxide at the downstream surface. The high enzyme concentration and short diffusion path maximizes capture efficiency and flux.
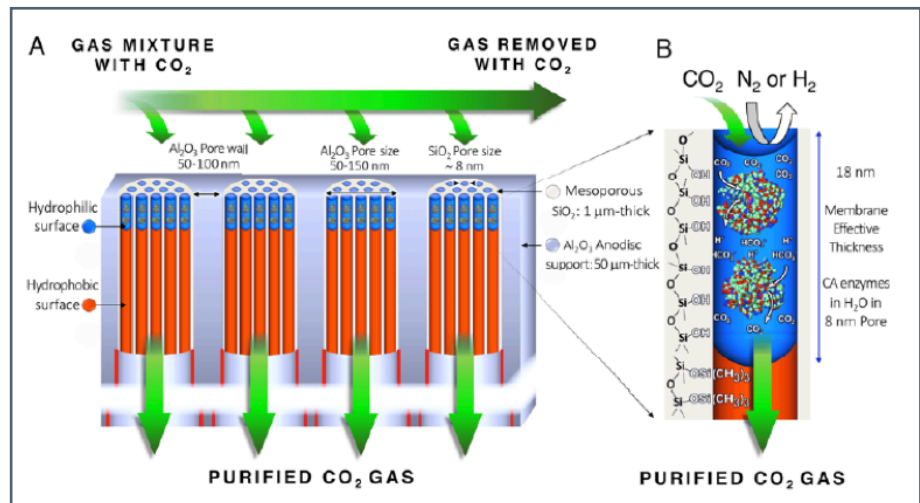
ATTRACTING, DEVELOPING AND RETAINING A WORLD-CLASS TECHNICAL WORKFORCE TO CREATE MISSION IMPACT

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 program support was important to many Sandia researchers who were recognized for their achievements this year. Additional awards for LDRD projects and researchers are listed in the Awards Section of this report.

DOE Early Career Research Program

Eric Cyr wins DOE Early Career Research Program award for 2018. The national award from the DOE's Office of Science is meant to "identify and provide support to those researchers early in their careers who have the potential to develop new scientific ideas, promote them and convince their peers to pursue them as new directions. "My role as an LDRD PI helped me understand how to develop a successful project. Not only in writing an innovative proposal, but how to set ambitious yet achievable goals and deliverables that externally convey the excitement of the project. Moreover, the technical knowledge that I developed and gained in my LDRDs was a direct antecedent of the technical work proposed by my DOE Early Career project," Eric said.

Sandia computational researcher Eric Cyr
(Photo by Randy Montoya)

Jill Hruby Fellowship

Mercedes Taylor and Chen Wang are Sandia's first Jill Hruby Fellows. The honorees have each been awarded a three-year postdoctoral fellowship in technical leadership, comprising national security-relevant research with an executive mentor. Susan Seestrom, chief research officer and associate laboratories director for Advanced Science and Technology, will mentor both Mercedes and Chen. The Jill Hruby Fellowship is meant to encourage women to consider leadership in national security as scientists and engineers. Jill Hruby served as Sandia's director from 2015 to 2017 and was the first woman to lead a national security laboratory.

Over the next three years, Mercedes' research will aim to develop new porous plastics that purify water by soaking up ions—electrically charged atoms and molecules—with an emphasis on negatively charged ions, called anions. Materials that can target an ion selectively, even in the presence of many other ions, could be especially useful to national security, by identifying chemical warfare agents, radioactive material or harmful natural impurities (e.g., in a water sample). Current technologies to remove various ions from water on an industrial scale leave much to be desired, so the work could also find practical use in desalination plants. As climate change and population growth are projected to make drinking water scarcer globally over the coming decades, Taylor hopes her work will provide relief and security. Mercedes earned a doctorate in chemistry from the University of California, Berkeley.

As a Jill Hruby Fellow, Mercedes Taylor will develop new water-purifying materials that capture potentially hazardous ions at Sandia. (Photo by Phil Bunting)

Cheng Wang says the Hruby Fellowship will help her continue to encourage public interest in science and environmental issues while promoting the public image of female scientists. As a graduate student and through the Association of Women in Science, she organized science activities for kids and families in downtown Riverside, California. She later expanded to large-scale workshops held at a Discovery Cube children's science museum in Santa Ana, California. "I saw it as an opportunity to do something more, to build the foundation of what the Hruby Fellowship will become in coming years." Chen earned a doctorate in materials science from the University of California, Irvine.

As a Jill Hruby Fellow, Chen Wang will analyze soot precursor molecules with microscopy, and design computational models for cleaner-burning combustion engines at Sandia. (Photo courtesy of Chen Wang)

Truman Fellowship

Sandia established the President Harry S. Truman Fellowship in National Security Science and Engineering to attract the best nationally recognized new PhD scientists and engineers. This three-year fellowship is named for President Truman who charged Sandia in 1949 with providing "an exceptional service in the national interest"—a motto that leads Sandia to excel to this day. Truman Fellows conduct independent ground-breaking research that supports Sandia's national-security mission. Fellows choose their own research topics and benefit by having access to Sandia's state-of-the-art facilities and collaborating with some of the nation's best scientists and engineers. Fellows may work at either of Sandia's principal locations in New Mexico and California. A member of Sandia's technical staff mentors each Truman Fellow. This emphasis on research mentoring enables Fellows to become integral members of Sandia R&D teams while acquiring unique skills during their early career development.

2018 Truman Fellows

Ethan Secor received his PhD from Northwestern University in materials science and engineering in September 2017. He earned his BS from Drake University, with a double major in chemistry and physics. He has received several awards including a National Defense Science and Engineering Graduate Fellowship. His graduate work on graphene inks resulted in a commercialization opportunity, two patents and several additional patent applications, and over ten journal papers. For his Truman Fellowship, "Nanomaterial Ink Development for Smart Manufacturing," Ethan is designing a digital additive manufacturing platform for simultaneous codeposition of nanomaterial inks. This could offer opportunities for bottom-up fabrication of functionally graded materials, printing of chemically reactive or incompatible precursors, and in situ composite synthesis.

2018 Truman Fellow Ethan Secor

Daniel Ruiz received his PhD in plasma physics from Princeton University in August 2017. He also has a MS degree in nuclear reactor physics from the Institut National des Sciences et Techniques Nucléaires in France and a BA degree in physics engineering from the Instituto Tecnológico de Monterrey in Mexico. During his PhD studies, Daniel's research was mainly focused on developing a new systematic approach based on variational principles to describe wave dynamics. Daniel's Truman Fellowship research will focus on developing a new theoretical model to better understand the basic physics of laser-plasma instabilities (LPI) processes relevant to the magnetized liner inertial fusion (MagLIF) experiment at Sandia.

2018 Truman Fellow Daniel Ruiz

Yiyang Li received his BS in Electrical and Computer Engineering from Olin College and his MS and PhD in Materials Science and Engineering from Stanford University. His thesis work, which used in situ characterization to understand ion insertion mechanisms in Li-ion batteries at the nanoscale, has been published in journals including Science and Nature Materials. Yiyang's Truman Fellowship extends electrochemical ion insertion beyond energy conversion and storage by developing a new class of materials whose properties can be dynamically changed through electrochemistry.

2018 Truman Fellow Yiyang Li
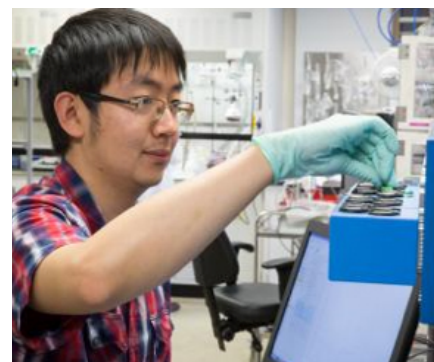
PROFESSIONAL RECOGNITION AWARDS
American Academy of Arts and Sciences Fellow

Sandia researcher Jeff Brinker elected fellow of American Academy of Arts and Sciences. Jeff Brinker, Sandia National Laboratories Fellow and University of New Mexico Regents' Professor, has been elected fellow of the oldest learned society and independent policy research center in the United States: the American Academy of Arts and Sciences. "My election into the academy would not have been possible without continued support from Sandia's Laboratory Directed Research and Development program, the Department of Energy's Office of Basic Energy Sciences, the Air Force Office of Scientific Research, the National Cancer Institute, the Defense Threat Reduction Agency, the National Science Foundation and the University of New Mexico."

Sandia researcher and American Academy of Arts and Sciences Fellow Jeff Brinker. (Photo by Randy Montoya)

American Physical Society Fellow

Sandia physicist Thomas Mattsson elected fellow of the American Physical Society. Mattsson was cited by the society "for contributions to the fundamental understanding of condensed matter at extreme temperatures and pressures through molecular dynamics and electronic structure simulations." In addition to contributing to LDRD work, Mattsson has led a fundamental science program at Sandia's Z machine—the most powerful generator of x-rays on Earth—since 2011.

Sandia researcher and American Physical Society Fellow Thomas Mattsson.

Sandia LDRD researcher Alex Talin elected fellow of the American Physical Society. Talin, from Sandia's California site, was honored "for the discovery of new electronic transport phenomena, materials and devices."

"The LDRD program has helped my career tremendously. In particular, it gave me the opportunity to answer fundamental question regarding mechanisms of charge transport in nanostructures and guest induced emergent phenomena in nanoporous materials. This work was responsible in large part for me getting the APS fellowship."

American Physical Society Fellow Alec Talin.

Asian American Engineer of the Year

Sandia measurements expert Hy Tran named a 2018 Asian American Engineer of the Year. The Chinese Institute of Engineers-USA awards Asian-American professionals in science, technology, engineering, and math who demonstrate exceptional leadership, technical achievements, and public service. Tran, whose family came to the United States from Vietnam during the Vietnam War said, "the values of education, hard work, and service" played a role in his desire to be an engineer. Hy oversees the LDRD Exploratory Express and New Ideas Investment Areas.

Sandia Senior Scientist and 2018 Asian American Engineer of the Year Hy Tran.

Sandia National Laboratories physicist Danelle Tanner.
(Photo by Randy Montoya)

National Organization of Gay and Lesbian Scientists and Technical Professionals

First Sandia employee honored as 2018 LGBTQ+ Scientist of the Year. Sandia physicist Danelle Tanner has been named the 2018 Scientist of the Year by the National Organization of Gay and Lesbian Scientists and Technical Professionals. She is the first Labs employee to receive the honor since the NOGLSTP created the award in 2004. In 1993, Tanner joined the microelectronics reliability group where she delved into reliability physics, redefining her career path. She received funding, in 1997, for a three-year LDRD project to establish MicroElectroMechanical Systems (MEMS) reliability as a differentiating strength for Sandia in this new developing technology. She spent the next decade as a leader in MEMS reliability, sharing her knowledge across the United States and Europe, before leading a team responsible for determining the root cause of a particularly challenging electrical component failure.

Society of Industrial and Applied Mathematics (SIAM)

Sandia computational scientist John Shadid elected Fellow of the Society of Industrial and Applied Mathematics (SIAM). Shadid's selection was based upon his research on solution methods for multiphysics systems, scalable parallel numerical algorithms, and numerical methods for strongly coupled nonlinear partial differential equations. He currently is investigating multi-scale methods, uncertainty quantification techniques, and preconditioning technology implementations as part of Sandia's LDRD Plasma Science and Engineering Grand Challenge.

Sandia National Laboratories computational scientist and mathematician John Shadid. (Photo by Randy Montoya)

Women of Color STEM

Sandia chemical engineer and LDRD researcher Rekha Rao received a peer-reviewed Women of Color Career Achievement Award at the annual Women of Color STEM Conference. Rao is a founding developer of Goma, multiphysics, open-source software developed for manufacturing. Goma excels at problems in capillary hydrodynamics, such as coating flows and liquid absorption by a porous material, and has extensive models as well for polymer and metal processing. The software won a 2014 R&D100 Award. Goma was funded by the LDRD program, the National Nuclear Security Administration, the National Science Foundation and others.

Sandia National Laboratories chemical engineer and LDRD researcher Rekha Rao.
(Photo by Lonnie Anderson)

PROGRAM OVERVIEW

Sandia National Laboratories Fellows

Sandia announced the appointment of six new Labs Fellows, including the first-ever female Sandia Fellow. Appointment as a Sandia Fellow recognizes a career of significant accomplishment for the Labs and for the nation. Of the six, three Fellows have made extensive contributions through Sandia's LDRD program.

Katherine Simonson has made important contributions to Sandia and the national security community in the field of statistics and data analysis. Katherine is well known and highly regarded in the Automatic Target Recognition and Space Mission communities; has received numerous Sandia awards (LDRD Award of Excellence, Employee Recognition Awards, and Classified Inventor awards); and was recently selected to serve on the US Air Force Scientific Advisory Board. Numerous statistical algorithms developed under the five LDRD projects that she has led have transitioned to operational national security systems, enabling orders-of-magnitude improvement over pre-existing technologies.

Sandia Fellow Katherine Simonson.

David Chandler is an internationally renowned gas phase physical chemist. He is a Fellow of the American Physical Society and has been elected by his peers to be chairman of the society's Division of Chemical Physics. He has been a principal investigator on six LDRD projects and has published over 120 refereed articles with more than 4,000 citations.

Sandia Fellow David Chandler adjusts equipment in his lab at Sandia's Combustion Research Facility. (Photo by Randy Wong)

Patrick Griffin has demonstrated expertise and expanded the state of the art in radiation effects, becoming an acknowledged leader in the international radiation effects community. Pat developed the NuGET code (a major tool for nuclear weapon qualification) and contributed greatly to the development of the radiation qualification process. He was the principal investigator on the Hostile Environments Grand Challenge LDRD project. Currently he is a thrust lead on the Radiation Hard Power Bus Grand Challenge LDRD project.

Sandia Fellow Patrick Griffin.

2018 R&D 100 Awards

Sandia won five R&D 100 awards this year, four of which were enabled at least in part by LDRD projects. The R&D 100 Awards are one of the most prestigious recognitions of innovation in the world. Since 1976, Sandia has earned 124 awards.

- **Detergent-Assisted Fabrication of Multifunctional Materials**. Application of ordinary detergents can produce uniform sizes and shapes of multifunctional materials at the nanoscale level, boosting their performance. Possible uses of the technique range from environmental cleanup to cancer treatment, while reducing costs. YouTube.

- **LAMMPS: Atomistic Simulation of Materials**. A widely used molecular dynamics simulation package that models materials from the atomistic to mesoscale to continuum scales. It can be run on desktop computers to the largest supercomputers to explore the structural and dynamic properties of materials and provide insights not easily accessible to experimental observation. YouTube.

- **Large Field-of-View Bench-Top 3D X-ray Phase Contrast Imaging (XPCI) System**. The system makes it possible to image low-density materials, such as the human body, polymers, epoxies, fillers, foams, plastics and other materials with as much as a thousand times more sensitivity than ordinary X-ray imaging. YouTube.

- **SWiCK Zoom**, or Sandia wide-angle quick zoom. The technology uses variable focal-length lenses or mirrors to toggle between high and low magnification almost instantly, enabling users to achieve true optical zoom with minimal power. Compact, lightweight and low-power systems are ideal where size, weight, speed or battery power come at a premium, including cameras on drones, cell-phones, and self-driving cars. YouTube.

Federal Consortium Awards

Sandia team wins Federal Laboratory Consortium award. Sandian team members Joey Carlson, Patrick Feng, and Huu Tran, and William Warburton from XIA, LLC, have won a Federal Laboratory Consortium award for "Outstanding Technology Development." The award recognizes the team's work to develop a radiation detector incorporating organic glass scintillators under DOE SBIR funding. The immediate use of the radiation detector will be used in cyclotron experiments. The organic glass scintillators were originally developed using NA-22 funding. Concepts crucial for the execution of the NA-22 work came from an Early Career LDRD project awarded to Patrick Feng at the beginning of his Sandia career. Thus, both the NA-22 and LDRD programs were key to the discovery and development of this new family of materials.

RESEARCH EXCELLENCE IN SERVICE TO THE NATION

LDRD supports Sandia's mission by investing in transformative research that advances the frontiers of science and engineering critical to national security. The program is 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

BIOSCIENCE

The Bioscience Investment Area pursues basic and applied research to develop solutions to national biosecurity challenges in two areas—defense against biological agents and emerging infectious diseases and biological production of fuels and chemicals. Biodefense research is directed toward improved approaches to detect, characterize, contain, and counter the effects of natural, intentional, or accidental biological events. An understanding of, and responses to, genomic threats are critical aspects of this effort. Research into the biological production of fuels and chemicals aims to achieve breakthroughs in the economic conversion of sustainable biomass into renewable fuels, chemicals, and materials, reducing the nation's reliance on fossil resources to produce these essential commodities. This research investigates two important sources of biomass: lignocellulose, or dry plant matter, and algae. Synthetic biology and microbiome-enabled approaches are key to this effort.

Exploiting the Microbial Achilles Heel for New Broad Spectrum Anti-Microbials
Project 190961, PI: Susan Rempe

Sandia developed a fundamental understanding of novel antibiotic function. Bacteria have developed resistance to every antibiotic currently available, triggering an urgent search for drugs with novel mechanisms that could alleviate the global crisis of bacterial resistance. Our studies on teixobactin (Txb), a recently discovered antimicrobial compound produced by a Gram-negative bacterium to combat Gram-positive bacteria, have produced new insights into the function of this molecule. By creating the first Txb molecular model and running molecular dynamics simulations in realistic bacterial membrane environments, we have identified how Txb binds to the membrane and inhibits cell wall biosynthesis[1]. We also have developed simpler and more efficient chemical synthesis approaches to produce Txb and variants that enable us to experimentally test the predictions of our modeling and simulations and to explore improved antimicrobial function of Txb variants. This should facilitate future development of novel compounds with broader, more potent, and resistance-delayed antimicrobial activity.

This graphic illustrates how teixobactin, a recently discovered antibiotic, binds to a lipid component in the bacterial membrane and inhibits cell wall biosynthesis
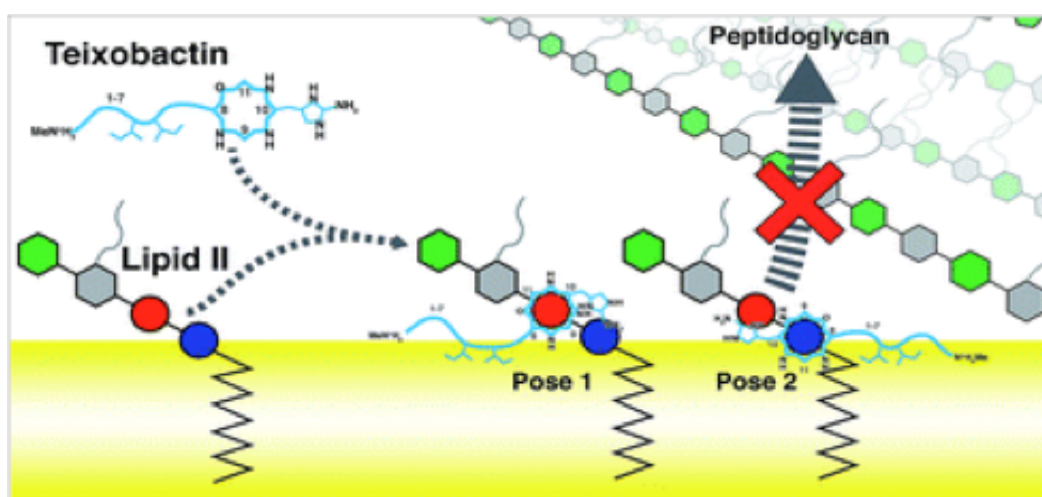
[1] Wen, *et al.*, "Probing key elements of teixobactin-lipid II interactions in membranes," **Chem. Sci.**, 2018, 9, 6997-7008.

PROJECTS

BIOSCIENCE

Analyzing and Understanding of Transporters to Control Lignin Transformation into Fuel

190958 | Year 3 of 3

Principal Investigator: J. A. Timlin

This project created analytical tools and biological methods to study and engineer the transport of specific lignin breakdown products into bacterial and fungal cells. The results provided the first-ever direct evidence of transport of a lignin dimer extracellularly and demonstrated enhanced transport of several lignin breakdown products into *E. coli*. The knowledge gained from this work has provided critical information that can be combined with lignin decomposition and biological conversion strategies to improve lignin upgrading into more valuable products for energy security.

Big Data, Machine Learning, and Dynamic Complex System Modeling to Improve Algae Cultivation

199975 | Year 2 of 3

Principal Investigator: R. W. Davis

This project will develop new fundamental understanding, experimental validation, and modeling capabilities to identify low-cost mechanisms for minimizing algae biomass productivity losses based on finite horizon environmental data. Understanding the fundamental interactions of fluid dynamics, microbial communities, and basic raceway management practices in variable environmental regimes will help to maximize algae biomass productivity to impact our nation's biomass resource potential.

Diagnostic Tool for Measuring Early Chemical Signatures of Pond Crash

199974 | Year 2 of 3

Principal Investigator: M. W. Moorman

Predators can significantly reduce the biomass yields of algal biofuel ponds if left untreated. Our research seeks to demonstrate that predation in algal ponds produces detectable chemical signatures. These gas phase chemical biomarkers are identifiable using Sandia's sensor technology and will be used as a diagnostic to reveal the health of the algal community. This will provide a powerful tool for biofuel producers to monitor the health of their ponds and increase yield and lower costs.

Diversified Therapeutic Phage Cocktails from Close Relatives of the Target Bacterium

209191 | Year 1 of 3

Principal Investigator: K. P. Williams

The rise of antibiotic-resistant bacteria is a national security problem that requires new countermeasures. We are isolating diverse bacteriophages for incorporation into cocktails to kill pathogenic bacteria. We mine a uniquely large Sandia database of mobile DNA sequences in bacterial genomes, isolate phages integrated into these genomes, and engineer the phages so that they can no longer integrate. Selecting phages from close relatives of the target bacterium ensures efficacy. This work will provide proof of principle on quick development of countermeasures that specifically target any bacteria emerging as national security biothreats.

Engineering Cells for Personalized Antimicrobial Therapy

209190 | Year 1 of 3

Principal Investigator: R. Krishnakumar

This project's goal is to develop a rapid and efficient method for converting readily available cells into therapeutic cells using gene editing tools, high-throughput screening, and data-driven optimization. If successful, this method could significantly impact our nation's ability to defend against antibiotic resistant or unknown pathogen threats, as a stand-alone treatment, a helper for existing therapies, and a prophylactic tool.

Engineering 'Green' Algae: Reducing Metabolic Waste for High Biomass Productivity

190962 | Year 3 of 3

Principal Investigator: A. Ruffing

The economic production of algal biofuels is limited by low natural biomass productivities. To improve biomass productivity in an industrially relevant alga, we developed genetic tools and engineered mutants that have reduced metabolic waste (i.e., carbon loss). Specifically, we targeted dark respiration, which accounts for carbon losses in the range of 20-60% on a daily basis.

Examination of Dual Use Concerns of Gene Editing

204977 | Year 2 of 3

Principal Investigator: J. A. Timlin

This project will develop biochemical, bioinformatic, and analytical tools, including assays and protocols to quantify the efficiency and accuracy of genome editing. This work addresses the growing need for robust diagnostics and therapeutics to support gene editing activities that are rapidly developing for translational medicine and to mitigate safety and dual use concerns raised by this technology.

Exploiting the Microbial Achilles Heel for New Broad Spectrum Anti-Microbials (NBSAMs)

190961 | Year 3 of 3

Principal Investigator: S. Rempe

Bacteria resist traditional antimicrobial drugs, which costs Americans their lives and the US $45B to fight these drug-resistant infections every year. Recent discovery of the first new class of antimicrobials in thirty years, Teixobactin, provides a potential game-changing opportunity for biodefense and public health. We developed the capability to synthesize and model Teixobactin variants and we discovered how Teixobactin binds with its rare lipid targets in the bacterial membrane. Those insights lay the foundation for development of more potent, broad-spectrum antimicrobials.

Modular Abiotic/Biotic Systems (MABS) for Understanding and Directing Biological Function

190960 | Year 3 of 3

Principal Investigator: C. J. Brinker

This project developed three new classes of modular abiotic/biotic systems: 1) synthetic biological cells constructed of synthetic/abiotic and natural/biotic components and designed to interact with living natural cells; 2) nanoparticle modified cells with retained viability but altered extremophile functions such as ultraviolet and osmotic stress resistance; and 3) completely synthetic red blood cells. Modular abiotic/biotic systems are more durable and chemically complex than natural cells and will enable new capabilities in detection, drug delivery, and detoxification for countering emerging chemical and biological warfare threats to our nation.

Rapid Antimicrobial Susceptibility Determination using Acoustic Resonance

209189 | Year 1 of 1

Principal Investigator: D. W. Branch

A method was presented to determine the antibiotic susceptibility of bacterial samples more rapidly than conventional methods to speed appropriate therapies and increase survival rate. We showed that *Escherichia coli* cell growth and adsorption are challenged by the antibiotic kanamycin when monitored using a shear-horizontal leaky surface acoustic wave resonator. This effect occurred on a time scale of thirty to sixty minutes. Of significance was the development of an active shunt capacitance cancelling oscillator for resonator parameter extraction. This oscillator actively removes the contribution of the shunt capacitance from the acoustic resonators, allowing precise tracking of the series resonant frequency.

Selection of Ribosomes from Infected Mammalian Cells to Identify Viral Pathogens

199973 | Year 2 of 3

Principal Investigator: K. J. Parchert

This project aims to improve the detection and identification of viruses by enriching for viral messenger RNA being translated by host ribosomes. Pathogen identification will be accomplished when viruses are emerging and/or early in infection, when identification of viruses is particularly challenging. Accurate identification of viruses is necessary to determine appropriate mitigating responses to natural outbreaks and biosecurity threats.

Three-Dimensional Multicolor Superresolution Microscopy for Imaging the Machinery of Cells and Capturing Biochemical Interfaces

199972 | Year 2 of 3

Principal Investigator: A. Backer

This project aims to enhance and re-imagine all facets of bioimaging technology. Using unconventional imaging system designs, we are working to increase the speed and sensitivity with which large datasets can be acquired, and biological pathogens identified. Furthermore, using novel optical materials, our work seeks to realize lightweight, small form-factor imaging/display devices for use by the armed forces.

Unmasking Hidden Compounds within Hyperspectral Images

190959 | Year 3 of 3

Principal Investigator: S. M. Anthony

This project developed software and hardware to improve the detection of weak signals within hyperspectral images. The capabilities developed with the hyperspectral stimulated emission depletion microscope allow super resolution and spatially resolved detection of pathogenic processes. These advances support the detection and treatment of infectious disease as well as biothreat agents. These software improvements can be applied more broadly to national security applications including remote sensing.

COMPUTING AND INFORMATION SCIENCES

The Computing and Information Sciences Investment Area (IA) champions innovative research and development that advances the state of the art in mathematics, information sciences, and computing relevant to Sandia's national security missions. As these applications continue to technically deepen and broaden, there is an ongoing need to innovate and advance underlying knowledge and capabilities. The scope includes computer and computational science and engineering (including high performance computing and computing architectures), and information and data sciences (including cognitive sciences).

Subsystem Reduced-Order Modeling and Network Uncertainty Quantification for Rapid, Agile, Extreme-Scale Simulation.

Project 190968. PI: Kevin Carlberg.

This project has enabled tractable modeling and simulation and uncertainty quantification (UQ) for decomposable systems at extreme scale. We considered systems composed of interconnected subsystems (e.g., components, subdomains), which characterize a wide range of mission-critical applications including electrical power systems, weapons systems (e.g., shock/vibration analysis), multiscale models, external cavity flows, and even non-physical systems such as emergency planning via suites of disparate modeling tools (i.e., SUMMIT). This project created two complementary methods—along with other supporting techniques—that perform extensive analyses at the subsystem level, and couple the results using ideas from domain decomposition (DD) to enable rapid full-system analyses. This divide-and-conquer strategy supports subsystem independence, as tailored uncertainty analysis, discretizations, solvers, and reduced-order model (ROM) techniques can be applied to each subsystem separately. The first method is a novel domain decomposition UQ (DDUQ) methodology. The second method is a domain-decomposition reduced-order model (DDROM) based on the least-squares Petrov-Galerkin projection method. The resulting strategy is affordable through the use of ROMs, agile by enabling subsystems to be swapped or reassembled, and provides assurance through uncertainty propagation.
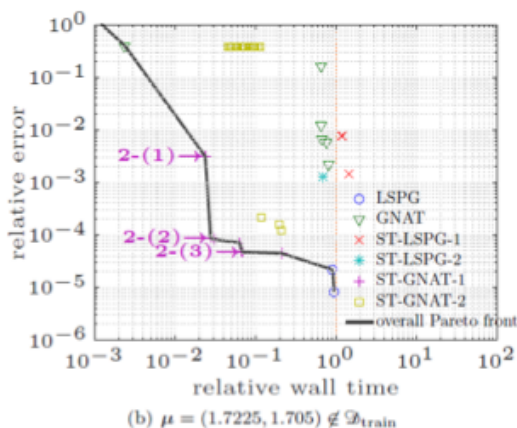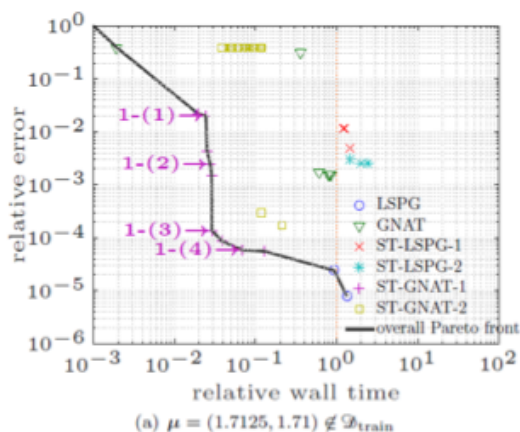
Quasi-1D Euler equation. Relative error versus relative wall time for varying model parameters. The newly created ST-GNAT (Space-Time Gaussian Newton with Approximate Tensors) method significantly outperforms all existing model-reduction methods in relative error and wall time.

P R O J E C T S

A Disaggregated Memory Architecture for Future High Performance Computing

199977 | Year 2 of 3

Principal Investigator: S. D. Hammond

This project will investigate novel approaches to the design of large-scale computing systems in which the storage/memory components of the architecture are placed directly into the high-speed interconnection fabric rather than being co-located with processors. The results will demonstrate how, or whether, such an architecture can provide benefit to Sandia's national security mission programs.

A Domain-Specific Language for High Consequence Control Software

203433 | Year 2 of 3

Principal Investigator: R. C. Armstrong

As a collaboration between the Jet Propulsion Laboratory and Sandia in the formal verification of high consequence controls, Sandia will concentrate research towards high assurance for time critical, single-threaded controls, using the Statechart language as input allowing interoperability. Sandia's focus is on formal refinement of timed events in controls that will improve the safety, security, and reliability of nuclear weapon controls. The Sandia work concentrates on single-threaded, very high consequence controls similar to those used in high consequence systems such as nuclear weapons, nuclear power plants, and the like.

Adverse Event Prediction using Graph-Augmented Temporal Analysis

190965 | Year 3 of 3

Principal Investigator: R. Brost

We sought methods for finding precursors to events of interest in temporal data streams. Our approach employed a combination of temporal analysis and graph analysis, focusing on temporal analysis. The temporal analysis identified candidate precursors to events of interest, which in some cases we refined using graph information. We explored several approaches, considering problems including disease outbreak prediction, wind power forecast error prediction, and identification of precursor signals in simulated network traffic data. We were able to demonstrate successful prediction capability, but prediction lead times were limited by the underconstrained nature of extrapolation. A key lesson learned was that including domain knowledge is a key tool to improve predictive capability.

An Exascale Computational Simulation Capability for Pervasive Fracture and Failure of Structures

203537 | Year 2 of 3

Principal Investigator: M. W. Heinstein

This project will develop the physics models and computational approaches to create computational simulations that answer questions about how structures fail in an explosion, and explore engineering design opportunities to mitigate the effects of a blast. Furthering the science of fracture modeling and simulation is important to our nuclear weapon and other national security programs.

Compatible Particle Methods: a New Paradigm for Structure-Preserving Discretization without a Mesh

199981 | Year 2 of 3

Principal Investigator: P. B. Bochev

This project will develop new classes of compatible meshless methods, which will provide advanced simulation tools for mission-relevant applications in subsurface, multi-material and atmospheric flows, climate, and energy storage. The project will develop new agile software libraries to support the new methods and to enable their demonstration on exemplar problems motivated by mission applications. The software also will be evaluated for other applications, such as meshfree data transfer for climate models. The main contribution of the project will be the development of compatible meshfree methods for partial differential equations that mirror the properties of compatible mesh-based discretizations.

Counter Adversarial Graph Analytics

190966 | Year 3 of 3

Principal Investigator: W. P. Kegelmeyer

Graph analysis algorithms, specifically community detection and node labeling, are a key part of many national security missions. This project asked: what vulnerabilities lurk in those algorithms, even when correctly applied? We discovered, studied, and quantifiably characterized such vulnerabilities, in the context of assuming the worst-case scenario of an informed, empowered adversary. We also developed countermeasures, and established their limits. Our project success has and will benefit the cybersecurity and counterintelligence communities.

Diffusion Maps: A Unified Framework for Reasoning about Imperfect Data

199984 | Year 2 of 3

Principal Investigator: M. Sarovar

This project will develop new fundamental techniques for algorithmically extracting structure from motion and reducing the dimensionality of large, time-dependent, noisy and incomplete datasets. The resulting computational understanding and representation of the structure present in data, as well as the minimal representation of its dynamics, will benefit national security needs for dynamical systems, big data analysis, and defense and space applications.

Distributed-In-Time Techniques for Optimization at Extreme Scales (DITTO-X)

209195 | Year 1 of 3

Principal Investigator: D. Ridzal

This project will pioneer parallelization across the time dimension as a transformative computational technique for parameter estimation, design optimization, and control of engineered systems driven by long-time scale dynamics. The project will develop new optimization algorithms and software geared toward extreme-scale computing, enabling the solution of critical–yet currently intractable–optimization problems in power grid, pulsed power, and reentry applications.

Efficient, Scalable Tomography of Many-Qubit Quantum Processors

209197 | Year 1 of 3

Principal Investigator: E. Nielsen

This project will create a foundation and implementation of a key enabling technology for the development and evaluation of quantum computing hardware: *efficient characterization of many-qubit quantum processors*. Success will constitute a breakthrough in quantum characterization. Our work is critical to national security missions through its potential to achieve and accelerate applications of quantum computing including cryptography, simulation, and beyond Moore computing.

Fast and Robust Linear Solvers Based on Hierarchical Matrices

199983 | Year 2 of 3

Principal Investigator: E. G. Boman

This project will develop and explore novel mathematical algorithms to solve large sparse linear systems based on hierarchical low-rank matrices. The goal is to develop new solvers/preconditioners that are both fast and robust for a wide range of problems from Sandia and DOE applications, such as ice sheet modeling, electromagnetics, and structural mechanics. Sandia is developing a parallel solver in collaboration with Stanford University.

Linear Programming in Strongly Polynomial Time

209194 | Year 1 of 3

Principal Investigator: M. S. Ebeida

We propose to design, analyze, implement, and rigorously test a new provably tractable, parallelizable algorithm for linear programming. If successful, our method would solve one of the greatest open math problems of the 21st century. A tractable solution would influence a wide range of mission-relevant applications in scheduling, nuclear weapon logistics, infrastructure analysis, nondestructive weapons testing, and sensor placement and management.

Mixed-Integer Partial Differential Equation Constrained Optimization (MIPDECO)

209196 | Year 1 of 3

Principal Investigator: C. A. Phillips

We propose to develop transformational mixed-integer partial differential equation constrained optimization (MIPDECO) methods by creating new mathematical concepts, modeling techniques, and algorithms. We will design and implement mixed-integer programming techniques that are aware of the underlying partial differential equations (PDEs), and create PDE techniques that exploit the discrete nature of the problem. This capability could impact many national security applications including energy harvesting for nuclear deterrent systems. We explicitly are targeting design of a system to transmit energy through a barrier. This is relevant for noninvasive container inspection at the border, protecting electronics from electromagnetic pulses, and nuclear deterrent applications.

Multi-Level Memory Algorithmics for Large, Sparse Problems

199982 | Year 2 of 3

Principal Investigator: J. W. Berry

This project explores the problem of computing with multiple levels of memory. The work is motivated by current and future DOE supercomputers, all of which are projected to have this feature. We approach the problem through co-design, which includes: theoretical modeling, design and analysis of algorithms, reference implementations, systems software considerations, and simulation. Our approach builds upon classical external memory algorithmics to significantly impact multiple national security missions.

Neural Algorithms for Low Power Implementation of Partial Differential Equations

209192 | Year 1 of 1

Principal Investigator: J. B. Aimone

Solving partial differential equations (PDEs) describing physical systems is a critical task within Sandia and NNSA's stockpile stewardship mission, and scaling high performance computing systems to necessary levels is increasingly limited by the power demands of modern computing technology. This research developed two new algorithms that enable the use of next-generation, low-power neuromorphic computing technology to be used to effectively solve diffusion-based PDE systems. These new mathematical approaches have the potential to dramatically reduce the power demands of national security simulation tasks.

Optimal Control and Design of Qubits

190970 | Year 3 of 3

Principal Investigator: G. J. von Winckel

This project developed a computational framework for novel quantum device characterization capabilities and determined optimal voltage schedules to improve fidelity of devices in the presence of process non-idealities. Resolving trapped charge and strain contributions to the potential from capacitance measurements requires imposing numerous nonlinear partial differential equation constraints, however, the software developed for this project provided efficient, scalable solutions for next-generation quantum computing and numerous scientific computing applications. The design philosophy has been carried out with the needs of the application specialist in mind and has leveraged and built upon Sandia's high performance computing software while providing a straightforward and accessible user interface.

Palletized Simulation Data for Traceability and Reproducibility

212649 | Year 1 of 1

Principal Investigator: G. F. Lofstead

Tracing a dataset back to all of the source materials that created it is difficult to impossible. We needed this capability to trust that the compute used for modeling and simulation represents the tests intended. Previous approaches cannot automatically encapsulate and tag a dataset with links back to source materials. This work investigated how to create such a system. It successfully demonstrated encapsulating data into a container annotated with the source environment information. The work also showed that we can use this containerized approach within our workflow system with minimal changes. The space and performance overheads were small and within acceptable limits.

Parallel Tensor Decompositions for Massive, Heterogeneous, Incomplete Data

199986 | Year 2 of 3

Principal Investigator: T. G. Kolda

Our goal is to develop a flexible hybrid parallel framework for tensor factorizations that lays the groundwork for meeting future mission requirements to process ever-larger and more complex data sets. A major goal of this project is to provide sure footing for current and emerging national security data analysis tasks.

Patterns of Analyst Attention

211913 | Year 1 of 1

Principal Investigator: L. E. Matzen

This project served as a proof of concept to assess the potential for developing compression algorithms for streaming sensor data based on patterns of analyst perception and attention. The goal of the project was to lay the groundwork for developing algorithms that could have broad applicability for improving system design and analyst performance. A set of four experimental paradigms were designed to assess the patterns of attention elicited by analysis of streaming sensor data. A dataset was collected, demonstrating that this approach, which combined eye tracking and electroencephalography, provides real-time information about analysts' attention to different features in the data. In future research, compression algorithms based on these patterns can be developed.

Quantum Optimization and Approximation Algorithms

190963 | Year 3 of 3

Principal Investigator: O. D. Parekh

This project advanced the emerging field of quantum optimization. Quantum computers are expected to outperform classical computers for certain types of problems, yet rigorous demonstrations of quantum superiority are relatively scarce. We developed some of the world's first quantum approximation algorithms that use quantum resources in novel ways to provide higher quality solutions to hard optimization problems than possible with the best-known classical algorithms. In addition, we discovered how to leverage classical discrete optimization techniques to design new algorithms that provide rigorous approximations of low energy states for problems arising in quantum physics. Our multi-disciplinary project brought together and trained DOE staff in both discrete optimization and quantum information science.

Statistical Uncertainty Quantification for Multivariate Physical Parameter Estimation with Multivariate Outputs

209193 | Year 1 of 2

Principal Investigator: L. Hund

This project will develop a generalized statistical approach for calibration of physical parameters in the presence of high dimensional uncertainties, model-form error, and multivariate outputs. A generalized calibration capability will increase the utility of computational simulation models for extrapolative prediction throughout the nuclear weapon space and will extract more information from data collected using Sandia's unique experimental facilities, including the Z-machine.

Stochastic Optimization to Enhance Resiliency and Response Strategies in Critical Infrastructure

199988 | Year 2 of 3

Principal Investigator: J. Watson

This project will develop advanced algorithms for considering uncertainty and nonlinearities in critical infrastructure operations and planning models. Addressing uncertainty and nonlinearities is crucial to critical infrastructure resilience, to address unknown impacts of extreme events, and to accurately reflect underlying physics (e.g., of power flow). Critical infrastructure resiliency is a pervasive national security issue for DOE, DoD, and DHS. Exemplar critical infrastructures considered by the project include the power grid and water distribution networks.

Subsystem Reduced-Order Modeling and Network Uncertainty Quantification for Rapid, Agile, Extreme-Scale Simulation

190968 | Year 3 of 3

Principal Investigator: K. T. Carlberg

This project developed a new methodology that enables rapid, scalable simulation, and uncertainty quantification (UQ) of decomposable systems. The approach: 1) models the system as a network of subsystems, 2) performs rapid uncertainty analysis via reduced-order modeling for each subsystem, and 3) couples subsystem uncertainties via network UQ. This has enabled a broad impact capability across mission-critical applications including gas-transfer 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.

High-Throughput Material Characterization via 6 Degrees of Freedom Loading and Material Parameter Feedback
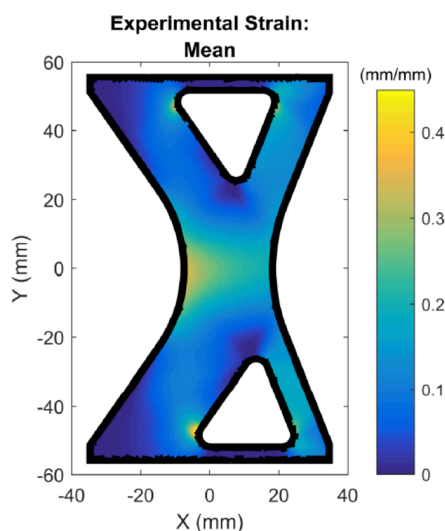### Project 191068, PI: Phillip Reu
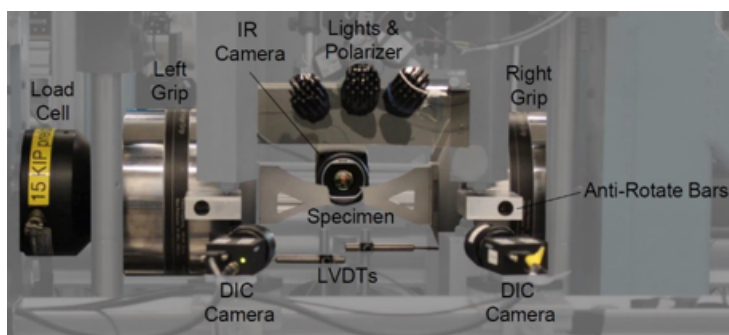
Experimental setup for full-field deformation and thermography measurements.

Full-field DIC measurements of the strain in a validation specimen of 304L stainless steel rolled sheet.

Modeling material and component behavior using finite element analysis (FEA) is critical for modern engineering. One key to a credible model is having an accurate material model, with calibrated model parameters, which describes the constitutive relationship between the deformation and the resulting stress in the material. As such, identifying material model parameters is critical to accurate and predictive FEA. Traditional calibration approaches use only global data (e.g., extensometers and resultant force) and simplified geometries to find the parameters. However, the utilization of rapidly maturing full-field characterization techniques (e.g., Digital Image Correlation) with inverse techniques (e.g., the Virtual Fields Method [VFM]) provide a new, novel, and improved method for parameter identification. We tested the idea: whether more parameters could be identified per test when using full-field data. The research successfully proved this hypothesis by comparing the VFM results with traditional calibration methods. Important products of the research include: verified VFM codes for identifying model parameters, a new look at parameter covariance in material model parameter estimation, new validation techniques to better utilize full-field measurements, and an exploration of optimized specimen design for improved data richness.

ENGINEERING SCIENCES

PROJECTS

A Unified Framework for Quantification of Margin and Uncertainty

209220 | Year 1 of 2

Principal Investigator: L. Hund

This project will develop a data integration framework for quantification of margins and uncertainties (QMU) by building statistical models to determine whether and how to combine information across data sources. Through measuring the added value of data integration, we will lay the groundwork for a streamlined approach to QMU across all types of information important to the nuclear weapon stockpile.

An Agile Design-to-Simulation Workflow using a New Conforming Moving Least Squares Method

209225 | Year 1 of 2

Principal Investigator: J. Koester

This project aims to disrupt the analysis process and enable agile simulations. The transformative idea is a numerical technique based on a recent discovery for handling boundaries in moving least squares methods. Simulation is ubiquitous in Sandia's core nuclear weapons and energy security activities. With this effort, simulation-based decisions will be made with higher confidence and at a lower cost.

Big-Data Multi-Energy Iterative Volumetric Reconstruction Methods for As-Built Validation and Verification Applications

191069 | Year 3 of 3

Principal Investigator: E. S. Jimenez, Jr.

This project developed new interrogation methods in x-ray imaging and new methods to reconstruct the data from the new interrogation method. Multi-energy iterative reconstruction (MEIR) acquires polychromatic x-ray images using a new energy-resolved detector and iterative reconstruction algorithms. The higher fidelity x-ray data and improved reconstruction has improved detection in 3D reconstruction and has yielded richer information for DOE, NNSA, and industrial computed tomography applications.

Connecting Polymer Physics and Microstructure with Large Deformation Polymer Foam Mechanics

209223 | Year 1 of 3

Principal Investigator: S. L. Kramer

This project will develop a new, large deformation constitutive model for polymer foams, unified across foam densities, and polymer glass transition temperatures, based on microstructural data, mesoscale deformation data, and solid polymer physics. This model, the associated data science tools, and the experimental approach will transform Sandia's ability to design and predict polymer foam deformation, necessary for national security applications.

Coupling of Laminar-Turbulent Transition Modeling with Reynolds-Averaged Navier-Stokes Computational Fluid Dynamics

209219 | Year 1 of 3

Principal Investigator: N. Bitter

This project will develop a much-needed new computational method for predicting laminar-turbulent transition on hypersonic reentry vehicles and coupling these predictions with aerodynamics simulation codes. This capability could significantly reduce risk and cost in the analysis and design of future reentry vehicle systems by decreasing uncertainty in predictions of thermal and aerodynamic loads.

Design of Acoustic Metamaterials for Shock and Vibration Control in Weapon Systems

200171 | Year 2 of 3

Principal Investigator: T. Walsh

This project will develop optimization strategies and design new tailored impedance materials for vibration mitigation applications. The ability to filter and deflect mechanical energy waves and ultimately shield structural components from harsh vibration environments will prevent costly over-design and result in better protection systems for mechanical vibration environments encountered in civil and defense applications.

Development of an Electromagnetic Resonance Dampener to Improve Shielding Effectiveness

209226 | Year 1 of 1

Principal Investigator: S. Campione

This project provided a preliminary investigation on the effect of loading high-quality factor cavities with absorbing materials to reduce the cavity's electromagnetic fields and quality factor over a given frequency band. The use of a 2 mm-thick magnetic absorber (occupying only 0.026% of the cavity volume) resulted in an improvement of shielding effectiveness larger than 19 dB and reductions in quality factor larger than 91% for four transverse magnetic modes. By reducing sensitivity to electromagnetic radiation, the concept's impact would be improvement in cavity shielding effectiveness and predictability for complex cavity systems.

Discovering the Physics of Blast and Fluid Structure Interactions: A Novel Experimental-Computational Approach

200170 | Year 2 of 3

Principal Investigator: J. Wagner

The primary goal of the project is to develop new spatially and time-resolved diagnostics to measure blast-structure and fluid-structure interaction. This includes detailed measurements of the shock-induced flow surrounding the structure as well as internal and external structural response. Such capabilities will improve the ability to predict weapons behavior in harsh delivery environments.

Explosive Challenge: Revolutionizing Spatial and Temporal Blast Characterization

209222 | Year 1 of 3

Principal Investigator: D. R. Guildenbecher

High-fidelity munitions modeling is needed to predict detailed behaviors to address national security challenges; however, current development cycles, which rely on limited data from large-scale tests, could require decades to complete. We seek to accelerate this using state-of-the-art, ultra-high-speed diagnostics of subscale environments. Data will be coupled with simulations to prove new pathways for experimentally validating intermediate phenomenological models.

High-Throughput Material Characterization via 6 Degrees of Freedom Loading and Material Parameter Feedback

191068 | Year 3 of 3

Principal Investigator: P. L. Reu

This project sought to change how material models and material properties are determined. The approach included optimized test specimen design, novel inverse techniques, and full field measurements. Outcomes of the project were software to optimize geometry, solve for properties using virtual fields, and an improved understanding of the mathematics of material models. The results going forward will impact our materials science and modeling capabilities for stockpile stewardship and other national security applications.

Physics of Discharge Initiation from Complex Surfaces

200172 | Year 2 of 3

Principal Investigator: C. H. Moore

This project will develop new fundamental mechanistic understanding of electron field emission from real surfaces with contaminant layers. This will be accomplished via comparison of newly developed modeling capabilities to experimental characterization of field emission from controlled surfaces, including adding controlled contaminant layers. Results will allow us to better understand breakdown initiation which is essential for modeling weapon components.

Pushing Continuum Reactive Capabilities through Novel Sub-Grid and Statistical Methods

200177 | Year 2 of 3

Principal Investigator: D. E. Kittell

This project will develop statistical and nonlinear physics-based analysis tools that will result in physics-based subgrid models for predicting the observed collective response of dynamic reactive materials. These models will address a critical gap in predictive capability by including the effects of microstructure, and will allow for optimized designs for energetic materials and components important in NNSA missions.

Reduced Order Models of Structures Incorporating Complex Materials

191074 | Year 3 of 3

Principal Investigator: R. J. Kuether

This project developed a novel model order reduction technique to lower the computational burden of predictive, high fidelity finite element models with viscoelastic materials. The method maintains high levels of accuracy for high consequence systems involving complex material behavior and is capable of speeding simulation times up to 10,000 times in comparison to directly solving the full-order equations. The newly developed capability permits Sandia engineers and analysts the opportunity to perform uncertainty quantification and optimization analyses for improved characterization of component-level designs in mechanical structures such as weapon systems and aerospace vehicles.

Residual Stress Inversion using Ultrasonic Surface Waves, X-Ray Diffraction, and Sacrificial Material

200175 | Year 2 of 3

Principal Investigator: J. E. Bishop

Residual stress in as-manufactured components can significantly impact structural performance such as fracture and fatigue. We are developing new experimental methodologies for quantifying the full 3D residual stress field of as-manufactured components with quantified uncertainty. Our primary experimental technique is semi-destructive relaxation with subsequent inverse modeling to obtain the residual stress field. These new techniques will improve predictive component simulations for current and future weapon systems.

Role of Phonon-to-Vibration Energy Transfer in Initiation of Energetic Materials

209224 | Year 1 of 3

Principal Investigator: K. Ramasesha

This project will test a major proposed mechanism for initiation of reaction in energetic materials. The goals of the project are to confirm/deny the mechanism, determine threshold conditions for reaction, and determine whether the mechanism explains variation in shock sensitivity between materials. Results (null and affirmative) are important to developing predictive models of initiation for explosive component development efforts.

ENGINEERING SCIENCES

Turbulent Flow Uncertainty Quantification using Machine Learning Techniques

191076 | Year 3 of 3

Principal Investigator: M. F. Barone

This project explored the use of machine learning techniques to develop improved models of near-wall turbulence. The research specifically targeted the improved prediction of surface pressure and shear stress loadings resulting from turbulent flow to enable simulation-based specification of design environments for weapon systems and many other engineered systems. Project outcomes included development and demonstration of a novel data-driven near-wall model for turbulent flows based on deep neural networks.

Understanding Soot Development and Thermal Stratification in Combustion Engines through Hyperspectral Nonlinear Optical Diagnostics

191060 | Year 3 of 3

Principal Investigator: C. J. Kliewer

This project developed new laser-based nonlinear optical probes and simulation tools for the study of next-generation combustion energy systems that operate at high pressures and temperatures with higher efficiency. We extended the capability of ultrafast coherent Raman spectroscopy, the gold standard for the measurement of temperature, pressure, and chemical speciation in the gas phase, to a previously unexplored pressure and temperature regime relevant to next-generation engine technology with well-controlled and validated measurements. The capability to probe and simulate novel engine technologies enables progress towards higher efficiency devices, thereby improving our nation's energy security.

Uncertainty Quantification of Microstructural Material Variability Effects

200176 | Year 2 of 3

Principal Investigator: R. E. Jones

This project is developing models of variability and performance to enable robust design and certification. Material variability originating from microstructure (e.g., grains and defects) has significant effects on component behavior and creates uncertainty in performance. The outcome will be a specific uncertainty quantification (UQ) enabled analysis of material variability effects on performance and a method to evaluate the consequences of microstructural variability in general.
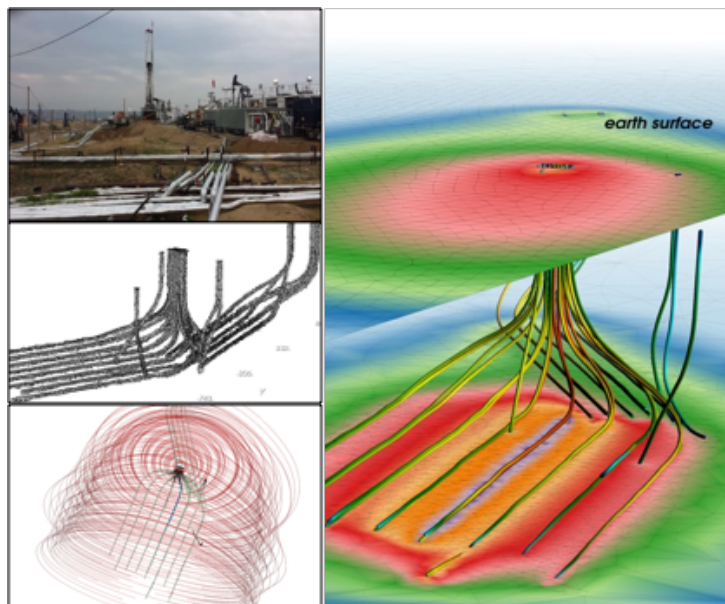
GEOSCIENCE

The Geoscience Investment Area seeks to expand the frontiers of knowledge about the earth's subsurface, surface, oceans, and atmosphere in the following areas: 1) advances in scientific understanding, 2) new sensing tools and methods that provide multi-dimensional information, and 3) numerical tools for mapping, parameterizing models, and integration of complex data streams and simulations. These earth science capabilities impact Sandia's national security missions.

Prediction and Inference of Multiscale Electrical Properties of Geomaterials

Project 200183, PI: Chet Weiss

By developing a computationally efficient, hierarchical representation of material properties in finite element analysis, Sandia researchers have demonstrated a scalable algorithm for simulating the geophysical response of small-scale features over physical distances many times their size. "A pervasive problem in electromagnetic (EM) geophysics applied to subsurface imaging and situational awareness is the extreme computational cost of estimating the scattering profile of thin, electrically conductive features such as geologic fractures, pipelines and cables in cases where the only viable observation points lie at distances 100s of meters to several kilometers away," says Sandia distinguished staff member Chester Weiss. "The hierarchical representation allows us to avoid explicit volume discretization of their thinness, but to retain their spatial extent, thus reducing the computational burden of computing their response by several orders of magnitude." This breakthrough in geophysical

Field-scale geophysical awareness in cluttered environments. Example computation of full electrostatic scattering from wellbore casing and geology over a 1 km3 Earth volume for remote drill-bit steering, formation permeability control and reservoir management.

simulation is one part of the project's larger objective in developing novel multi-physics simulation capabilities for multi-scale systems, where the dynamics at the micro-scale have significant influence on overall behavior at the meso- and mega-scale. These results in direct, multi-scale modeling inform and speak directly to mathematical concepts in non-local operators and fractional calculus, which the researchers are currently advancing with outside collaboration from George Mason University. "The ramifications of the hierarchical and fractional work are potentially huge, especially for optimization," according to co-PI Bart van Bloemen Waanders, "and have already begun to influence our thinking of transport on complex network systems, whether those systems are physical, biological, or even informational." This work was published in the journal, *Geophysics*.[1]

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[1] Chester J. Weiss (2017). "Finite-element analysis for model parameters distributed on a hierarchy of geometric simplices." *Geophysics*, 82(4), E155-E167. https://doi.org/10.1190/geo2017-0058.1

PROJECTS

Active Tracers for In Situ Computing in Porous and Fractured Media

209236 | Year 1 of 1

Principal Investigator: R. P. Jensen

We investigated methods to transform porous media into unconventional computational systems. We sought a paradigm shift in geoscience engineering from a workflow of sequential monitoring and post-processing to one of "in situ computing", meaning a system that, due to its make-up and components added to it, performs calculations to gain useful and actionable information. We used autocatalytic reactions to generate nonlinear chemical waves, which respond to aspects of the porous media through which they traverse. We used microfluidic systems and computational fluid dynamic simulations. We demonstrated logic gates in fracture networks. In situ computing may impact national and energy security through the systems doing self-monitoring of health and performance.

An Advanced Persistent Homology Toolbox for Real-Time, Automatic Classification of Seismic Signals

211067 | Year 1 of 1

Principal Investigator: J. E. Heath

Robust, real-time, automated interpretation of seismic data directly impacts national and energy security. This project developed new algorithms using topological signal processing for the classification of seismic events such as underground explosions or earthquakes. We developed a new form of persistent homology, called concurrent persistent homology (CPH). Persistent homology is a tool from algebraic topology that analyzes the connectivity structure of data. Our results show that the concurrent dominant trends in motion of a three-component seismogram can discriminate seismic events. Our algorithms for CPH discrimination of seismic events were implemented in MATLAB, and these algorithms may also be useful for seismic event detection.

Arctic Tipping Points Triggering Global Change

209230 | Year 1 of 3

Principal Investigator: K. J. Peterson

This project will develop computational methods enabling Arctic-focused tipping event prediction. Tipping events, or small magnitude changes with state-altering effects, are anticipated in the Arctic with the potential to disrupt the global Earth system. The proposed framework will support early warning of critical events with uncertainty quantification by leveraging unique Sandia data analytics capabilities and the Energy Exascale Earth System Model.

Attribution of Methane Emissions in the Arctic and Continental US

200182 | Year 2 of 3

Principal Investigator: R. Bambha

This project will develop a novel data analysis approach for quantifying regional methane emissions and estimating the contributions from different methane source types. The project addresses a general problem relevant to national energy, nonproliferation, and defense needs using atmospheric measurements to estimate the emissions of a substance by a collection of sources and including heterogeneous measurements to improve emissions estimates.

Characterization and Sampling of Ultralow Permeability Geomaterials using Electrokinetics

209234 | Year 1 of 3

Principal Investigator: K. L. Kuhlman

This project will develop new transient electrokinetic laboratory methods to sample and characterize properties of fractured ultralow permeability geomaterials (e.g., granite or cement). These methods will fundamentally contribute to physical understanding of transient electrical phenomena in rocks and will revolutionize Sandia's ability to understand and control ultralow permeability geomaterials that are critical to advanced energy, infrastructure, and nuclear waste disposal missions.

Chemical-Mechanical Modeling of Subcritical-to-Critical Fracture in Geomaterials

191133 | Year 3 of 3

Principal Investigator: L. Criscenti

We developed molecular simulation and experimental approaches to understand how fluid composition affects fracture initiation and propagation. These methods can be used to improve our capability to control fracturing in rock for gas and oil extraction, assess the long-term viability for carbon dioxide or nuclear waste sequestration, and, more generally, to predict stress-corrosion in materials. We specifically showed that with a reactive force field, we can predict the dissolution mechanisms for silica over a range of pH values and calculate distinct fracture toughness values for silica exposed to different aqueous environments. This capability is important to DOE's Fossil Energy, Nuclear Energy, and Basic Energy Sciences.

Developing Fugitive Emissions Sensor Networks: New Optimization Algorithms for Monitoring, Measurement, and Verification

193231 | Year 3 of 3

Principal Investigator: K. A. Klise

Sensor placement optimization is an important field of research given the inherent variability of sensor performance based on environmental variables, sensor location, and sensor operating conditions. This project developed algorithms and software for sensor placement optimization to maximize monitoring effectiveness. While this research was focused on methane emissions, the research can be applied to a wide range of applications, including the placement of surveillance cameras, chemical, and fire detectors. This work aligns with DOE goals to increase the safety and resilience of natural gas infrastructure by improving the way sensors are deployed in the field.

Developing the Color Key for "Hyperspectral Google Earth"

209233 | Year 1 of 1

Principal Investigator: T. A. Reichardt

This project demonstrated the utility of a Sandia-developed physical model for the interpretation of hyperspectral imaging (HSI) data relevant to geosciences and security remote sensing. Given the demonstrated progress, there remains the potential to develop an integrated HSI-analysis model that will fuse Sandia expertise in HSI, geochemistry, spectroscopy, analytics, and security, preparing Sandia for the future ubiquity of HSI data (HSI "Google Earth").

High Fidelity Hybrid Method for In Situ Borehole Stress Determination

191087 | Year 3 of 3

Principal Investigator: M. D. Ingraham

This project sought to improve the accuracy of in situ hydraulic fracture measurements of stress through inclusion of thermo- and chemo-mechanical coupling. Current uncertainty of in situ measurements is on the order of 50%–we sought to reduce this to 40% or less. Depending on conditions and rock type, we have achieved reductions in uncertainty on the order of 10-20% through the use of advanced constitutive/numerical models that include intermediate principal stress dependence, as well as thermal and chemical effects. In situ stress affects all subsurface activities for energy security, including fossil and geothermal energy, nuclear waste disposal, and geologic storage.

Integrated Geomechanics and Geophysics in Induced Seismicity: Mechanisms and Monitoring

200180 | Year 2 of 3

Principal Investigator: H. Yoon

This project will develop new fundamental mechanistic understanding of geomechanical and geophysical processes of fracturing that lead to induced seismicity in fractured systems. The project will also develop a physics-based machine learning approach to characterizing fracture evolution through the integration of multichannel acoustic emission (AE) data, digital image correlation (DIC) and micro-computed tomography (micro-CT) data. This research will lead to the new groundwork for remote characterization of rock failure by identifying the precursors to the induced seismicity in fractured systems, which will significantly impact DOE missions in subsurface resource extraction, waste storage, and energy storage.

Monitoring and Repair of Damaged Cement-Geomaterial Interfaces in High Pressure High Temperature Repository and Borehole Scenarios

200181 | Year 2 of 3

Principal Investigator: E. N. Matteo

This project will develop fundamental understanding of chemical and mechanical degradation at cement-geomaterial interfaces via a study that includes novel code development to model coupled reactive transport and solid mechanics codes and state-of-the-art experimental characterization. Understanding from the project is critical to ensure seal integrity (wellbores, nuclear waste repository seals) during subsurface operations that are central to securing our nation's energy future.

Optimizing Electromagnetic Signal Transmission for Distributed Embedded Wireless Sensors for Geoscience Applications

209235 | Year 1 of 1

Principal Investigator: J. E. Heath

This project developed concepts to enable remote charging of wireless sensors for real-time and long-term monitoring of subsurface engineered environments. Such sensor systems would improve national energy security and environmental protection. Subsurface environments may include fracture networks, near-wellbore environments, aquifers, hydrocarbon reservoirs, and nuclear waste storage sites. Specifically, the project investigated: 1) energy delivery to subsurface wireless sensors and 2) sensor designs for energy harvesting. We modeled power density in the direct current (DC) mode for realistic scenarios based on a field site. Our findings indicate that power delivery to sensors can be on the order of tens of milliwatts per meter cubed, for which power harvesters can be designed.

Prediction and Inference of Multi-Scale Electrical Properties of Geomaterials

200183 | Year 2 of 3

Principal Investigator: C. J. Weiss

This project will develop a computational capability for predictive forward modeling and optimization of electromagnetic geophysical data in situations where fine scale structure—either engineered or naturally occurring—has a profound effect on the data, but is computationally explosive to model with traditional numerical methods. Application spaces include border security, nonproliferation, and energy research. New breakthroughs therein will provide a computational ability unmatched elsewhere in the DOE complex.

Real-Time Subsurface Event Assessment and Detection

209237 | Year 1 of 3

Principal Investigator: G. Bettin

This project seeks to establish preeminent capabilities through the design and implementation of autonomous, self-powered, self-monitoring wellbore systems, rapid failure event detection via embedded sensor networks, machine learning and smart deployment, and repair methods. This will uniquely position Sandia to be the national leader in wellbore integrity, working as an impartial partner with industry, academia, governmental agencies, and the public.

Unlocking Real Time Infrasound Event Classification Abilities using Machine Learning

209231 | Year 1 of 2

Principal Investigator: S. Albert

This project will leverage state-of-the-art machine learning methods and pre-existing Python tools to develop an algorithm to categorize infrasound (low frequency sound) events by type. The final product will consist of an event classification code package that can be implemented alongside real-time detection algorithms. This will create the ability for national security agencies to deduce the nature of an event immediately after its detection, aiding in important decision making.
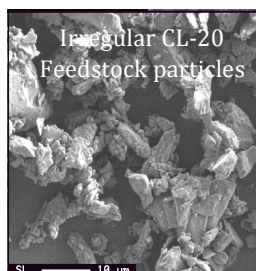
MATERIALS SCIENCE

The Materials Science Research Foundation (MSRF) sustains and nurtures Sandia's materials science capabilities needed to: 1) enable science-based engineering decisions for Sandia's mission areas, 2) provide the materials discovery, synthesis and processing to underpin current and future Sandia materials applications, 3) respond to emerging national security needs including military, terrorism, cyber, economy, and energy, and 4) execute foundational R&D to develop new insights and understanding to meet current and future mission objectives and maintain Sandia's leadership in the international scientific community. The MSRF makes investments that differentiate and strengthen our materials capabilities. We emphasize bold initiatives and innovative science that couple theory, computation, and experiments to gain new insights, fostering new ideas and collaborations that position Sandia to be a leader in emerging areas of science and technology.

Cooperative Self-Assembly for Structure and Morphology Control of Energetic Materials

Project 191194, PI: Hongyou Fan

This project developed fundamental understanding of self-assembly of energetic materials and effective control of their morphology. A detergent assisted self-assembly process was developed to manufacture ~1-gram quantities of energetic material nanoparticles with controlled size and microparticle morphologies. The ability to control morphology at this level of production represents a completely new capability in energetic material processing. This research has the potential to eliminate inconsistent performance of energetic materials by providing a trusted and reproducible method to improve energetic materials for nuclear weapon applications, which will enable significant improvements in design confidence, surveillance approaches, and predictive models of energetic materials reliability. This work contributed to a 2018 R&D 100 award for Detergent-Assisted Fabrication of Multifunctional Nanomaterials.

Feedstock before Self-Assembly / After Self-Assembly / Monodisperse / Various controlled morphologies

PROJECTS

PROJECTS (continued)

An Interfacial Synaptic Transistor for Fast Neuromorphic Computing

209249 | Year 1 of 3

Principal Investigator: Y. Li

This project will develop an interfacial synaptic transistor (IST) for neuromorphic computing, which provides an advanced framework to process unstructured data and identify future national security threats. The IST modulates the electronic conductivity by storing electrons and ions at interfaces, and will be programmed at megahertz frequencies while retaining nonvolatility and low power consumption.

Assessment of an Energy-Release Process for Point-Defect Migration in Group-III Nitride Semiconductors

211434 | Year 1 of 1

Principal Investigator: S. R. Lee

This project developed improved mechanistic understanding of previously unstudied physical processes for point-defect migration in wide-bandgap Group-III-nitride semiconductors, where the energy released by carrier capture at point defects drives defect transport via localized, nonequilibrium heating of the crystal lattice. These processes may be important to accurately model defect diffusion when wide-bandgap semiconductor devices are exposed to ionizing radiation; understanding them will improve our nation's ability to qualify advanced national security systems.

Characterizing Ferromagnetic/Antiferromagnetic Interfaces for Ultrafast Spintronics

209247 | Year 1 of 1

Principal Investigator: C. Chan

This project developed a new, unique, world-class capability that uses an ultraviolet laser to enable polarization-dependent materials imaging with photoemission electron microscopy (PEEM). Such a system enabled novel ultraviolet magnetic circular dichroic imaging (UVMCD-PEEM) and ultraviolet magnetic linear dichroic (UVMLD-PEEM) imaging of ferromagnetic and antiferromagnetic materials. Understanding how the properties of ferromagnetic and antiferromagnetic materials and interfaces impact spin dynamics in ultrafast spintronics enables faster and more efficient devices. These materials are at the forefront of basic research into novel, high-density, high-speed, robust computing and memory paradigms.

Cooperative Self-Assembly for Structure and Morphology Control of Energetic Materials

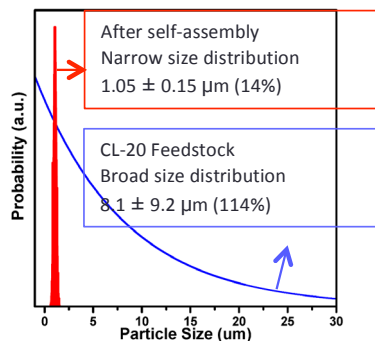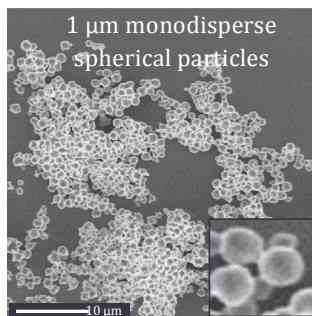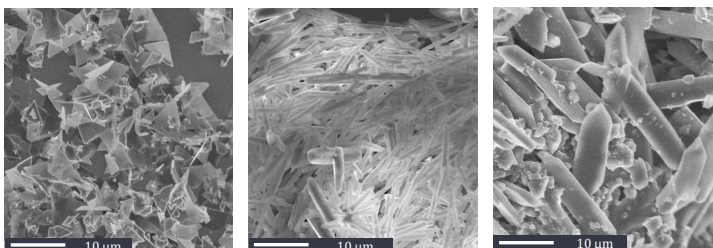**191194 | Year 3 of 3**

Principal Investigator: H. Fan

This project developed fundamental understanding of self-assembly of energetic materials and effective control of their morphology. A detergent assisted self-assembly process was developed to manufacture ~1 gram quantities of energetic material nanoparticles with controlled size and microparticle morphologies. Ability to control morphology at this level of production represents a completely new capability in energetic material processing. This research has the potential to eliminate inconsistent performance of energetic materials by providing a trusted and reproducible method to improve energetic materials for nuclear weapon applications, which will enable significant improvements in design confidence, surveillance approaches, and predictive models of energetic materials reliability.

Describing the Chemical Steps of Hydrogen Incorporation in Metal Hydrides using Time-Resolved Environmental X-Ray Photoelectron Spectroscopy

209243 | Year 1 of 3

Principal Investigator: F. El Gabaly Marquez

This project will develop environmental x-ray photoemission spectroscopy to determine the molecular processes of hydrogen incorporation and evolution in hydrides under meaningful gas overpressures. New insight will come from unique experimental setups that will enable gas/surface interrogation. Knowledge of these processes will impact technologies in hydrogen purification, hydrogen solid storage, and isotopic gas handling systems important to NNSA's nuclear security mission.

Designer Quantum Materials

209242 | Year 1 of 2

Principal Investigator: S. Misra

This project leverages Sandia's unique atomic precision fabrication capability to engineer tunable arrays of dopants that mimic the electronic behavior of quantum materials. This work could revolutionize the understanding of quantum material physics by pursuing the first-ever systematic approach to complement existing ones based primarily on trial and error. This project impacts quantum science and addresses the DOE's mission through innovation in science and technology.

Development of Alternative Lattice-Matched Buffer Layers and Optimization of Metalorganic Chemical Vapor Deposition Growth for III-Nitride Power Electronics

212413 | Year 1 of 3

Principal Investigator: B. P. Gunning

This project addresses the mitigation and understanding of material defects in aluminum gallium nitride and gallium nitride films, a major hurdle for III-nitride device realization. Understanding and overcoming this high defect density will lead to the demonstration of state-of-the-art ultra-wide bandgap materials, enabling new device architectures with radiation hardness and high-voltage/power handling at reduced size, weight, and power, for DOE and NNSA applications.

Discovering a New Aging Mechanism in Lamellar Solid Lubricants

211670 | Year 1 of 1

Principal Investigator: M. T. Dugger

This project resulted in a new model for predicting the temperature-dependent shear properties of a solid lubricant from calculated energy barriers to atomic motion. This ability to predict macroscale performance based on fundamental atomic scale processes is expected to be applicable to other lamellar solids as well, resulting in impact beyond national security applications. This model forms the foundation for both predicting performance of solid lubricants in weapon components as a function of age, and for the design of more age-resistant materials for future weapon component applications.

Electrochemical Model of Humidity-Driven Corrosion

191187 | Year 3 of 3

Principal Investigator: E. J. Schindelholz

This project aimed to advance scientific understanding of atmospheric corrosion, a little understood but primary materials degradation mode in many DOE systems, from weapons to spent nuclear fuel canisters. An approach framework and tools were developed to define the properties of electrolytes on atmospherically exposed surfaces and their linkage to electrochemical processes driving atmospheric corrosion. A mechanistic damage model for copper atmospheric corrosion was demonstrated. This approach and understanding have been leveraged for development of next-generation corrosion service life prediction models, including atmospheric stress corrosion cracking of spent nuclear fuel canisters and corrosion of aluminum components in microelectronics.

Enabling Hydrogen Infrastructure through Surface Passivation of Structural Materials

200197 | Year 2 of 3

Principal Investigator: R. Kolasinski

This project will develop the science basis for surface passivation as a remediation for hydrogen-assisted fatigue crack growth in pipeline steels. Over-designing pipelines to protect against hydrogen embrittlement presents a significant barrier to the adoption of fuel cell electric vehicles. Our research explores a low-cost solution, impacting our nation's ability to field low-carbon, renewable energy sources for transportation.

Engineering Next-Generation Zero Thermal Expansion Composite Materials for Additive Manufacturing Technologies

200199 | Year 2 of 3

Principal Investigator: N. C. Burtch

This project will develop new fundamental understanding of negative thermal expansion materials that can robustly compensate for positive thermal expansion in additive manufacturing technologies. Positive thermal expansion can lead to mechanical failure modes in materials used in high consequence applications. New negative thermal expansion material innovations would mitigate such problems and bring significant value to Sandia's materials science and engineering capabilities as well as advance DOE's goal to strengthen the connection between advances in fundamental science and technology innovation.

High Entropy Alloys: A Materials Solution to Metals Additive Manufacturing

209246 | Year 1 of 3

Principal Investigator: A. Kustas

This work will establish new fundamental understanding of the unique properties of high entropy alloys and open a new route for the fabrication of additively manufactured metal parts able to meet stringent engineering qualifications associated with high consequence applications. Successful completion of this work could significantly impact our nation's ability to realize next-generation aerospace, automotive, and power generation systems.

High Power Solid State Li-ion Batteries through Interface Engineering

191191 | Year 3 of 3

Principal Investigator: F. El Gabaly Marquez

Engineering interfaces can critically improve performance of very small, all solid state lithium-ion batteries that can be integrated with other microelectronics. We focused this project on tailoring the interfacial structure and chemical composition of solid state lithium-ion batteries and achieved lower interfacial resistance and higher power capability. The improved solid state rechargeable micro-batteries resulting from this project are now much closer to meeting the technical requirements needed to improve our nation's ability to field maintenance-free sensors, antennas, and other power-hungry microelectronics.

Identifying Rare, "Disqualifying" Flaws in AM Components

209244 | Year 1 of 3

Principal Investigator: J. Carroll

Additively manufactured (AM) components exhibit rare, disqualifying flaws that are problematic for reliability. This project takes a practical approach to nondestructively inspect AM parts within a damage tolerant paradigm. Probabilistic modeling, high throughput materials characterization, and nondestructive evaluation will define allowable flaws and optimal inspection techniques. This project will inform reliable AM components for high consequence nuclear security related applications.

Inkjet Printing Metal Organic Frameworks for Next-Generation Electronics and Optoelectronics

204725 | Year 2 of 2

Principal Investigator: A. L. Benin

This project utilized inkjet printing to deposit functional materials, particularly metal organic frameworks (MOFs), onto low-cost substrates such as glass, silicon/silicon dioxide, and polyethylene terephthalate (PET) polymer. New synthetic methods were developed to achieve nanosized MOF crystallites and stable, printable inks. Deposition of electronically conducting organic polymer and silver ink were optimized on PET. Fabrication of an organic electrochemical device on a flexible substrate and demonstration of device operation have also been accomplished. These advancements in capabilities would support several national security missions including faster creation of "smart" devices, and advancements in flexible electronic and photonic devices with potential impacts in sensors, low-power electronics, and multi-material structures.

Interfacial Effects on the Microstructure and Morphology of Energetic Materials

191188 | Year 3 of 3

Principal Investigator: E. C. Forrest

The microstructure and morphology of energetic materials strongly influences detonation characteristics. We engineered and leveraged interfacial characteristics at atomic-to-microscopic length scales to study the effects of surface energy and microtopography on properties of explosive films created with physical vapor deposition. This enabled control of explosive performance at length scales of interest, representing a paradigm shift in explosive science for national security applications.

Investigating Phase Evolution in Chemical Wavefronts Subject to High Heating Rates (~1e6 K/s)

200204 | Year 2 of 3

Principal Investigator: D. P. Adams

This project explores the atomistic mechanisms that underly propagating wavefront stability in reactive solids. The team is combining dynamic transmission electron microscopy, predictive thermal modeling, molecular dynamics simulations, and advanced material design to research key unknowns of reactive solids. This fundamental research should ultimately lead to new, improved, reliable material designs needed for joining, microsystems, and energy applications.

Magnetic Nanocomposites for High Performance Inductor Materials

200203 | Year 2 of 3

Principal Investigator: D. L. Huber

This project will develop magnetic nanocomposites for high performance inductor materials. The magnetic nanocomposites will be optimized for specific applications by tuning the particle size and spacing. These new inductors have applications in power electronic circuits for military and civilian applications where size, weight, and power density are of critical importance.

Making Density Functional Theory Work for all Materials

200202 | Year 2 of 3

Principal Investigator: A. Cangi

This project will develop predictive density functional theory approximations for all materials, including heavier elements such as rare earths, lanthanides, actinides, and transition metal oxides. This work will improve advanced calculations and allow the extension of model-based design and engineering to the unique properties of d- and f-electron materials crucially important to the NNSA's national security mission. Potential applications include electronics, computer/communication systems, transportation, health care, and national defense.

Mechanistic Origins of Stochastic Rupture in Metals

200201 | Year 2 of 3

Principal Investigator: B. Boyce

The project explores the microstructural conditions that give rise to void nucleation during quasi-static ductile rupture of metals. After inducing progressive damage states through mechanical testing, pedagogical metallic materials are dissected to characterize the local microstructure and defect state. Complementary atomistic and dislocation dynamics models help explore the critical conditions that give rise to emergent void nucleation. Ductile failure assessment and prevention is relevant to the nuclear weapons mission.

Mitigation of Point Defects in Wide-Bandgap Semiconductors by Photo-Modification of Fermi Level during Growth

209248 | Year 1 of 3

Principal Investigator: M. H. Crawford

The purpose of this project is to unambiguously and quantitatively prove that tailored optical excitation of a semiconductor surface during growth can significantly reduce point defect incorporation through the mechanism of Fermi-level control. This effort will gain new fundamental understanding, surmount long-standing III-N semiconductor materials limitations, and enable record performance from power electronics and ultraviolet optoelectronics for broad-ranging mission impact.

Modeling Energy Transfer and Melting Efficiencies in Fusion Metal Additive

209652 | Year 1 of 2

Principal Investigator: D. J. Tung

This project will develop laser energy efficiency defect relationships in additive manufacturing through making small-scale builds in an integrating sphere. Understanding these relationships and mitigating defects through process parameter variations will provide a technique to increase build consistency and confidence, which in turn will allow additively manufactured components to be viable candidates for a larger range of energy and weapons applications.

Nanomaterial Ink Development for Smart Manufacturing

209245 | Year 1 of 3

Principal Investigator: E. B. Secor

This project will address the challenge of integrating disparate electronic materials using a single additive manufacturing process by developing chemistries, manufacturing tools, and feedback software to rapidly explore the design space of co-printed materials. This work could impact national security efforts to develop next-generation printed electronics, sensors, energy transducers, autonomous systems, etc., using high-throughput and trusted manufacturing approaches.

Predicting the Friction Behavior of Body-Centered Cubic Metal and Alloys

200200 | Year 2 of 3

Principal Investigator: M. E. Chandross

This project aims to develop a model of microstructural evolution in body-centered cubic metals under applied cyclic stress. A quantitative model connecting atomistic processes to macroscale mechanical behavior (friction) would be a paradigm shift in the design of mechanical contacts found in nuclear weapons (e.g., stronglinks, accelerometers), power (e.g., electric vehicles, wind turbines) and aerospace, enabling a systematic methodology that greatly improves reliability. In FY 2018, we compared our first prediction from the model to experiment, and quantitatively matched the stress limit above which we expect plowing (i.e., material removal) to dominate the frictional response in single-crystal Tantalum.

Quantum Nanofabrication: Mechanisms and Fundamental Limits

191196 | Year 3 of 3

Principal Investigator: G. T. Wang

The project goal was to provide a detailed understanding of the mechanisms and ultimate limitations of quantum-size controlled photoelectrochemical etching and to explore its applicability over a wider range of semiconductor materials. Key understandings were gained on the time-dependent etch process and the impact of nanoscaling on the etch process. New experimental demonstrations of the etching of nanowires and multiple quantum dot layers were also achieved. This work established a foundation for the controlled fabrication of epitaxial semiconductor quantum dots, with relevance to numerous mission areas including: high efficiency lasers, single and entangled photon sources and detectors, and radiation hard devices for space, and nuclear weapons applications.

Self-Assembly Assisted Additive Manufacturing of Thermoset Materials

209505 | Year 1 of 2

Principal Investigator: K. Manning

This project developed the use of thermosetting polymers, which are largely unprintable, in additive manufacturing through the creation of novel chemistries with tunable material rheology and cure dynamics via self-assembly. The approach addressed the fundamental gap in development of additive manufacturing thermosetting polymers. The impact of this work was establishment of a new class of thermosetting polymers amenable to additive manufacturing as options for national security applications.

Sequential Design of Experiments for Accelerated Life Testing

195881 | Year 3 of 3

Principal Investigator: S. V. Crowder

This project developed methodology for optimal accelerated test plans under a limited number of samples. This methodology allows test planners to best use their limited time and resources to understand product performance so that they can ensure US weapons and other products perform as intended in the field.

Topological Quantum Material for Quantum Computation

203429 | Year 2 of 3

Principal Investigator: W. Pan

Topological quantum materials (TQMs) are a rapidly emerging field in materials research, with a potential to profoundly impact the nation's information and energy technology applications. Here, we seek to understand the following quantum properties of TQMs that can propel the electronics industry into a whole new topological quantum electronics area: topologically created Majorana fermions, topological superconductivity, and topologically modified photoconductivity.

Understanding Pulsed Laser Surface Annealing for Advanced Semiconductor Materials

210202 | Year 1 of 1

Principal Investigator: M. P. Siegal

This project will advance pulsed laser surface annealing via ultraviolet light pulses to deliver the energy necessary to anneal (or crystallize) a film (or coating) with negligible heat transfer to the substrate or other co-located device materials. Critical problems in advanced semiconductor materials science will be studied; successful development could enable novel architectural designs for power electronics and silicon-based cyber applications.

Understanding Transport and Aging Mechanisms to Optimize Sandia's Ion-Conducting Electrolytes for Energy Applications

191186 | Year 3 of 3

Principal Investigator: A. Frischknecht

In this project, we developed an understanding of the relationships among polymer chemistry, morphology, and proton conductivity, in a proton-conducting polymer developed at Sandia. We used computational methods including molecular dynamics simulations, along with experimental methods including nuclear magnetic resonance spectroscopy and x-ray scattering, to understand the increase in conductivity with increasing levels of sulfonation and hydration of the polymer. This understanding will lead to better design of polymer membranes for use in fuel cells and in flow batteries to improve energy storage devices, applications of interest to DOE's energy mission and specifically the Fuel Cell Technologies Office (fuel cells) and Office of Electricity (flow batteries).

NANODEVICES AND MICROSYSTEMS

The Nanodevices and Microsystems Research Foundation (NMRF) strives to discover new phenomena at the nanoscale and microscale and to create new concepts, devices, components, subsystems, and systems that leverage science in the nano-to-microscale domain. Its objective is to foster a bold, ground-breaking science and technology base needed to support wide-ranging future national security missions. Major technical thrust areas include: 1) trusted radiation-hardened microsystems, 2) Beyond Moore's Law computing technologies, 3) optoelectronics of the future, 4) advanced microsystem sensor technologies, and (5) nanoscale and microscale-enabled performance.

Scandium Aluminum Nitride for Advanced Piezoelectric Sensors, Actuators, and Filters

Project 191198, PI: David Henry

This project investigated and solved a significant scientific and industrial problem involving fundamental material challenges of piezoelectric aluminum nitride (AlN) films. These challenges presently limit application of acousto-electric filters in high bandwidth mobile communications. Theoretical studies and modeling suggested that fundamental changes in the atomic and crystalline structure of AlN films were needed to reach the necessary performance for commercial markets. If other atoms, such as scandium (Sc), could be substituted for Al in the wurtzite crystal, electromechanical coupling could increase by more than 200%. Earlier attempts with ScAlN were met with unexpected inclusions and unwanted crystallographic orientations that substantially degraded device performance. Through material science and fabrication experiments, the team identified secondary growth mechanisms that degrade film quality and then established techniques to control them. The team then overcame other device-architecture challenges to demonstrate ScAlN acousto-electric resonators with record performance.

This project generated multiple patents, created new collaborations with industrial and academic partners, and placed Sandia at the forefront of the piezoelectric ScAlN field.

Replacing an Al atom in AlN with Sc (left) to improve film properties can produce undesirable crystallographic phases (top and right). Sandia helped to identify this problem, developed patented methods to control film growth (center), and applied these advances to make high-performance acoustic-electrical devices (bottom).
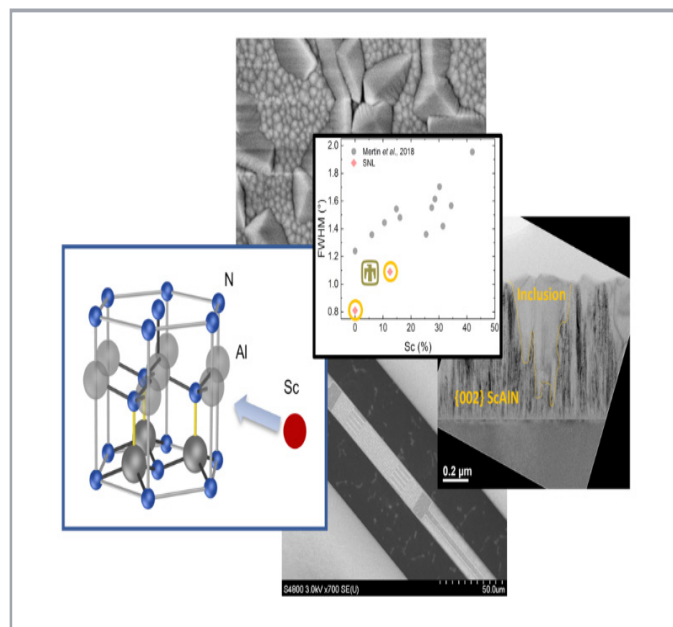
PROJECTS

A Compact, Spectrally Tunable Source of Entangled Photon Pairs for Quantum Sensing

192786 | Year 3 of 3

Principal Investigator: I. Brener

We proposed a new source for generation of entangled photon pairs in the near infrared (~1.5 μm) based on semiconductor heterostructures (III-nitrides) coupled to metamaterials. This combination can create giant, gated, and tunable optical nonlinearities, thereby enabling control of the entangled photons wavelength and the ability to switch photon generation on/off using a bias voltage. We showed record optical nonlinearities that can lead to new light sources useful for sensing of trace chemicals and chem/bio weapon threats.

A New Paradigm in Chem/Bio Threat Detection: Evaluating Threats based on Biological Function Rather than Chemical Form

191203 | Year 3 of 3

Principal Investigator: K. Achyuthan

This project was engaged in the development of robust sensors to detect chemical and biological threats based on their biological function rather than their chemical form. The operating principle was to mimic biological membranes with robust polymer amphiphiles on nanowire field-effect transistors (FETs), and correlate changes in conductivity to exposure to chemical and biological threats. Toward this goal, a sensing system was developed to detect pH changes due to membrane perturbations. Membrane perturbations are the first indications of several chem/bio threat agents or attack. Thus, this technology paved the way for the creation of a portable sensor for national and homeland security missions to detect chemical and biological threat agents.

A Truly Micro-Scale Low Cost, Size, Weight, and Power Gyroscope based on Optomechanical Oscillation

200231 | Year 2 of 3

Principal Investigator: A. J. Grine

We are building a rotation sensor that, through design and scaling, breaks trends in current technologies. Namely, we aim to show that by scaling down to microscale dimensions (goal: 10 μm< active radius<100 μm), we can simultaneously improve sensitivity while reducing cost, size, weight, and power (CSWaP). The sensor is promising in applications requiring agile navigation, guidance, and control.

Active and Nonreciprocal Radio Frequency Acoustic Microsystems

200229 | Year 2 of 3

Principal Investigator: M. Eichenfield

This project will develop novel radio frequency (RF) amplifiers using the acoustoelectric interaction between piezoelectric thin films and semiconductors. Success will allow orders of magnitude reduction in size, weight, and power of RF signal processing units by having active and passive components on one chip. This allows dramatic size, weight, and power reduction for RF devices impacting a broad range of national security and other RF applications.

Asynchronous Ballistic Reversible Computation with Superconducting Josephson Junctions

209250 | Year 1 of 3

Principal Investigator: R. M. Lewis

A reversible approach to computation can reduce the fundamental energy required to process a single bit of information below the thermal limit of kBT log 2 (Landauer). Reversible logic will be demonstrated using novel asynchronous ballistic designs for reversible logic gates based on superconducting Josephson junction switches and interconnects. Reversible logic would strongly impact national security computing tasks, as current supercomputers are limited in size by power consumption. A reversible supercomputer could be several orders of magnitude more computationally powerful with the same power budget allowing a paradigm shift in what problems are considered computationally tractable.

Demonstrating Robustness of Analogue Quantum Simulators

209254 | Year 1 of 3

Principal Investigator: P. L. Maunz

We will make analog quantum simulation (AQS) robust against environmental noise with active logical cooling and develop a viable hardware platform for precise analogue simulation in a Sandia-developed microfabricated ion trap chip. If successful, the project will provide the knowledge to design and build a robust AQS for applications in chemistry, medicine, and material science.

Developing a Solid State Technology for Electron Spin Qubits on Liquid Helium

191210 | Year 3 of 3

Principal Investigator: E. A. Shaner

The project explored electron spin qubits and the foundations of a silicon integrated circuit-based advanced computing technology by integrating electrons on helium with complementary metal-oxide-semiconductor structures and demonstrating spin-to-charge conversion for single spin readout. While not the main focus, a new breakthrough was realized in this effort using amorphous conducting layers to allow ultra-shallow channels to enable nanoscale structures. Progress was made on gated quantum dot structures, but full realization of functional quantum dot devices was not realized. If further efforts in this area are successful, it may be an important building block in eventual advanced quantum information sciences, a key element critical to the US government's national security missions.

Digital Electronics at the Atomic Limit (DEAL)

200232 | Year 2 of 3

Principal Investigator: S. Misra

The Digital Electronics at the Atomic Limit (DEAL) project seeks to leverage Sandia's atomic-precision fabrication capability to realize the theorized orders-of-magnitude improvement in operating voltage for tunnel field effect transistors (TFETs) compared to complementary metal–oxide–semiconductor (CMOS) transistors. Not only are low-power digital circuits a critical element of many national security systems (e.g., satellites), TFETs can perform circuit functions inaccessible to conventional CMOS electronics (e.g., polymorphism).

Graphene-Enabled On-Chip Spectroscopy for Massive SWaP Gains

209252 | Year 1 of 1

Principal Investigator: M. Goldflam

This project aimed to develop a path towards a portable on-chip spectroscopy system. This goal required two advances. First, improvement and miniaturization of the spectrally sensitive elements of the spectrometer, which was explored through simulation work. Second, our extremely sensitive detectors required further development with a proof-of-concept completed in this project. When combined, these technological advances should provide a route to expanded deployability of infrared spectroscopy systems, thereby strengthening the nation's ability to assess chemical/biological threats.

High-Voltage Power-Transistors Enabled by Selective Area Regrowth of p/n Junctions using Ultra-Wide Bandgap Nitride Semiconductors

209253 | Year 1 of 3

Principal Investigator: A. A. Allerman

This project will develop a mechanistic understanding of how crystalline defects at a regrown p/n junction interface influence reverse electrical leakage in AlGaN-based diodes. This understanding will enable selective-area-regrown p/n junctions with low leakage current and will be used as the core element necessary to demonstrate the first AlGaN-based vertical power-switching transistor, an enabling capability for next-generation high-power electronic systems.

Highly Efficient Solar-Blind Single Photon Detectors

191199 | Year 3 of 3

Principal Investigator: A. Armstrong

We demonstrated the first AlGaN-based quantum dot floating gate high electron mobility transistors (FG-HEMTs). Visible-blind detection with responsivity > 108 A/W and solar-blind detection with responsivity > 104 A/W was achieved. Low voltage and 297 K operation of AlGaN FG-HEMT photodetectors simplifies systems integration compared to high voltage and cryogenic commercial options. This new technology benefits a variety of national security applications requiring high sensitivity ultraviolet photodetection in the visible-blind and solar-blind spectrum, including non-line-of-sight communication and fluorescence-based bio-agent sensing.

Low-Power High-Speed Transistors Enabled by Ferroelectric Hafnium Oxide

209251 | Year 1 of 3

Principal Investigator: P. Davids

This project seeks to develop a new transistor device architecture based on negative differential capacitance of a ferroelectric oxide gate stack using a new replacement metal gate process. This recently discovered phenomena has the potential to greatly reduce integrated circuit power consumption and improve device performance and density, offering the possibility of new low power, high-performance, custom integrated circuits for nuclear weapons and defense sciences mission areas.

MilliKelvin High-Electron-Mobility Transistor Amplifiers for Low Noise, High Bandwidth Measurement of Quantum Devices

200233 | Year 2 of 2

Principal Investigator: L. A. Tracy

This project developed ultra-low power cryogenic amplifiers for improving measurement of quantum devices. The low power consumption (less than 1 microWatt) allows the amplifier to be located near the device, at the coldest cryostat stage, typically less than 100 milliKelvin. Developing the technology for fast, accurate measurement of quantum devices is of importance for quantum computing applications.

Nano-Engineering of Detector Surfaces to Offer Unprecedented Imager Sensitivity to Soft X-Rays and Low Energy Electrons

203202 | Year 2 of 3

Principal Investigator: M. O. Sanchez

In a collaborative effort with NASA's Jet Propulsion Laboratory (JPL), this project will explore how to maximize the sensitivity of a silicon detector surface to shallowly absorbed radiation by using electric field shaping techniques and surface passivation with JPL's Delta Doping process. This will provide insight on how to create silicon detectors that respond to low energy radiation with high efficiency.

Near Infrared Nanophotonics through Dynamic Control of Carrier Density in Conducting Ceramics

200228 | Year 2 of 3

Principal Investigator: D. K. Serkland

The goal of this project is to realize a new class of high-speed nanophotonics through active control of carrier densities in unconventional plasmonic materials. If successful, we will develop nanophotonics devices with size, weight, and power performance far superior to existing III-V/silicon photonics, enabling a new generation of optical communications technologies relevant to high performance computing platforms that will impact multiple national security applications.

Optimization of Sputtered Aluminum Nitride for the Seeding of Metal Organic Chemical Vapor Deposition Gallium Nitride Films

191204 | Year 3 of 3

Principal Investigator: K. Knisely

The goal of this project was to develop gallium nitride on silicon capabilities using sputtered aluminum nitride (AlN) buffer layers. This project evaluated AlN, aluminum scandium nitride (AlScN), and AlN/metal bilayers as buffer layer candidates. The films were characterized for texture, morphology, and stress, including how film properties evolved as the films thickened. A method for controlling the stress properties in AlN films was developed, allowing local control of the AlN surface strain. This work improved the mission capabilities at MesaFab by developing sputtered AlN buffer layer capabilities for optoelectronics applications and by expanding piezoelectric sensor capabilities by improving AlN and AlScN deposition and integration capabilities.

Rad Hard Devices Science using Quasi-Electric Fields

200226 | Year 2 of 3

Principal Investigator: G. A. Vawter

This project explores new semiconductor devices for harsh radiation environments by creating "rad-hard by band-structure" design concepts for transistors and diodes. The core concept is to use bandgap engineering to establish quasi-electric fields in compound semiconductors, which act differently on majority and minority carriers, to push excess populations of minority carriers in the same direction as majority carriers so that no undesired current flows in these layers.

Scandium Aluminum Nitride for Advanced Piezoelectric Sensors, Actuators, and Filters

191198 | Year 3 of 3

Principal Investigator: R. W. Reger

This project investigated alloying of Scandium into aluminum nitride piezoelectric films to enhance the piezoelectric properties of the film. The observed improvement in the piezoelectric material properties impacts our nation's ability to field advanced radio frequency systems, ultrasonic imagers, sensors for extreme environments, and near zero power wakeup devices.

Understanding the Physics of Silicon-Germanium Heterojunction Bipolar Transistors for Cutting-Edge Electronics at Deep Cryogenic Temperatures

193422 | Year 3 of 3

Principal Investigator: T. D. England

The purpose of this project was to discover new device physics and to create cutting-edge analog and radio frequency circuits with silicon germanium heterojunction bipolar transistors operating at 4 Kelvin. The project successfully generated new knowledge about the physics of these devices. It showed the dominate collector current transport to originate from tunneling currents and created models to match that current. This new understanding paves the way for improvements in future circuits operating at 4 Kelvin and below for quantum information applications. Project success relates to DOE Strategic Objective 5 by the creation of cutting-edge technology.

Vertically Injected Ultraviolet Laser Diodes

188288 | Year 4 of 4*

Principal Investigator: M. H. Crawford

This project targeted materials roadblocks to extending laser diodes (LDs) into the deep-ultraviolet (DUV) region. Such DUV LDs could enable compact, robust light sources for applications including fluorescence-based bioagent sensing, atomic clocks, and technologies in the solar-blind region (< 280 nm). Major materials challenges include the lack of low-defect, electrically conducting substrates, thereby prohibiting low-resistance vertical-injection geometries, and lack of insight into origins of high optical loss. We demonstrated electrically conducting AlGaN-on-GaN substrates with threading-defect densities ~10x lower than standard, electrically insulating AlGaN-on-sapphire substrates. Optically pumped lasing studies confirmed Mg-doping contributed substantial optical loss and provided insight into optimal doping profiles. This work developed key elements and understanding toward demonstration of vertically injected DUV LDs.

* This project did not exceed the maximum period of performance of 36 months

What is Happening in Narrow-Band-Gap Devices? Radiation Induced Defects and Recombination

200230 | Year 2 of 2

Principal Investigator: P. A. Schultz

This project developed and demonstrated new experimental techniques (time-resolved microwave reflectance for defect levels) and modeling methods (bandgap-discriminating density functional theory) to probe and characterize radiation-induced defects in narrow bandgap systems such as InAs(Sb). These capabilities were used to discover fundamental understanding of radiation sensitivities in InAs/InAsSb-based superlattice devices, that will impact the ability of the nation to qualify and deploy these next generation technologies in space applications (e.g., focal plane arrays for thermal imaging).

Wide-Range Solid State Tuning for Acoustoelectronics

209255 | Year 1 of 3

Principal Investigator: D. W. Branch

Electric field-based frequency tuning of acoustic resonators at the material level provides an enabling technology for building complex tunable filters. Tunable acoustic resonators were fabricated in thin plates (h/l ~ 0.05) of X-cut lithium niobate (90°, 90°, y = 170°). We demonstrate the effect of a direct current (DC) bias to shift the resonant frequency by ~0.4% by directly tuning the resonator material. The mechanism is based on the nonlinearities that exist in the piezoelectric properties of lithium niobate. Devices centered at 332 MHz achieved frequency tuning of 12 kHz/V through application of a DC bias.

A Platform for Quantum Information and Large-Scale Entanglement with Rydberg Atoms in Programmable Optical Potentials

191211 | Year 3 of 3

Principal Investigator: S. A. Kemme

This project demonstrated reconfigurable arrays of individually trapped ultracold atoms, thus realizing a platform that could demonstrate large-scale quantum entanglement with the addition of strong inter-atomic interactions. Arrays with up to 100 trap sites were formed via digital holography and a high numerical aperture imaging system that featured in situ trap diagnostics and single atom imaging resolution. We further discovered a new implementation of a controlled-phase gate that utilized coherent excitation to Rydberg states. This method will enable robust entanglement protocols in many-atom systems such as the one developed here.

NEW IDEAS

While all LDRD projects are required to perform creative, innovative R&D focused on challenging, high-risk science and engineering problems with potential impact to Sandia and DOE/NNSA's national security missions, most projects are focused toward problems identified and supported by a traditional Investment Area (IA). By contrast, the New Ideas IA is intended for those daring ideas that lie outside Sandia's current research focus areas and have potential for exceptional contributions to Sandia's strategic goals over the long term. New Ideas supports pioneering basic research unlikely to be funded by other IAs that may lead to game-changing breakthroughs for Sandia's national security mission.

Electro-Optical Control over SiV Center Emission in Diamond

Project 200240, PI: Edward Bielejec

We developed and characterized silicon vacancy (SiV) defect centers in diamond. Using Sandia's nanoImplanter, we fabricated single atom devices by implanting impurity atoms, in this case Si, into high quality electronic grade diamond substrates. These impurity atoms form optically active defect centers that can be used for quantum information sciences (QIS) including single photon sources, quantum sensors, and quantum computation. These defect centers can also be used for applications such as high resolution magnetic and electric field sensors and bio-compatible temperature sensors.

Three follow-on projects resulted in >$9M dollars of funding. Based on defect centers in diamond, we added the University of Chicago, Purdue, Naval Research Lab, Argonne National Lab, etc., to our existing external user base. We published or were coauthors on eight papers, including one *Science* and two *Nature Communication* articles using Sandia's focused ion beam implantation capability. Highlighted below is an example of one of these collaborations.

In this latest research[1], a team of researchers from Harvard University, University of Cambridge, and Sandia developed a new approach to decouple the SiV quantum system from its environment minimizing thermal decoherence. SiV centers were created at Sandia using a focused ion beam to precisely implant silicon ions in an array on a diamond substrate. This type of device usually would be subject to the thermal decoherence unless the quantum system is operated at cryogenic temperatures. The team took advantage of the fact that the cause of the thermal decoherence arises from a high susceptibility of the electronic orbitals to lattice strain and devised a way to increase control of the strain. We designed a single-crystal diamond cantilever with metal electrodes patterned above and below it. An opening in the top electrode allows optical access to the SiV qubits. DC voltage applied across the electrodes deflects the cantilever downwards and generates controllable static strain. Through strain control, the team reduced the electron-phonon coupling and demonstrated six-fold improvement in the spin coherence time.
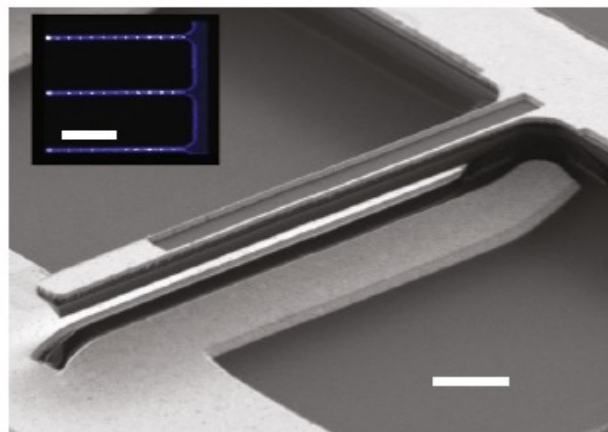
An example of a nanocantilever implanted using focused ion beam implantation at Sandia.

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[1] Y-I. Sohn, S. Meesala, B. Pingault, A.A. Atikian, J. Holzgrafe, M. Gündogan, C. Stavrakas, M.J. Stanley, A. Sipahigil, J. Choi, M. Zhang, J.L. Pacheco, J. Abraham, E. Bielejec, M.D. Lukin, M. Atatüre and M. Loncar, "Controlling the coherence of a diamond spin qubit through its strain environment." *Nature Communications* 9, 2012 (2018).

PROJECTS

2D and 3D Real-Time Visualization of Magnetic Fields using Quantum Optics

209278 | Year 1 of 2

Principal Investigator: D. R. Farley

This project will develop the technical basis to noninvasively image magnetic fields for noble gases using the quantum optical effect of Coherent Population Trapping by tuning laser beams to the Zeeman splitting of metastable krypton atoms. This capability applies to atom traps (nuclear forensics), and has utility in other applications where fields should be noninvasively imaged, potentially in nuclear weapons.

A New All-Dielectric Nanolaser

191223 | Year 3 of 3

Principal Investigator: M. B. Sinclair

This project explored the use of high-quality factor dielectric metasurfaces as a platform for a new type of nanolaser. We extensively characterized the photoluminescence from metasurfaces fabricated from III-V semiconductor materials with embedded quantum heterostructures. We found that quantum dots-in-a-well provided substantially improved photoluminescence yield due to reduced surface recombination. We later determined that quantum wells in the InGaAsP material system provide even stronger emission, and pursued a flip-chip bonding fabrication path for fabricating metasurfaces with these materials. Development of new nanolaser arrays based on this concept could address sensing, imaging, and communication needs for DoD and DHS missions.

Developing Thermally Activated Acid Release Agents

200236 | Year 2 of 2

Principal Investigator: T. N. Lambert

This project developed molecular control and a new fundamental understanding of chemical bonding concepts that allowed for the development of compounds that are stable at room temperature but release a variety of protic substances (contain a hydrogen atom bonded to an oxygen atom) upon thermal exposure. Control of the type and the amount of protic release was demonstrated. Additionally, we demonstrated that we could release mixtures of protic species. Such thermally activated compounds could find use in several applications, including molecular switches and in lithography, as well as a benign way to store corrosive materials.

Electro-Optical Control over SiV Center Emission in Diamond

200240 | Year 2 of 2

Principal Investigator: E. S. Bielejec

Our goal was to develop and characterize silicon vacancy (SiV) defect centers in diamond. We developed a microfabricated structure to enable electrical emission of the SiV. The ability to electrically control the optical emission of the defect centers in diamond opens up a wide range of potential applications in cybersecurity and quantum information processing. While we were unsuccessful in demonstrating electroluminescence, the techniques developed including surface cleans, terminations, etched alignment markers, high temperature annealing, and diamond processing will be useful in the future. Over the course of this project, we published or were coauthors on eight papers including one Science and two Nature Communication articles using focused ion beam implantation.

Engineering Spin-Orbit Interaction in Si

200238 | Year 2 of 2

Principal Investigator: T. Lu

This project studied, theoretically and experimentally, a new engineered quantum material using silicon, which has weak spin-orbit coupling, and nanoscale magnets. The newly developed artificial material possesses an energy-momentum dispersion that currently only exists in materials with strong spin-orbit coupling. Nanoscale magnets with the required alternating magnetization configuration were demonstrated experimentally. When coupled to a conventional superconductor, this material can host so-called Majorana fermions, which can be used for fault-tolerant topological quantum computing, which could be critical in the future for national security.

Enhance Substrate Binding of Organophosphorus Hydrolase (OPH) via Unnatural Amino Acids utilizing Advanced Transition State and Allosteric Modeling

209275 | Year 1 of 2

Principal Investigator: D. Ye

This project will develop revolutionary organophosphorus hydrolase protein variants with 100-fold increases in nerve-agent binding. Success will provide new understanding to develop detoxification countermeasures and demonstrate the feasibility of allosteric/chemical modeling and the power of unnatural amino acid replacements to greatly enhance enzyme properties. Success of the project will impact our nation's ability to develop nerve agent countermeasures.

Microwave Doppler Charge Velocimetry for Narrow and Wide Bandgap Semiconductors

209279 | Year 1 of 2

Principal Investigator: E. A. Shaner

Infrared sensors based on III-V superlattices are desirable to replace HgCdTe for many applications. The lack of fundamental understanding of vertical transport in these structures is set to become a giant technological problem as the industry transitions. We seek to develop Doppler velocimetry for vertical mobility transport measurements in novel heterostructures. Success will allow more rapid materials development and enable leapfrog advances in infrared sensors and national security mission capabilities for intelligence, surveillance, and reconnaissance.

Phonon Blockade of the Superconducting Transition

209277 | Year 1 of 2

Principal Investigator: I. F. El-Kady

This project will engineer the superconducting transition width by suppressing the phonon population responsible for the Cooper-pair decoherence below the superconducting transition temperature (Tc) via phononic bandgap engineering. A phononic crystal will be used to engineer a phononic frequency gap suppressing the decohering thermal phonon population. Fundamentally, this will result in suppressing the phonon heat capacity near Tc and lead to single phonon detection schemes with performance rivaling the state-of-the-art detectors but with much shorter dead times. Success will carry tremendous impact to superconducting electronics and interconnects pivotal for both beyond Moore's law and quantum computing, encryption, and secure communications.

Topological Photonics: The Quest for Ultimate Photon Control

191221 | Year 3 of 3

Principal Investigator: G. S. Subramania

Approaches that exploit topological properties of the phase space of a system can offer stability and robustness to the system of interest from external disturbances such as scattering or decoherence. We achieved a topological photonic crystal designed to operate at telecom frequencies (1550 nm) exhibiting helicity dependent unidirectional light transport on a silicon-insulator platform guided by electromagnetic modeling. We also developed an approach for topological photonic structures in III-nitrides that can be used for topological light emitters. This project has leveraged Sandia's established strength in nanophotonics to achieve fundamental understanding, positioning us strongly for future mission needs such as fault-tolerant quantum computing and quantum communications vital for national security.

Understanding Si-Decorated Nanoporous Carbon Anodes for High Performance Li-Ion Energy Storage

200237 | Year 2 of 3

Principal Investigator: K. L. Harrison

This project will develop composite anode materials for lithium-ion batteries consisting of silicon and a Sandia-invented form of carbon (nanoporous carbon). These composite materials are expected to perform better than traditional silicon-carbon composites. In addition to improving lithium-ion batteries, synthesis of these materials is amenable to thin-film battery fabrication, which is of particular interest for energy security applications.

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 sciences, dynamic material properties, high energy density science, and pulsed power science. The goal of the radiation effects sciences area is to ensure that engineered systems can operate as intended in radiation environments they encounter, with interest in developing pulsed power technologies, innovative experimental techniques, and novel diagnostics that could scale to higher energy drivers.

Time-Resolved X-Ray Diffraction Measurements on Laser-Compressed Polycrystalline Samples using a Multi-Phase, Short-Pulse Laser Generated X-Ray Source

Project 191235, PI: Marius Schollmeier

Materials, when exposed to high pressures and temperatures, can change their crystal structure. For example, graphite turns into diamond at approximately 150,000 atmospheres pressure. At even higher pressures, materials are exposed to conditions similar to those found in hypervelocity impacts, planetary and stellar interiors, or in inertial confinement fusion research. Key information on the mechanical properties of materials at these extreme conditions can be obtained with x-ray powder diffraction, which allows material investigations on an atomic scale due to the correlation between solid state structures and their associated diffraction patterns. At Sandia, the 100-feet diameter, 20-feet high Z Pulsed Power Facility is used to compress material samples to extreme pressures on a sub-microsecond time scale. Following compression, the material disintegrates in a violent explosion equivalent to the energy released by a few sticks of dynamite. Performing an x-ray diffraction measurement in such a harsh environment requires an intense, nanosecond x-ray source, and a well-protected x-ray detector that can survive the nearby explosion. In an LDRD project that ended in 2018, Sandia researchers developed a dynamic x-ray powder diffraction platform utilizing the warehouse-sized Z-Beamlet or Z-Petawatt laser system to create a plasma x-ray source coupled to a polycapillary x-ray lens. A laser pulse from a third laser is used to simultaneously shock compress a sample, mimicking a Z experiment. Lessons learned from this platform guided the design of a dynamic diffraction diagnostic for Z, which led to the first successful dynamic diffraction measurement on Z in November 2018.
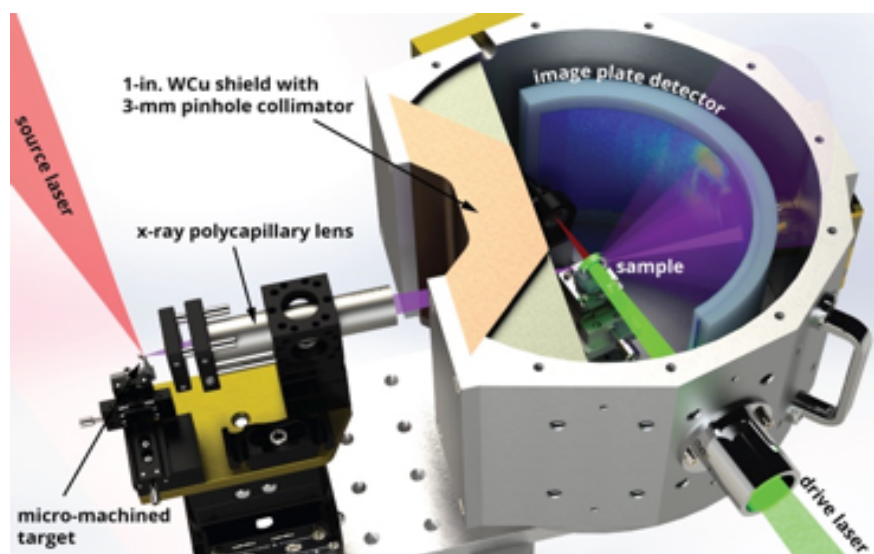
An intense laser pulse directed to a micro-machined metal foil creates a plasma x-ray source. X-ray line radiation emitted by the plasma is guided to a material sample by an x-ray polycapillary lens. This lens increases the x-ray flux 100-fold compared to a conventional pinhole aperture while reducing background radiation emitted by the plasma. The material sample inside the shielding box is shock-compressed by irradiating it with another laser pulse. An image plate detector detects the diffraction pattern; a fiber-based photonic Doppler velocimetry probe measures the sample pressure.

PROJECTS

3D-Magnetohydrodynamic Simulations of Electrothermal Instability Growth by Studying Z-Pinches with Engineered Defects

200269 | Year 2 of 3

Principal Investigator: T. J. Awe

This project will generate new data on the nonuniform heating of conductors driven with intense current. Data will constrain 3D-magnetohydrodynamic simulations, accelerating the development of an advanced computational model of instability growth on magnetically driven implosions relevant to radiation effects science and inertial confinement fusion experiments. The research will identify the type of resistivity perturbation that most aggressively drives nonuniform heating—knowledge vital for mitigating magneto-Rayleigh-Taylor instability growth.

Advancing the Understanding of Laser-Plasma Interactions in High Energy Density Plasma

209289 | Year 1 of 3

Principal Investigator: D. E. Ruiz

This project will focus on the physics behind laser scattering processes, such as stimulated Raman scattering (SRS) and stimulated Brillouin scattering (SBS), relevant to Magnetized Liner Inertial Fusion. The deeper understanding of the basic physics involved in these processes will lead to novel ways in which these processes can be controlled or even exploited in creation of high energy density plasmas.

Correlating the Structural and Electrical Performance of Microelectronics during a Radiation Event

191240 | Year 3 of 3

Principal Investigator: K. M. Hattar

Radiation damage affects performance and reduces lifetimes of microelectronics used in space electronics, nuclear reactors, and weapons. After the cascade is done (picoseconds), the resulting defects will diffuse and interact over timescales from nanoseconds to the lifetime of the device, affecting the material properties and reliability. Our project provides fundamental understanding of the initial creation, fast reaction, and long-term evolution of collision cascades in materials.

Coupled Electron-Photon Monte Carlo Radiation Transport for Next-Generation Computing Systems

195880 | Year 3 of 3

Principal Investigator: K. Bossler

This project explored two concepts for Monte Carlo radiation transport better suited to the single instruction, multiple data (SIMD) paradigm used by accelerators such as graphics processing units (GPUs) that are expected to be installed on upcoming exascale systems. The first was how to process tallies effectively on the GPU, and the second was using event-based particle tracking instead of the traditional history-based approach. Exploring these two concepts has established a stronger foundation for maintaining our ability to provide accurate Monte Carlo radiation transport results, which are essential for helping drive engineering design and qualification of the nuclear weapon stockpile.

Current Loss in 0.1 - 100 Terawatt Vacuum Transmission Lines: Next-Generation Experiments and Physics-Based Simulations

191237 | Year 3 of 3

Principal Investigator: B. T. Hutsel

This project developed new understanding of electrical power flow in high power density magnetically insulated transmission lines (MITLs). In support of this project, we conducted pulsed power experiments and developed physics-based theoretical models of the experiments with the goal of developing predictive circuit and fully electromagnetic, fully relativistic, 3D particle-in-cell models of a MITL system. Developing an understanding of current loss will aid in the design of powerful next-generation pulsed power accelerators relevant to DOE missions.

Development of Fast Pulse Intense Neutron Generation Capability by Beam-Target Interaction on Hermes-III for Radiation Effects Testing

200267 | Year 2 of 3

Principal Investigator: T. J. Renk

This project, if successful, will result in a key addition to radiation effects testing, a source of high energy pulsed neutrons based on beam-target interaction on Sandia's HERMES III radiation test facility. Understanding circuit effects resulting from such a pulsed neutron flux should result in increased reliability of the US nuclear stockpile to respond to adversary threats.

High-Energy X-Ray Detectors using Fast, High-Z Semiconductors

200271 | Year 2 of 3

Principal Investigator: D. K. Serkland

This project combines radiation physics theory, materials science studies, and electro-optic device engineering to develop high-speed compound-semiconductor high-energy x-ray detectors. These new x-ray detectors will benefit national security by enabling high-fidelity measurements of time-dependent photon spatial distributions and power history for radiation effects science and inertial confinement fusion experiments.

Illumination of Damage with High-Strength Alloys in Abnormal Mechanical Environments

200174 | Year 2 of 3

Principal Investigator: M. Hudspeth

This project will illuminate fundamental failure behavior of both solid and distended media experimentally subjected to extreme states of dynamic loading. This work will provide enhanced understanding of these failure phenomena that will be incorporated into continuum and mesoscale modelling environments utilized in national security applications such as protective armor materials, explosives, and weapon system design.

Modeling Low Density Plasma in Electrode/Target Systems for High Current Pulsed Power

209287 | Year 1 of 3

Principal Investigator: M. Martin

This project will develop next-generation advanced plasma simulation codes that will have a transformative impact on the development of pulsed power inertial fusion target design and our understanding of the power flow on our current and future pulsed power drivers. We will overcome known limitations in our existing simulation codes by implementing more descriptive plasma models and creating new algorithms to allow for the first-time efficient simulation of the fully coupled pulsed power driver and fusion target behavior in all three dimensions. This will lead to advances in fusion target behavior and more efficient pulsed power designs.

Polynomial Chaos Methods in Xyce for Embedded Uncertainty Quantification Circuit Analysis

200265 | Year 2 of 3

Principal Investigator: E. R. Keiter

This project will develop embedded uncertainty quantification approaches based on intrusive polynomial chaos expansions in the Xyce circuit simulator. These nonsampling-based approaches will allow for a more scalable, verifiable, accurate, and computationally efficient uncertainty quantification analysis for circuit simulation. This will improve confidence in Xyce qualification evidence and will benefit various nuclear weapon programs.

Prediction and Design of Nonlinear Systems and their Emergent Behavior

200275 | Year 2 of 3

Principal Investigator: M. E. Glinsky

This project will develop models of turbulent mix and self organization (through the novel application of a state-of-the-art mathematical transformation) to more confidently model the evolution of complex, nonlinear systems. The project will also revolutionize data analysis and code verification, providing quantitative metrics to compare both simulated and experimental images of complex multiscale systems, impacting the design and computational verification of our nation's nuclear stockpile.

Single Event Effects in Sandia's Semiconductor Devices and Acceptance Testing in Integrated Circuits

200264 | Year 2 of 3

Principal Investigator: J. Black

The Single Event Effect (SEE) project made significant achievements towards its ultimate goal in FY 2018. A comprehensive technology computer-aided design (TCAD) simulation campaign of complementary metal-oxide-semiconductor (CMOS7) sequential circuit transistors led to the creation of Monte Carlo Radiative Energy Deposition (MRED) models. These models were able to reproduce existing SEE test data (heavy ion and neutron) from those same circuits. The work identified several interesting areas of study and led to four submissions for conference presentations and publications.

Stochastic Shock in Advanced Materials

200268 | Year 2 of 3

Principal Investigator: N. W. Moore

This project will develop new fundamental mechanistic understanding, experimental characterization, and modeling capabilities to explain shock generation, propagation, and failure in stochastic media (e.g., flame-sprayed metal films) that are porous and highly anisotropic. This will enable tailored design and science-based qualification of these and potentially other new additively manufactured materials with properties optimized for a wide range of defense applications.

Testing Effects of 14 MeV Neutrons on Materials and Devices at the Sandia Ion Beam Laboratory

209290 | Year 1 of 2

Principal Investigator: W. R. Wampler

The goals of this project are to optimize the design and operation of tritide targets used to produce 14 MeV neutrons, elucidate the underlying material science determining target lifetime, and establish the feasibility of testing response of electronic devices to 14 MeV neutrons at the Sandia Ion Beam Laboratory (IBL) for qualification of nuclear weapon survivability in hostile radiation environments. Results from the first year exceeded all milestones and validated the proposed model for predicting target lifetime. Neutron production now exceeds $2x10^{15}$ neutrons per target. The new capability is being used to test response of electronics to 14 MeV neutrons.

Time-Resolved X-Ray Diffraction Measurements on Laser-Compressed Polycrystalline Samples using a Multi-Pulse, Short-Pulse Laser Generated X-Ray Source

191235 | Year 3 of 3

Principal Investigator: M. Schollmeier

This project investigated whether material properties are different in nanosecond-scale compression compared to static compression. Two laser pulses were used to dynamically compress samples and to generate an x-ray source for x-ray diffraction measurements on these samples. These measurements provided data to benchmark atomic scale modeling of dynamic phase transitions, which is a key contribution to the advancement of predictive capability. These capabilities could benefit the NNSA's nuclear security mission.

RADIATION EFFECTS AND HIGH ENERGY DENSITY SCIENCES

Towards Multi-Fluid Multi-Physics Continuum Plasma Simulation for Modeling Magnetically Driven Experiments on Z

200276 | Year 2 of 3

Principal Investigator: J. N. Shadid

Our goal is the development of a unique, robust, and accurate implicit/explicit computational approach for continuum multifluid multiphysics shock-hydro electromagnetic plasma modeling for fast waves and moderate-to-high density plasmas, enabling longer-time-scale simulations for pulsed power applications. This capability is not only critical as a continuum model, but is also foundational for multiscale kinetic-continuum models for coupling of kinetic/particle in cell (PIC) and continuum/fluid scales.

ADVANCED SCIENCE AND TECHNOLOGY

The Advanced Science and Technology (AST) LDRD Investment Area (IA) invests in Sandia's expertise to advance the science of the possible for science and engineering applications addressing national security missions (including energy) that are *beyond the strategic horizons of Sandia's other mission portfolios. LDRD funding is used to mature scientific concepts* relevant to the needs of DOE's Office of Science (SC); *develop differentiating capabilities* that can be used to advance the impact SC investments have at Sandia; and *deepen the intellectual impact* and reputation of current Sandia Principal Investigators.

A Fundamental Study on the Physicochemical Process of Soot Particle Inception
Project 191017, PI: Scott A. Skeen

Modern engine designers rely heavily on computational fluid dynamics (CFD) codes to optimize piston bowl geometries and in-cylinder flows, among other things, to maximize fuel efficiency and minimize pollutant emissions. Predictive soot modeling over a range of design configurations is key to the development of advanced, clean engine designs; however, the use of oversimplified, non-physical soot models often leads to incorrect results when compared to designs selected for prototyping. Identification of species associated with the nucleation of incipient soot and the physicochemical process by which this occurs represent the greatest knowledge gap preventing the development of more accurate soot models.

Work conducted on this project has led to the development of new scientific capabilities enabling the identification of macromolecules associated with the soot nucleation event and novel experimental techniques developed to characterize soot formation at engine relevant pressures for a variety of fuels and under previously unexplored pyrolytic conditions. The data have led to new discoveries including measurements and modeling of coronene binding energies, the first experimental imaging of low-pressure soot nuclei with atomic resolution, confirmation of the existence of aliphatically-bridged aromatics as soot precursors, the ruling out of soot nucleation by pyrene dimerization (a widely used method in soot modeling), and the identification of a pressure-invariant soot onset temperature. As cost-efficient development of advanced engines is expected to rely heavily on predictive engine simulations, these discoveries represent critical steps toward establishing the necessary predictive soot modeling capabilities.
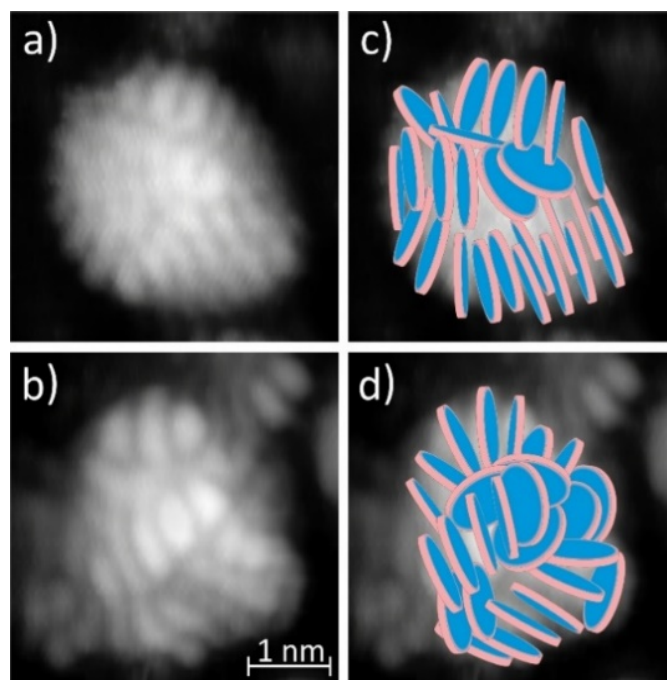
Internal structure of 3D coronene aggregates. a) and b) Detailed scanning tunneling microscope images of individual 3D coronene aggregates, c) and d) Estimated internal structure of these aggregates, deduced from the ripples seen in a) and b). In these schematics, each coronene molecule is represented by a blue/pink disk with a diameter of 1 nm.

PROJECTS

A Fundamental Study on the Physicochemical Process of Soot Particle Inception

191017 | Year 3 of 3

Principal Investigator: S. A. Skeen

This project developed new scientific capabilities toward the identification of the macromolecules associated with the soot nucleation event and established novel experimental techniques to characterize soot formation at engine-relevant pressures for a variety of fuels and under previously unexplored pyrolytic conditions. The data led to new discoveries including the confirmation of aliphatically bridged aromatics, the ruling out of soot nucleation by pyrene dimerization (a widely used method in soot modeling), and the identification of a pressure-invariant soot onset temperature. These discoveries represent critical steps toward establishing predictive soot modeling capabilities for the design of advanced engines.

Deciphering Atmospheric Ice Nucleation using Molecular-Scale Microscopy

200149 | Year 2 of 3

Principal Investigator: K. Thurmer

This project develops and applies nanoscale-microscopy procedures to provide a realistic understanding of ice nucleation in Earth's atmosphere, which affects the climate via precipitation and cloud albedo. This novel insight into key steps of ice nucleation under atmospheric conditions informs an improved parametrization of a global climate model (Energy Exascale Earth System Model/E3SM, formerly Accelerated Climate Modeling for Energy/ACME), advancing our nation's capability to predict the evolution of Earth's atmosphere.

Exploring Fundamental Limitations of Manganese Oxide Cathodes for Reversible Zn/MnO2 Batteries

200168 | Year 2 of 3

Principal Investigator: T. N. Lambert

This project is developing new fundamental mechanistic understanding, experimental synthesis, characterization, and computer modeling capabilities in order to understand the chemical and physical changes that occur when cycling zinc-manganese oxide batteries in alkaline electrolyte. Additionally, we will develop new materials with improved performance such that new high capacity batteries relevant to grid storage and mobile applications can be realized.

High-Resolution Modeling and Measurements in the Arctic

191055 | Year 3 of 3

Principal Investigator: E. L. Roesler

This project helped close the gap between atmospheric in situ measurements of Arctic boundary-layer clouds via sensors on tethered balloon systems and atmospheric models' representation of these clouds by testing four unique model configurations over multiple resolutions. These prevalent clouds play an important role in the Arctic climate, and improving their representation in climate models will inevitably reduce uncertainty in the Arctic's climate projections, which benefits DOE's energy security missions. As predicted, the project found spatial resolution was a key factor in improving simulated cloud amount. Future work in model physics and retrieval algorithms could reduce model bias of cloud phase partitioning.

Molecular Modeling of Pressure Directed Assembly

211149 | Year 1 of 1

Principal Investigator: G. S. Grest

This project used large scale molecular dynamics simulations to assess the degree of structural control in nanoparticle self-assembly that can be exercised through variation of the self-assembly process, nanoparticle size, and organic ligand length and graft density. The research benefited the design of structured materials for applications in national security, including solar energy, effective ion/electron transporting membranes, and sensors.

Novel Microelectromechanical-System-Enabled Nanofracking of Subsurface Minerals

192762 | Year 3 of 3

Principal Investigator: K. L. Jungjohann

This project pioneered the development of unique instrumentation to quantitatively study the mechanisms of chemical-mechanical fracture in materials by atomic-scale imaging within an environmental cell. Experimental testing from the atomic scale to bulk scale of chemo-mechanical properties of materials in liquid environments determined that layered minerals drastically changed in fracture toughness as a result of the chemical environment, resulting in many fractures under high pH (basic) solutions. The localized corrosion initiation mechanisms of low-carbon steel were determined with nanoscale accuracy and complete identification of the most susceptible microstructural features. This knowledge is relevant to DOE's energy security mission for extraction of natural gas and oil from the subsurface.

DEFENSE NUCLEAR NONPROLIFERATION

Preventing the proliferation of nuclear, chemical, and biological weapons of mass destruction (WMD) and reducing the threat of WMD terrorism around the world are key US national security strategic objectives. The US government must have a strong technical base to meet its nonproliferation, counterproliferation, and counterterrorism responsibilities. As the threat becomes more sophisticated and creative, we must identify effective solutions that mitigate current and future risks. Thus, the Defense Nuclear Nonproliferation Investment Area invests in research and development efforts that advance our ability to meet our vision to deliver innovative engineering solution.

Emulating Genome Security Risks in Realistic Genomics Data Ecosystems
Project 209211, PI: Corey Hudson

This project was taken on to apply cybersecurity techniques to secure genomic systems and prevent broad attacks on genomic data. Genomic systems are large and complex involving numerous pieces of laboratory equipment, large high-performance computers and a variety of software tools. Genomic systems are important and attacks on them would undermine forensic, medical, and agricultural capabilities in the US. Modeling these systems is complex and difficult to do in ways that are realistic. In this project, we used Sandia's LDRD-developed Emulytics™ capabilities to build a reusable platform to model genomic systems. With help from the University of Illinois, we modeled their large-scale genomic facility. The platform is general purpose. It can arbitrarily model other facilities, creating a new genomic security capability that can be applied in a variety of contexts. By modeling our emulated genomic facility in combination with a modeled database server, we explored the possibility of a malicious attacker exploiting this vulnerability to attack a genomic system to change raw data behind a secure firewall, leading to a malicious clinical outcome. This work is in the process of responsible disclosure. We are issuing a patch to the software and providing the community with a description on how to mitigate this problem using best practices. These suggest what steps large governmental genomic database providers should take to provide a more secure environment for genomics.
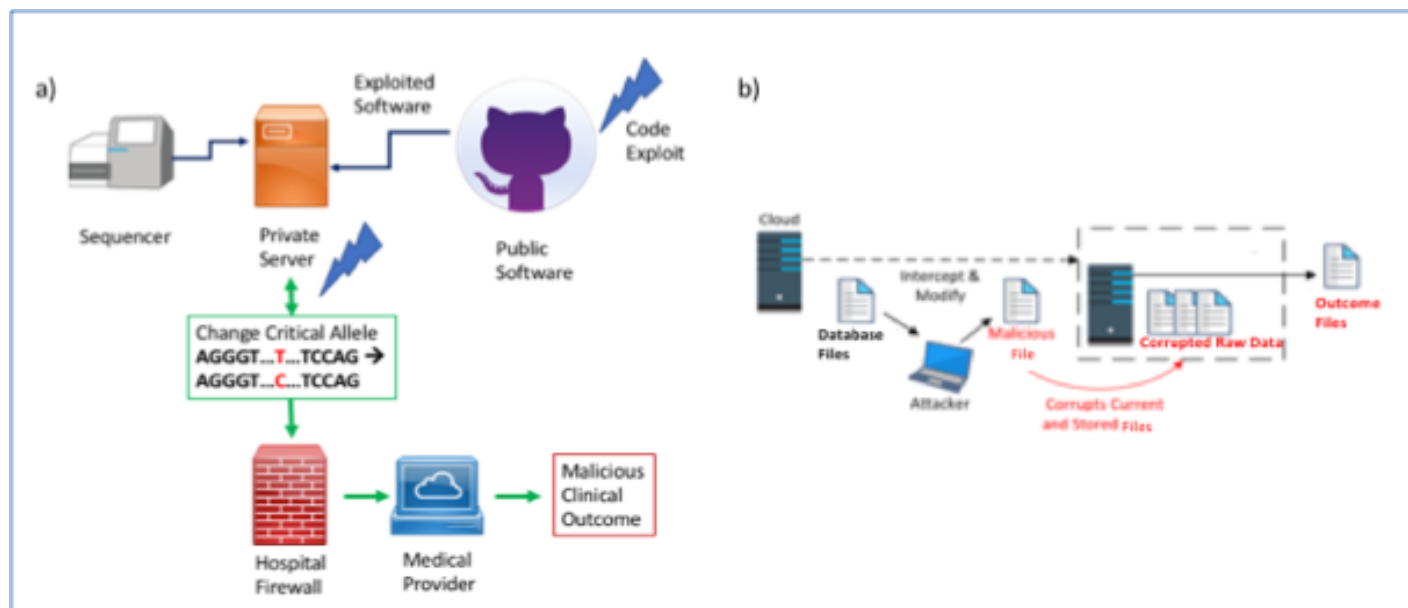
Realistic threat scenarios using Emulytics. a) In this description of a genomic security vulnerability, we define a scenario in which the clinical outcome of a sequencing test is made vulnerable. b) This scenario is modeled using Sandia's Emulytics platform to model a multipart system to discover potential weaknesses in standard processing that create the threat of subversion of clinical outcomes in real genomic environments.

DEFENSE NUCLEAR NONPROLIFERATION

LDRD

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PROJECTS (continued)

3D Printed Waveguide Optics for Transformative Sensors

209206 | Year 1 of 3

Principal Investigator: E. J. Skogen

This project will develop a new method for manufacturing optical waveguides similar to optical fiber using 3D printing. Using this technique, we have demonstrated light pipes that guide light from input to output characterized by optical microscopy and Fabry-Perot cavity optical loss measurements. Using this technology, we plan to demonstrate curved optical waveguides to map a curved surface to a planar one which will allow new camera systems to be realized, enabling new remote sensing systems in support of future national security missions.

A 1V, 1W, 100 GHz Electrooptic Modulator on Silicon for Space Applications

200134 | Year 2 of 3

Principal Investigator: A. L. Lentine

This project will develop and demonstrate the world's highest performance optical modulator using electro-optic materials on silicon. Challenges include optical and semiconductor modeling, optimization of the design, and microsystems fabrication to make devices with repeatable performance predicted from the models. This project provides a solution to a rapidly growing big data national security/DOE mission problem and addresses a technology gap that is not being addressed by industrial vendors.

A Novel Joint Hierarchical Model for Hyper-Spectral Target Prediction

200098 | Year 2 of 2

Principal Investigator: D. Z. Anderson

This project developed new optimization algorithms and software for supervised tensor factorization to better detect and classify hyperspectral signatures. Incorporation of supervisory information into model formulation boosts predictive power, facilitating the use of hyperspectral imagery for a wide range of national security mission applications from target detection to treaty monitoring and verification.

A Parallel Optics Approach to Snapshot Hyperspectral Imaging

209199 | Year 1 of 2

Principal Investigator: D. Bossert

This project will advance the state of the art in hyperspectral imagery by enabling the single frame collection of an entire hyperspectral image data cube at high spatial and spectral resolution. The new capabilities offered by this work exceed what is currently available and will open up proliferation detection and surveillance mission spaces that were previously unrealizable.

Additively Manufactured, Athermal, Broadband, and Light-Weight Optical Telescope

200063 | Year 2 of 3

Principal Investigator: J. Choi

This project will pioneer the development of materials and new processes to additively manufacture lightweight, reflective, optical components using ceramic materials. This project has the potential to reduce the weight, fabrication time, and integration time of reflective optical systems, enabling more agile and resilient optical systems for DOE/NNSA national security missions.

Arming and Firing System Charge State Determination using Unintended Radiated Electromagnetic Emissions (URE)

191150 | Year 3 of 3

Principal Investigator: J. T. Williams

The overarching goal of the project was to develop techniques that allow for the remote detection and automatic classification of the operating states of general arming and firing systems based on their inherent electromagnetic signatures. As part of this effort, the feasibility of remotely detecting low-level "partial discharge" phenomena in charged high-voltage capacitors was also investigated. The results from this research effort have high potential to improve our ability to remotely assess weapons of mass destruction threats and to critically inform stabilization, render safe, and consequence management operations.

Autonomous Detection and Assessment with Moving Sensors (ADAMS): A Foundation for Future Physical Security Systems

209210 | Year 1 of 3

Principal Investigator: S. Buerger

This project will develop foundational intrusion detection and assessment technology for future physical security systems that autonomously optimizes the behavior of dynamic/moving sensors to resolve most alarms without operator attention. This will address several technical issues while also reducing infrastructure costs.

Avalanche Photodiode Arrays for High Dynamic Range Infrared Detection

200137 | Year 2 of 3

Principal Investigator: D. K. Serkland

This project seeks to develop low-noise avalanche photodiodes using novel compound semiconductor materials. If successful, this work will eventually lead to focal plane arrays with improved performance for remote sensing missions and other DOE applications.

Building the World's First Laser Refrigerated Sensor

209200 | Year 1 of 3

Principal Investigator: S. Melgaard

This project seeks to design and build the world's first optically cooled sensor. Optical refrigeration is the only cryogenic solid state refrigeration process in the world. We seek to advance this technology in order to develop a novel, practical solution for cooling sensors in remote sensing. If successful, our technology will be applicable to a variety of domestic and defense applications.

Chip-Scale Nano-Optomechanical Platform for High-Bandwidth, High-Efficiency Radio Frequency Signal Processing

209205 | Year 1 of 3

Principal Investigator: C. M. Reinke

We propose to demonstrate a practical nano-optomechanical radio frequency signal processing platform that offers bandwidth exceeding 100GHz with channel resolution as sharp as 1MHz and size, weight, and power constraints that far exceed what is currently possible with today's electronic systems. If successful, this work will have ground-breaking applications in the fields of electronic warfare and electromagnetic situational awareness.

Cognitive Information Environments for International Safeguards Inspections

200188 | Year 2 of 3

Principal Investigator: Z. N. Gastelum

This project conducts human performance experiments to examine the types, quantity, and mechanism for providing information to support enhanced performance and situational awareness of international safeguards inspectors in the field. It leverages Sandia's expertise in international nuclear safeguards, information platforms, and cognitive science. The outcomes of this research will inform safeguards inspector training, information provision to safeguards inspectors, and if/how advanced information systems should be developed to support international safeguards. Enhancing safeguards inspector performance and situational awareness will support the International Atomic Energy Agency's expanding role in detecting global nuclear proliferation activities.

Efficient Real-Time Cognition at the Point of Sensing

209208 | Year 1 of 3

Principal Investigator: E. A. Shields

This project will demonstrate that machine learning algorithms can operate on signals acquired with compressive sensing systems. Such systems allow information to be collected with fewer measurements than traditional theory dictates, but the data are in a form that requires a computationally intensive reconstruction to put the data into a form a human can interpret. We will demonstrate that machine learning tasks can be performed on the raw data, obviating the reconstruction operation. This new sensing paradigm will enable faster, more efficient automated systems for a wide variety of national security missions.

Electromagnetic (Optical/Radio Frequency) Signatures Associated with Atmospheric Discharges and Plasma Generation in Explosive Events

195868 | Year 3 of 3

Principal Investigator: R. Tang

This project aimed to develop experimental plasma generation and diagnostics methods to increase our understanding of electromagnetic phenomena associated with plasma events, such as in explosive, nonproliferation processes, and nuclear weapon system component breakdown failure. A nanosecond arc discharge served as our surrogate system to investigate radio frequency (RF) and optical characteristics associated with breakdown under various background conditions. Leveraging findings from work in other programs, we explored new techniques for collecting and assessing RF signatures beyond passive detection. These techniques offer the potential ability to detect these events remotely or perform nondestructive sensing using plasma-related signatures. The study also helped mature modeling capabilities through investigation of underlying physics mechanisms.

Engineered Materials for Deactivation of Chemical Agents in Non-Aqueous, Non-Corrosive Environments

200196 | Year 2 of 3

Principal Investigator: D. F. Sava Gallis

This project aims to develop chemistries to degrade organophosphates in water-free environments via an iterative feedback loop between materials synthesis and characterization, with molecular modeling and analytical testing. The fundamental understanding of the relationship between materials structural properties and decontamination activity will improve technology for decontaminating sensitive electronics exposed to chemical warfare agents in national and homeland security applications.

Enhanced Single-Frame Closely Spaced Object Processing

200014 | Year 2 of 2

Principal Investigator: S. M. Anthony

This project developed a robust algorithm that provides a state-of-the-art capability to detect and extract objects beyond the resolution limit of a sensor system from a single image. The resulting algorithm impacts a variety of electro-optical and/or infrared sensing systems, including those used for DOE national security mission areas.

Eyes on the Ground: Visual Verification for On-Site Inspection

191161 | Year 3 of 3

Principal Investigator: R. Brost

This project sought to develop tools to assist an International Atomic Energy Agency inspector when he or she visits a facility. After studying task requirements, we developed a preliminary prototype Inspector's Assistant tool to take 3D measurements of facility equipment and document related semantic information. The resulting data could then be used to help fulfill inspection tasks and communicate inspection data within a 2D and 3D context for localization, relationship identification, and understanding of multi-modality data in context. Once completed and deployed, the proposed Inspector's Assistant would increase inspector efficiency, improve communication between the inspector and International Atomic Energy Agency headquarters, and could increase safeguards assurance.

Implementing Neural Adaptive Filtering in Detection Systems

190993 | Year 3 of 3

Principal Investigator: F. S. Chance

The objective of this project was to develop novel neural-inspired adaptive algorithms, guided by the neural circuitry of the retina, to adaptively filter information at the sensor level. The developed algorithms will enhance the performance of detection systems by allowing them to filter a range of distractor signals, potentially at the sensor-hardware location, leaving more bandwidth for transmitting signals-of-interest. Successful outcomes will apply to DOE/national security remote sensing systems limited by size/weight/power restrictions.

Improving Render Safe Capabilities for National Security from Chemical and Biological Dissemination Devices

191151 | Year 3 of 3

Principal Investigator: A. L. Sanchez

This project addressed informational gaps in chemical/biological dissemination devices, specifically, source term data used by modelers and first responders. Project outcomes advanced experimental data for improved plume modeling performance and render safe techniques, which enabled better predictions for decision makers, decreased time for first responders, and improved consequence management following the release of a weapon of mass destruction.

Inferring Proliferation from Supply Chain Signals

200185 | Year 2 of 3

Principal Investigator: N. J. Brown

This research will advance ideas from supply chain modeling and network analysis to develop modeling methods that use sparse and uncertain signals to characterize and understand proliferation networks. In year one, significant progress was made on network modeling. In year two, an improved approach to probability distribution fitting of temporal data was developed to aid in outlier detection. Year three will focus on combining indicator data with network analysis and outlier detection using Bayesian Belief Networks. If successful, the resulting research could benefit the State Department and DOE in support of arms control verification and nonproliferation.

Information-Theoretic Algorithms to Quantify Genomic Information for Genomic Security

209198 | Year 1 of 2

Principal Investigator: C. Ting

This project will develop new computational methods for identifying higher order dependencies in the genomic sequence that may lead to unintended release of personally identifiable information to an adversary. We will apply machine learning and information theoretic algorithms to simulate an adversarial inference attack scenario and explore how different prioritization schemes for masking the genome affect the prediction ability of the adversary's classifier. We will focus on prioritization schemes based on methods for identifying higher order dependencies. This work addresses national security missions to increase security and to prevent abuse of the rapidly increasing volume of highly personal genomic information.

Microelectronics-Based Neutron and Spectroscopic Gamma Detectors using Compound Semiconductors

209263 | Year 1 of 3

Principal Investigator: G. Pickrell

This project will develop high-efficiency neutron and spectroscopic gamma detectors capable of operating at room temperature. Integration with electronics leads to revolutionary, ultra-low power, imaging arrays for location/characterization of special nuclear materials. This work enables a new sensor class for detection/identification of emerging threats and provides widely distributable, networked detectors for pre/post-detonation scenarios or integration with tags/seals for safeguards and arms control.

Multilayered Solid State Neutron Detector for Nonproliferation Applications

200136 | Year 2 of 2

Principal Investigator: W. C. Rice

This project developed a solid state neutron sensor that uses a stacked multilayer to achieve high efficiencies within a small volume. This sensor will provide an advanced neutron detection capability for a variety of applications such as radiation dose monitoring and control for safety, as well as nuclear material detection in nonproliferation applications for national security.

Neural Inspired Computation Remote Sensing Platform

200106 | Year 2 of 3

Principal Investigator: C. M. Vineyard

This project explores using neural-inspired computation to evaluate, filter, and process remote sensing data at the sensor rather than downstream where the costs (system cost, system volume, system weight, power consumption, and response time) are much higher. Understanding what computational advantages neural-inspired computing can afford for remote sensing will impact our nation's ability to monitor and maintain national security.

Polarimetry for Extended Persistence and Range in Fog for Infrastructure Protection

191184 | Year 3 of 3

Principal Investigator: J. B. Wright

Extending optical capability in numerous scattering environments remains an important subject for research in security and situational awareness scenarios. Using simulation and experiment, this research sought to demonstrate tailored wavelength and polarization selection for increased persistence and range in fog compared to intensity-based techniques. To prove our model, we designed, built, and validated new experimental setups at different wavelengths in Sandia's fog tunnels, which are capable of creating and sustaining controlled fog that can simulate specific fog conditions. The fog tunnel capability enables testing of systems for enhanced performance in degraded visual environments. Our work has shown that circularly polarized light has improved persistence over linearly polarized light in fog.

Polarized Radar for Detection and Automatic Nonvisual Assessment of Unmanned Aerial Systems

200190 | Year 2 of 3

Principal Investigator: J. A. McVay

This technology development project uses polarized radar processing algorithms to differentiate among biological targets, such as birds, weather, and man-made targets (e.g., unmanned aircraft systems (UASs)). The approach studied here makes use of orthogonal polarized radar returns such that processing can be performed that will avoid the false and nuisance alarms caused by birds or other returns that are not UASs, such as weather, and should not be acted against with valuable counter-measure resources. This project makes use of the fact that while targets such as birds and UASs can possess similar radar cross section magnitudes, the responses of these structures can indeed be distinguished.

Shock Tube Measurements of Hot Dense Gas Luminosity and Opacity for Constructing Opacity Tables

209201 | Year 1 of 3

Principal Investigator: J. Wagner

This project will develop new techniques to measure the optical properties, temperature, and density of air and other gases shocked in a "free-piston shock tube" to emulate the conditions in fireballs from conventional explosions. The resulting experimental data could then be used to construct opacity tables for NNSA's computer codes to model fireball optical emission supporting multiple national security applications.

Spiking/Processing Array (SPARR) for Wide Dynamic Range and High Resolution Photonic Sensing

200135 | Year 2 of 3

Principal Investigator: P. Hays

This project will improve national security by strengthening key technologies for remote sensing, detection, and signal processing. Spike-based signal processing embedded in the microelectronic architecture of focal plane arrays will improve sensor dynamic range and effective sample rates while reducing power consumption. The spike-based signal representations connect seamlessly to modern low-power neural-inspired processing and allow low total power systems useful in DOE missions.

The Chemical Composition of Vaporized Ground Materials

200015 | Year 2 of 2

Principal Investigator: D. E. Kittell

The chemical composition of vaporized ground materials was studied in an effort to further improve the equations of state used in conventional and nuclear detonation simulations. This work was focused primarily on Tuff, a geological material composed of silicon, aluminum, iron, and oxygen. Improved Tuff models were exercised in a shock physics hydrocode, where it was determined that a significant amount of the material behavior is dominated by a solid equation of state (rather than vapor); the Tillotson model was extended to approximate the solid/vapor transition on-the-fly. A hypervelocity impact experiment utilizing a three-stage gas gun was also designed to perform model validation.

Ultra-Efficient Sensing System through Holistic Design

209202 | Year 1 of 3

Principal Investigator: G. C. Birch

This project seeks to establish a new paradigm that involves determining what measurements a sensing system needs to make in order for a machine learning or deep learning algorithm to maximize performance, while minimizing the amount of data required to make accurate decisions. We will develop techniques to create a physical optical element that directly collects these optimal measurements and demonstrate an improved sensing system. Development of sensing systems built explicitly for machine interpretability rather than human analysis has a wide range of applications in the creation of advanced autonomous systems, sensing at the edge, and creating low size, weight, and power consuming systems.

Xenon Atom Trap Trace Analysis Enabled by Optical Isotopic Enrichment

200195 | Year 2 of 3

Principal Investigator: T. J. Kulp

This project will develop a new method to allow atom trap trace analysis (ATTA) to be useful for the quantitative analysis of noble gas isotopes whose abundances are extremely low (<1 part in 1013). The method will be accomplished by developing a high-efficiency metastable generator, based on multi-photon laser excitation, that will enhance the counting performance of ATTA by up to four orders of magnitude. If successful, this project could directly benefit the NNSA's nuclear nonproliferation mission.

ENERGY AND HOMELAND SECURITY

The Energy and Homeland Security Investment Area (IA) promotes innovative research and development that strengthens our nation's energy security and resilience, accelerates transformative innovations in the transportation sector, protects our digital and physical critical infrastructure, and reduces our vulnerability to chemical, biological, radiological and nuclear weapons. The IA seeks R&D that leverages Sandia's differentiating capabilities to create opportunities that can be transformational and provide real solutions to the most pressing mission challenges.

Water Treatment System for Resilient Energy Production

Project 191051. PI: Laura Biedermann

Sandia Team Develops Robust Graphene Oxide (GO)/Polymer Desalination Membranes. Water scarcity threatens energy security and exacerbates geopolitical conflict. Desalination membranes enable recycling of scarce water resources and productive use of abundant saline water supplies. Current nanofiltration membranes having polyamide salt rejection layers effectively reject salt ions, yet are prone to biofouling and intolerant to chlorine bleach used in water treatment. Low-fouling, chlorine-tolerant desalination membranes are needed to treat diverse water supplies. Graphene oxide nanosheets offer the necessary chlorine tolerance and have biocidal properties.

Sandia researchers designed and optimized GO/polymer membranes with a focus on durability, scalability, and green chemistry. In these membranes, a laminar GO structure, ~50-150 nm thick, replaces the chlorine-intolerant polyamide layer of conventional desalination membranes. These overlapping GO sheets create a dense network of nanometer-tall channels that permit water flow while blocking salt ion passage. With these GO/polymer-based membranes, filtration of diverse waste waters, including cooling tower water from natural gas fired power plants and simulant waste waters containing contaminates of emerging concerns, was demonstrated. These GO/polymer membranes have sulfate (>97 %) and ibuprofen (>98%) rejections comparable to commercial nanofiltration membranes. A scalable multilayer membrane structure that preserved GO/polymer membrane integrity in month-long tests was developed. First, the laminar GO layers are assembled on porous polymeric ultrafiltration membrane supports. These stiff membrane supports minimize lateral strain that could fracture the GO layers. Uniquely, a siloxane-based adhesion promoter covalently links the first GO layer to the ultrafiltration membrane surface, preventing GO delamination at high operating pressures (up to 650 psi). GO/polymer membranes demonstrated excellent durability, filtering high volumes (10s of liters of test solutions) under flow conditions that simulate spiral-wound membrane operation. The two-stage aqueous chemistry process to assemble these GO/polymer membranes uses techniques compatible with current membrane manufacturing methods.
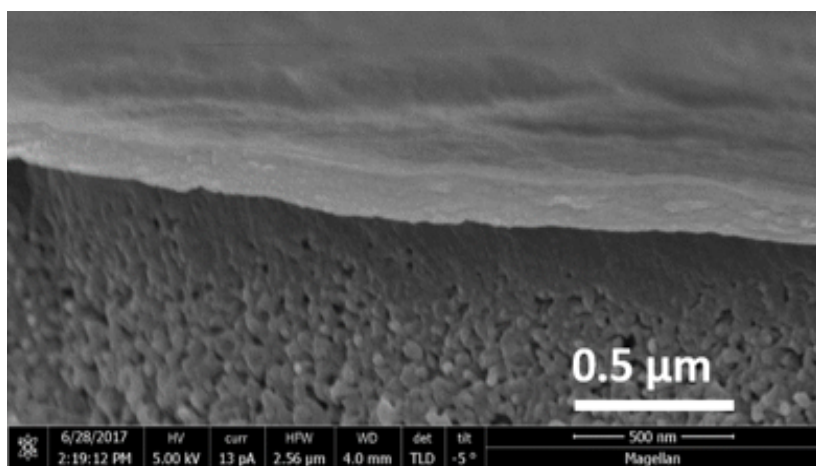
This scanning electron microscope image of a GO/polymer membrane cross-section shows the laminar GO atop the porous ultrafiltration support.

PROJECTS

PROJECTS (continued)

A New Method to Contain Molten Corium in Catastrophic Nuclear Reactor Accidents

200165 | Year 2 of 3

Principal Investigator: D. Louie

This project will develop an injectable new granular sacrificial material system to cool and contain molten corium from release to the environment during a catastrophic nuclear reactor accident. The understanding of the interactions of the new granular sacrificial material and corium surrogate will enable us to develop a new safety feature for both existing and future nuclear reactor plants for the national energy security and sustainability.

A Novel Approach to Foot-and-Mouth Disease Early Detection, Epizootic Surveillance, and Differentiating Infection from Vaccination Status

200193 | Year 2 of 3

Principal Investigator: B. Carson

This project will develop a new method for quickly developing and producing diagnostic reagents for infectious diseases. Specifically, we will identify antibody targets in bovines that allow diagnosis of foot-and-mouth disease virus infection and vaccination status that are specific to virus serotype. We will adapt the reagents we develop to an inexpensive and readily field-deployable test. If successful, this work will benefit the DHS biosecurity mission and provide a platform for rapid, pathogen-agnostic diagnostic development.

A Predictive Model for Arctic Coastal Erosion

209217 | Year 1 of 3

Principal Investigator: D. L. Bull

Accelerating Arctic coastal erosion rates (20 meters per year) have placed existing military detection and warning infrastructure and at least thirty-one Alaskan towns in imminent risk of destruction. This project will deliver a field-validated predictive model of thermo-abrasive erosion for the permafrost Arctic coastline. The event-based projections will provide a quantitative tool for guiding military and civil infrastructure investments.

Applying Biological Immune-System Concepts to Improve Electronic Biosurveillance System Performance

191183 | Year 3 of 3

Principal Investigator: P. D. Finley

This project generated new analytical methods that can improve the ability of national-scale electronic biosurveillance systems to rapidly identify bio attacks and emerging infectious disease outbreaks. By developing and testing state-of-the-art complex systems and artificial intelligence data analytics methods, this project documented possible game-changing improvements in timeliness and specificity of initial alerts for possible bioweapon events or deadly infectious disease outbreaks. As this groundbreaking research is further validated and incorporated into the national defense surveillance systems, the resulting improvements in disease detection are projected to have significant impacts for national security.

Automated Threat Modeling for Cybersecurity Analytics and Emulation

209273 | Year 1 of 3

Principal Investigator: V. Urias

Threat modeling is the first step in developing any security solution. It is necessary to understand the potential vulnerabilities of a system and ultimately inform the quality of any defensive strategy. In short, cyber does not exist in the absence of an adversary. This project has two goals. First, we will develop the capability to generate traffic (both malicious and benign) from a variety of sources that is representative of human actors. Second, we will produce a threat landscape, a mechanism to create, provision, and instrument application layer artifacts for use by generated threat models.

Bio-Inspired Ion-Selective Electrodialysis Membranes

200167 | Year 2 of 3

Principal Investigator: S. Rempe

This project will draw inspiration from biological systems to design advanced, ion-selective membranes for water purification via electrodialysis. Lessons learned from modeling biological systems will be leveraged to design nanostructured, synthetic membranes using a variety of materials chemistry, electrochemistry, and chemical vapor deposition techniques. Superior electrodialysis membranes will enable cost competitive water purification from produced and inland brackish water supplies furthering DOE's goals to reduce the energy and cost requirements of desalination to provide clean and safe water.

Co-Optimization to Integrate Power System Reliability Decisions with Resiliency Decisions

191057 | Year 3 of 3

Principal Investigator: B. J. Pierre

This project developed new models and algorithms for the selection of electrical infrastructure improvements that simultaneously co-optimize reliability and resilience. The project developed five separate optimization models to inform utilities and their stakeholders, DHS, DOE, and policy makers of the best decisions available to improve power system reliability and/or resilience. The five models were tested on Institute of Electrical and Electronics Engineers (IEEE) systems and utility data sets. The five optimization models use stochastic mixed integer programs, generalized dynamic programming techniques, generalize disjunctive programming, and co-optimization techniques to determine the optimal investments to improve power system reliability and/or resilience.

Controlling the Activity of Gene Editing Tools

200186 | Year 2 of 3

Principal Investigator: B. N. Harmon

Inhibitors that block CRISPR (clustered regularly interspaced short palindromic repeats) gene editing activity in vivo could ensure the safety of CRISPR-based gene therapies and provide an antidote in the event of unwanted exposure. This project will leverage Sandia's experience in computational biology, high-throughput screening, and gene editing to develop a pipeline to discover clinically useful inhibitors that block CRISPR-Cas9 activity for use in treatment or prophylaxis when Cas9 containing agents are encountered. The innovative screening technology developed can be extended and used for new natural or synthetic threats, which will significantly advance our capability to detect and mitigate chemical and biological dangers.

Cost-Competitive, Scalable and Safe Grid Storage: Sandia's Radical Ion Flow Battery Technology

210403 | Year 1 of 3

Principal Investigator: J. P. Koplow

This project will investigate the feasibility of the electrochemical half reaction of nitrogen dioxide plus an electron to form the nitrite anion in molten sodium nitrite for low-cost battery-based grid storage. This half reaction is hypothesized to provide very efficient charging/discharging and freedom from side reactions (battery capacity fade). Grid storage is required to address the intermittency problem of photovoltaic solar and wind power. To make exploitation of the nitrogen dioxide to nitrite redox couple practical, this project is also directed towards the development of a new composite sodium electrode structure that addresses the problem catastrophic mechanical failure in prior art sodium electrodes.

Developing Process-Microstructure-Property Correlation of Radiation-Tolerant Nanoporous and Nanostructured Materials for High Irradiation Environments

200150 | Year 2 of 3

Principal Investigator: R. P. Dingreville

This project seeks to develop a novel, integrated capability to design and engineer novel radiation-tolerant and thermally stable materials operating in irradiated and high temperature environments. Optimization of microstructural features to improve their tolerance to radiation effects will be informed through an iterative process combining multiscale modeling and a corresponding suite of experimental techniques to characterize their thermo-mechanical properties under irradiation.

Development of Detection and Mitigation Algorithms for False Data Injection Cyberattacks against Nuclear Facilities

193419 | Year 3 of 3

Principal Investigator: C. Lamb

This project proposed the development of a fundamentally new philosophy for cyber physical defenses, aimed to protect digitally controlled critical infrastructure at the physical process level rather than the levels which are typically protected using information technology defenses. This new defense philosophy introduced a new line of defense, covertly embedded in communication from the digital control system. The project implemented a one-time-pad inspired digital defense via randomly generated signatures hidden within digital control traffic that effectively prove the integrity of marked control traffic. The approach was shown to be effective against sophisticated, simulated cyberattacks against known reactor models.

Distributed Computational Algorithms Focusing on Modeling and Demonstration of Transformer Cyber Resilience

212430 | Year 1 of 2

Principal Investigator: J. P. Eddy

This project will develop fundamentally new topology, experimental characterization, and modeling capabilities for solid state transformers and their impact on the electrical grid, such as prevention of cascaded failures from natural or intentional man-made disruptions through frequency/phase decoupling. Solid state transformers also provide other important benefits, such as power factor correction and voltage support for grid stability and resilience.

Efficient and Scalable Modeling of Nontraditional Devices for Emulytics

200189 | Year 2 of 3

Principal Investigator: D. J. Fritz

This project will advance the state of the art in emulytics by creating a novel Internet-of-Things description, modeling, and emulation capability. The primary focus will be on providing a scalable non-information technology communication framework that can support millions of devices communicating with the physical world and information technology infrastructure. Successful project completion will impact DOE/NNSA missions in national cyber strategy and could also provide benefits to the DHS, DoD, and the intelligence community.

Enhancing Power Plant Safety through Coupling Plant Simulators to Cyber Digital Architecture Model

200152 | Year 2 of 2

Principal Investigator: R. J. Bruneau

This project developed an understanding of how nuclear power plant operators would respond to a cyberattack on the digital controls within the plant. The research utilized a simulated environment for the plant coupled to a nuclear power plant training simulator. Experiments were conducted with licensed operators to understand their perceptions and response to attacks. The pilot experimental run revealed some lessons learned and gained perspective from the operators. Initial indications include insights into targeted false readings which create delayed response on the part of operators and that, for this set of scenarios, the operators were able to keep the plant in a safe condition.

Fundamentals of Pellet-Clad Debonding

191056 | Year 3 of 3

Principal Investigator: R. P. Dingreville

This project enabled a new fundamental mechanistic understanding of the complex degradation mechanisms associated with pellet/clad debonding through the use of a unique suite of in situ nanoscale experiments on surrogate interfaces, multi-modeling, and characterization of decommissioned commercial spent nuclear reactor fuel. Understanding metal/ceramic interfaces' degradation significantly impacted the technical basis related to the safety of high burn-up fuel, a problem of interest to DOE.

In-Cylinder Diagnostics to Overcome Efficiency Barriers in Natural Gas Engines

200166 | Year 2 of 2

Principal Investigator: M. P. Musculus

The objective of this project was to solve national security problems associated with petroleum use, cost, and environmental impacts by enabling more efficient use of natural gas fueled internal combustion engines. A natural gas optical engine facility was built to provide in-cylinder imaging and pressure data on "knock," which is detrimental to fuel efficiency. Chemical-kinetic modeling isolated the role of autoignition chemistry on efficiency. Combustion imaging revealed six categories of knock. Modeling predicted knock well, thereby validating state-of-the-art kinetic mechanisms. The results closed a gap in the science base on the factors that affect efficiency in natural gas engines to enable more fuel-efficient designs.

Innovative Technologies for Optical Detection of Stress Corrosion Cracks

209216 | Year 1 of 1

Principal Investigator: C. R. Bryan

This project developed new algorithms for combining and optimizing camera movements and super-resolution image processing, with the specific goal of developing improved visual corrosion inspection protocols for hazardous or restricted access applications. Potentially of wide applicability, one immediate use for this technology is visual inspection of spent nuclear fuel dry storage canisters for stress corrosion cracks. With that in mind, a camera motion module was developed and mated with a robotic delivery system, and the technology was demonstrated in a mock-up of a spent nuclear fuel storage system.

Integrated Cyber/Physical Resiliency Analysis

212770 | Year 1 of 1

Principal Investigator: L. A. Dawson

This project explored coupling modeling and analysis methods from multiple domains to address complex hybrid (cyber and physical) attacks on mission critical infrastructure. Robust methods to integrate these complex systems are necessary to enable large trade-space exploration including dynamic/evolving threats and mitigations. Reinforcement learning employing deep neural networks (e.g., the AlphaGo Zero solution) was used to identify "best" (or approximately optimal) resilience strategies for operation of a cyber/physical grid model. The machine learning algorithm was made to play itself in a game of 'hurt the grid.' This mod-sim platform relies on a high fidelity, but small, grid model.

Investigating the Chemistry, Physics, Wear and Aging in Rolling Electrical Contact

191053 | Year 3 of 3

Principal Investigator: W. L. Staats, Jr.

Twistact technology comprises a novel rotary electrical contact to eliminate the need for rare earth magnets in wind turbines, making wind energy more competitive and directly contributing to US energy independence. This project demonstrated that Twistact technology provides the required longevity for wind turbine applications and developed a mechanistic understanding of the electro-tribo-chemistry of extended rolling electrical contact.

Networked-Based Cyber Analysis using Deep Packet Inspection (DPI) for High-Speed Networks

209257 | Year 1 of 2

Principal Investigator: B. P. Van Leeuwen

This project will develop new cybersecurity solutions for high-speed networked systems applicable to our nation's computer network systems. The solutions will enhance network intrusion detection systems (NIDS) and enable detection of advanced content-based threats that exploit application vulnerabilities and require deep packet inspection (DPI) for detection of the threat. The solutions will benefit entities that depend on commercial communication infrastructure during emergency or crisis scenarios.

Novel Zoned Wasteforms for High-Priority Radionuclide Waste Streams

200151 | Year 2 of 3

Principal Investigator: C. R. Bryan

This project will develop innovative, zoned wasteforms, based on a rare class of substances (zirconium tungstates and related materials). These wasteforms shrink upon amorphization, with radionuclide-rich cores and barren shells that isolate the radionuclide even when core amorphization due to radiation damage occurs. These wasteforms will provide a critical disposal option for hard-to-handle radioactive waste streams containing technetium or weapons-grade plutonium.

Passive Magnetoelastic Smart Sensors for a Resilient Energy Infrastructure

200169 | Year 2 of 3

Principal Investigator: T. Monson

We are developing a novel, passive, autonomous microsensor for indirect detection of microamp currents at a cost of < $10/sensor, installed. These wireless, magnetoelastic smart sensors can be integrated in close proximity to current-carrying conductors and are capable of detecting small changes in their magnetic field via frequency shifts. These sensors can be used to detect leakage currents, faults, and monitor assets to enhance the resilience of energy infrastructure.

Probiotic, Optimized Strains of Specifically Engineered (POSSE) Bacteria

209218 | Year 1 of 3

Principal Investigator: T. Lane

Developing methodology to mitigate and ultimately prevent predation of algae will increase biomass production, substantially drive down costs for algae culturists, reduce the risk involved with algae cultivation, and ultimately increase biofuel production. This will serve to enhance the energy security of the US by reducing the economic barriers to renewable energy production. The goal of this project is to identify natural products from bacteria that are harmful to algal predators but do not inhibit algal growth, productivity, or survival and that can be used to reduce the frequency of crop failure in algal ponds.

Quantifying Uncertainty in Emulations

200191 | Year 2 of 3

Principal Investigator: J. Crussell

Emulated testbeds aid in our understanding of large-scale cyber systems, yet we have only begun to understand how well they represent the real world and how much we can rely on them to support DOE, DHS, and DoD national security missions. This project aims to discover the usefulness of emulytics for modeling multi-node network phenomena. We will develop a fundamental understanding of the accuracy and limitations of these testbeds.

Rapid Assessment of Autoignition Propensity in Novel Fuels and Blends

209215 | Year 1 of 3

Principal Investigator: L. Sheps

This project will develop a combined experimental and modeling approach to measure autoignition propensity for transportation fuels and fuel blends. This capability will enable efficient screening of existing candidate fuel compounds and create the fundamental knowledge for intelligent design of future fuels and blends, significantly accelerating fuel diversification efforts and the development of fuel-efficient engines.

Rapid Automated Pathogen Identification by Enhanced Ribotyping (RAPIER)

191175 | Year 3 of 3

Principal Investigator: M. Bartsch

This project sought to adapt cutting-edge nanopore sequencing technology to rapid broad-spectrum pathogen diagnostics with potential impact to Sandia missions in biodefense and biosurveillance of emerging infectious diseases. In particular, we developed a novel real-time selective sequencing architecture that we anticipate will dramatically reduce time-to-detection and enhance sensitivity and specificity when identifying and characterizing pathogens in clinical samples.

Water Treatment System for Resilient Energy Production

191051 | Year 3 of 3

Principal Investigator: L. Biedermann

This project developed chlorine-tolerant, fouling-resistant graphene oxide/polymer desalination membranes to reduce the system-level energy cost of desalination and water reuse. In this project, we optimized the porous polymer support and covalent linkage chemistry to develop membranes robust to month-long operation fabricated using green, scalable chemistries. Decreasing the thickness of the salt-rejecting laminar graphene oxide layer increased both clean water permeation and ion rejection. These graphene oxide/polymer membranes effectively reject scale-forming divalent ions when recycling cooling tower blowdown water, decreasing freshwater demands of thermoelectric power plants. Target pesticide and chemical warfare simulants are rejected with 94-98% efficiency. Water reuse technologies may potentially be used to support forward deployed warfighters worldwide.

NATIONAL SECURITY PROGRAMS

The National Security Programs (NSP) Investment Area (IA) delivers advanced science and technology solutions to detect, deter, track, defeat, and defend against threats to our national security. NSP provides trusted, threat-informed pathfinder systems, products, and analysis. The work develops innovative systems, sensors, and technologies for the nation's defense communities. This IA draws upon Sandia's state-of-the-art science, technology, and engineering capabilities through focused investments in three strategic program areas covering cyberspace, innovative technologies and defense products. NSP also focuses on developing leading edge technologies and capabilities to respond to emergent national security challenges.

Creating an Interprocedural, Analyst-Oriented Data Flow Representation for Binary Program Analysis

Project 200071, PIs: Michelle Leger and Karin Butler

Protecting our national computer infrastructure from attackers often requires manual vulnerability analysis and reverse engineering of compiled (binary) computer programs. This analysis is extremely challenging when considering data inputs and data flow. An interdisciplinary Sandia-Georgia Tech team enabled visual analytics for this binary data flow analysis, creating visualizations for representing data flow like that in the example figure. While still complex, these visualizations help human analysts to interact intuitively with data flow, reducing the human time burden for binary vulnerability analysis and reverse engineering. The Sandia team derived visualization requirements by applying human factors techniques to binary analysis, modifying the techniques as needed. By representing the limited number of important data flow primitives and relationships identified in these requirements (see the key in the figure), the team-developed revolutionary user-centric visualizations of data flow. These visualizations enable novel code navigation, information presentation supporting rapid decision-making,
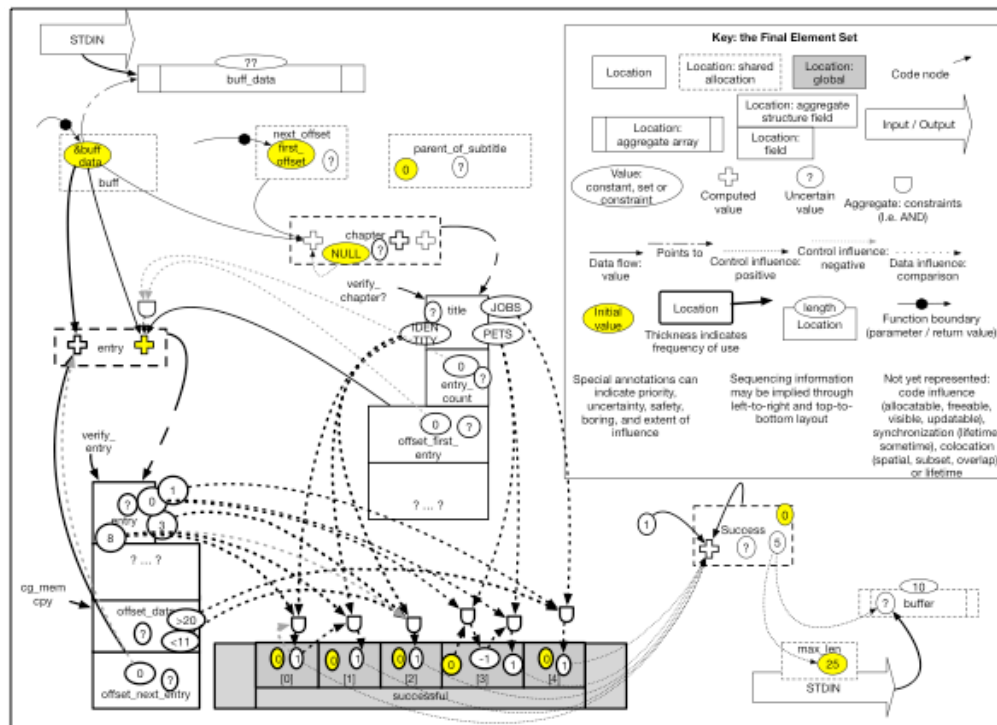
and information sharing between human analysts and automated binary analyses. Georgia Tech collaborators proved out some of these capabilities, creating a proof-of-concept automatic data flow fact generator and a proof-of-concept visualization supporting interactive exploration, annotation, and update of such graphs.

PROJECTS

P R O J E C T S (continued)

Activity Waveforms: Measuring and Comparing the Rhythms of Complex Behaviors

209261 | Year 1 of 3

Principal Investigator: D. J. Stracuzzi

We propose to supplement expert opinion, which frequently forms the basis for activity analysis in nonproliferation missions, with a rigorous statistical analysis of available remote sensing data. Our approach improves the accuracy and sensitivity of activity analysis by characterizing detection uncertainties into a multidimensional time series, and then comparing among current and historical time series to predict future activities.

Advanced Synthetic Aperture Radar Exploitation

200022 | Year 2 of 3

Principal Investigator: R. D. West

We introduced a mathematical framework for discriminating between different types of change within a coherent change detection (CCD) image. We utilized the extra degrees of freedom provided by the elementary scattering physics information from polarimetric synthetic aperture radar (PolSAR) data and PolSAR processing techniques to demonstrate change-type discrimination in CCD images. Many intelligence, surveillance, and reconnaissance missions could benefit from successful completion of this research, which is highly relevant to DOE/DoD missions.

Autonomous Sensor Tasking and Scheduling across Multiple Platforms

209274 | Year 1 of 3

Principal Investigator: J. Richards

The goal of this effort is the development of sensor tasking and scheduling algorithms to enable effective autonomous use of multi-platform, multi-sensor systems. The scope of this research includes not only concepts of operation in which centralized control is possible, but also those in which communication constraints or mission requirements dictate that all tasking and scheduling must happen in a distributed fashion. Successful development of these approaches will fill a critical capability gap, enabling the coordination of platform and sensor resources for emerging autonomy applications in intelligence, surveillance, and reconnaissance (ISR) missions for the warfighter and intelligence community.

Autonomy-Enabled, Real-Time, Rapid Trajectory Generation for Highly Dynamic Hypersonic Missions

211148 | Year 1 of 2

Principal Investigator: M. J. Grant

This project will develop a new fundamental understanding of the interaction between machine learning and classical optimization methodologies that may enable real-time rapid trajectory generation onboard hypersonic flight systems. Understanding this interaction will develop enabling capabilities for autonomous hypersonic vehicles to successfully operate within highly challenging flight environments. This project will create new flight software algorithms that can perform computationally intensive trajectory generation calculations with minimal flight hardware computing resources.

Blockchain Derived Secure Computing

209272 | Year 1 of 3

Principal Investigator: N. D. Pattengale

This project will explore the feasibility of a new approach to garbled computation capable of efficiently and correctly operating, with strong protections against reverse engineering, in hostile/untrusted computer network environments. This work dovetails Sandia's significant history of impactful code obfuscation research, thereby inheriting its myriad applications. Implementing in Ethereum smart contracts is simultaneously challenging and enabling, thus offering compelling risk/reward. The relevance of this project to national security missions is the development of techniques that increase the resiliency of the current cyber environment. Developing tools that cryptographically protect sensitive operations from malicious tampering can be used to protect critical infrastructure, as well as other sectors dependent upon cyber.

Broadband Extremely Low-Profile Antennas

200067 | Year 2 of 3

Principal Investigator: G. D. Wainwright

At low frequencies, physical antenna heights can be large (e.g., 2.5 meters for a monopole at 30MHz). The proposed antenna will replace these monopoles and reduce the height to mere inches instead of meters. An expected impact, among others, is that communication system antennas will be less apparent physically, which would enable new national security missions or capabilities.

CAPS (Configurable Additive Packaging Solutions)

210650 | Year 1 of 1

Principal Investigator: A. Cook

Advanced packaging solutions may be required to support integration of electronics components with device level assemblies. By combining high resolution printing techniques with ink-based pattering processes, a configurable additive packaging solution (CAPS) was established. Once matured, this capability will support prototyping and low volume delivery of specialized functional hardware.

Clandestine Facility Detection and Characterization with a Compact Low-Power Chemical Detector

200114 | Year 2 of 3

Principal Investigator: M. P. Siegal

This project will develop/demonstrate a method to indicate the presence of nuclear production activities via a miniaturized, low-power, high-fidelity passive sensor technology for specific byproduct fission gas detection by combining Sandia-developed, US-patented nanoarray electrochemical sensors with highly selective materials that preconcentrate specific ions/gases to yield part-per-billion level detections. This proposed technology represents a nuclear materials detection breakthrough for sensitivity and minimization of false positives.

Convolutional Scattering Networks for Autonomy

209256 | Year 1 of 3

Principal Investigator: M. W. Koch

This project will create foundational work for extending the convolutional neural network (CNN) architecture to solving problems in national security. Our approach will take advantage of their unique structure, but improve their weakness to spoofing and requiring large annotated data sets for training. We will demonstrate this with a CNN solution to a problem in synthetic aperture radar target recognition.

Creating Automatic Information Theoretic Analysis to Assist in Reverse Engineering Binary Image Formats

209298 | Year 1 of 2

Principal Investigator: T. L. Bauer

We propose to significantly reduce the latency and human time burden in reverse engineering the structure of unknown binary data such as firmware images. We will do this by developing algorithms that leverage statistical data compression measures to automatically discover structural components. These algorithms will be built and tested with the assistance of reverse engineers who would benefit from them. Reducing the latency and human time burden in reverse engineering would improve the ability to evaluate and protect our critical information systems.

Creating an Interprocedural Analyst-Oriented Data Flow Representation for Binary Program Analysis

200071 | Year 2 of 2

Principal Investigator: M. A. Leger

Our goal was to significantly reduce the human time burden for binary vulnerability analysis (reverse engineering) by allowing humans to intuitively interact with data flow in static binaries. We used human factors techniques to design visual representation requirements, resulting in two primary accomplishments: a revolutionary user-centric representation of data flow and a new human factors method for achieving consensus about mental models across diverse tasks. Representations implementing our requirements should enable novel: 1) code navigation, 2) information presentation supporting rapid decision making, and 3) information sharing between human analysts and automated binary analyses, addressing national security missions to protect information systems by dramatically increasing the efficacy of binary analysts.

Cryogenic Ingress and Egress of Optical Signals for Cyber

200145 | Year 2 of 2

Principal Investigator: C. DeRose

This project successfully developed a new understanding of optoelectronic device physics of low energy ingress and egress of optical signals in a cryogenic environment. New multiphysics models were developed and validated by experimental characterization of silicon photonic modulators and detectors at cryogenic temperatures.

Diagnosing and Destroying Non-Markovian Noise in Qubits

209266 | Year 1 of 3

Principal Investigator: K. Young

Quantum computing is an essential pillar of the nation's next-generation cybersecurity. Quantum systems, however, are plagued by often unidentified but pervasive time-dependent noise. This project develops and deploys tools to detect and eliminate this noise. Success in this project will deliver a unique, world-leading, essential capability at Sandia for characterizing, diagnosing, and improving as-built qubits.

Diversity for Microelectronics Lifecycle Security

200147 | Year 2 of 2

Principal Investigator: J. Hamlet

We identified and analyzed several architectures for incorporating implementation diversity in microelectronic circuits. We studied the impact of the architectures on attacker's probability of successfully attacking the circuit, as well as the area and performance penalties incurred to implement each of the architectures. We also identified a general approach for selectively modifying circuit designs to eliminate or randomize portions of the circuit that are not required to implement the circuit's intended functionality. Such unnecessary circuitry can result from hardware trojans, design errors, or from the use of configurable intellectual property cores. We demonstrated the effectiveness of this approach by implementing it and testing it on a collection of trojan benchmarks.

Donor Quantum-Dot Four-Qubit Assessment Platform

200143 | Year 2 of 2

Principal Investigator: M. S. Carroll

This project developed new quantum bits in a form, which is compatible with metal oxide semiconductor transistors. The ability to integrate quantum information systems with classical silicon electronics has the potential for significant impacts to quantum information processing, quantum sensing, and cybersecurity.

Enabling Atomic Layer Precision during Circuit Edit and Global Back-Side Ultra-Thinning: A Path to Improved Failure Analysis of State-of-the-Art Microelectronic Devices

209271 | Year 1 of 3

Principal Investigator: R. J. Shul

Shrinking semiconductor device nodes have far surpassed the ability of conventional failure analysis (FA) techniques to reliably analyze device failures and preform circuit edits (CEs). Development of atomic layer etching (ALE), material removal with atomic layer precision, will provide the ultimate FA tool not only for current state-of-the-art devices but potentially for Si-based microelectronics. This work will enhance Sandia's role as a leader in FA activities and enable FA of emerging, sub-14 nm devices that will become essential to a variety of national security applications. Processes developed here will accelerate the qualification and testing of such devices and attract new customers.

Enabling Novel, Game-Changing Radar Sensing via Ultra-Wideband Polarimetry

200060 | Year 2 of 3

Principal Investigator: B. H. Strassner, II

The goal is to design a planar, lightweight, dual-polarized antenna array. The array should provide 3 GHz of instantaneous bandwidth in Ku-band, cross-polarization levels of about 30 dB, and port-to-port isolations at around 30 dB. The polarimetric antenna will provide radiation characteristics that will enable novel modalities such as maritime imaging, coherent change detection in high-clutter environments, and foliage-penetration algorithm development relevant to DoD defense and DOE energy security missions.

Entity Resolution at Large Scale: Benchmarking and Algorithmics

200105 | Year 2 of 2

Principal Investigator: J. W. Berry

This project addressed "Entity Resolution," a collection of problems shared by many data analysis problems at DOE and its customers. References (such as names, electronic addresses, etc.) to entities (such as people, computers, concepts) in mission data are observed, and these references must be mapped to the underlying entities before analysis can proceed. We worked with top academics to develop unclassified algorithms, software, and benchmarks for entity resolution. The final status as of project completion was a set of guidelines for evaluating the quality of solutions provided by entity resolution algorithms. A notion of recall was completed; a notion of precision was in development.

Event Correlation using Spatio-Temporal Point Processes

196390 | Year 3 of 3

Principal Investigator: J. D. Tucker

This project developed new theoretical statistical modeling in spatio-temporal point processes in which the observations contained missing data. By extending spatio-temporal point process methodologies to develop inferences about the correlation of events in both space and time, one can provide a more complete and nuanced picture to the analyst in near-real time for intelligence and surveillance applications.

Exploring the Effects of Silicon Ultra Thinning on Integrated Circuit Behavior

200016 | Year 2 of 2

Principal Investigator: C. R. Friedman

Silicon ultra thinning is an emerging capability that has the potential to enhance spatial resolution of laser-based failure analysis techniques. This project developed a deeper understanding of the effects of ultra thinning on circuit behavior that is necessary for the success of the failure analysis approaches. This project also developed modeling tools and experimental practices that can be applied to future projects. This supported our nation's cross-cutting microelectronics work in both research and fielded technologies for DOE/NNSA missions.

Extreme Power Radio Frequency Amplifiers

200138 | Year 2 of 3

Principal Investigator: P. D. Coleman

The fundamental goal of this work is to demonstrate the feasibility of gigawatt class high-power amplifiers capable of radiating complex "smart" waveforms. Successful demonstration of this new amplifier capability would greatly expand the options available for reducing global nuclear security threats and securing cyberspace. This will position Sandia as a leader in providing revolutionary high-powered electromagnetic capability to the nation.

Generative Models for Synthetic Aperture Radar Target Synthesis

210570 | Year 1 of 1

Principal Investigator: J. J. Coon

This project explored generating statistically and visually realistic synthetic aperture radar (SAR) data for difficult and denied targets by training a generative adversarial network (GAN) to generate SAR imagery from a small number of input images. It is anticipated that this work will impact DoD and intelligence-gathering communities.

Geospatially Aware System of Systems Decision Capability

200140 | Year 2 of 3

Principal Investigator: H. D. Le

This project will develop a new capability to integrate discrete event stochastic simulation with geospatial information system databases to aid military decision makers. These hybrid simulations will allow assessments of locations, logistics, and national security missions while streamlining the model-building process by using existing databases to pre-populate key data and eliminate the need to convert spatial information into time-based representations.

Highly Sensitive Atomic Electrometry for Noninvasively Detecting and Diagnosing Electronics

200194 | Year 2 of 3

Principal Investigator: Y. Jau

This project aims to understand the foundations for realizing ultrasensitive atomic electrometry to improve electric-field sensing technology, which is highly significant for nuclear security missions. Atomic metrology has demonstrated the best performance in time keeping, magnetic-field sensing, measurements of acceleration and rotation, etc. We propose to conduct relevant modeling work, computer simulations, and experiments to develop atomic electrometry based on atomic vapor systems to detect electric-field signals from static to MHz frequency with sensitivity beyond the other existing technology.

Improved Industrial Control Systems Resilience through Automated Detection and Response

206861 | Year 2 of 3

Principal Investigator: J. M. Henry

This project will investigate indicators of cyber events and subsequent autonomous reactions to improve industrial control system (ICS) resilience. This technology will enable automated detection and responses, providing situational awareness and autonomous adaptation for cyber conditions. ICS device intrinsic security is weak, so newly developed indicators and autonomous reactions will improve critical infrastructure resilience which is imperative to US national security.

Improved Mobile Device Positioning via Contextual Awareness

200020 | Year 2 of 3

Principal Investigator: A. J. Patterson

Given a relative trajectory with associated activities, we sought to establish an absolute geolocation by matching features extracted from the trajectory with those in a contextual database (e.g., OpenStreetMaps, light detection and ranging (LiDAR), building floor plans). This provided a new analysis technique that enhanced situational awareness in support of US nuclear (NNSA) and national security (DoD/intelligence community) missions.

Language-Independent Software Analysis

209269 | Year 1 of 3

Principal Investigator: D. P. Ghormley

Historically, automated software analyses intermingle mission and target language dependencies throughout their code, making re-use of components for different mission question or different target languages impractical. This project will answer the question of how real-world, mission-relevant, static software analyses can be designed and constructed in a language-independent fashion, dramatically increasing the reusability of software analysis investments. Activities this year focused on investigating the feasibility of the approach by examining specific features of dynamic languages (which we envision to be the most challenging) including JavaScript and Python.

Latent, Passive, Low-Energy X-Ray Exposure Indicator

199992 | Year 2 of 2

Principal Investigator: L. Biedermann

This project developed unique optical sensing capabilities based on coupled optical and chemical amplification to indicate if an object has been x-ray interrogated. These x-ray sensors comprised alternating active and inert layers in an all-polymeric Bragg crystal. We evaluated the optical sensitivity, thermal stability, and processing conditions for a variety of polymer formulations containing chemically active photoresists blended with iodonium-based photoacid generators (PAGs). The greatest optical sensitivity was achieved with PAGs that released a strong triflic acid upon exposure. Three Bragg crystal fabrication methods were evaluated. Tape-cast block copolymer films showed the greatest reflectance change following optical exposure and thermal development.

Mitigating Charge Carrier Generation in Silicon to Enhance Backside Laser Failure Analysis

203539 | Year 2 of 2

Principal Investigator: C. R. Friedman

This project developed a technique to enhance failure analysis (FA) capabilities by minimizing the impact of undesired electrical signals in backside laser-based FA approaches such as light-induced voltage alteration. The outcome of this project is an improved ability to detect opens and other types of failures. This work benefits a broad set of national security sponsors by expanding microelectronics hardware capabilities and developing critical technical understanding of the physics that governs various laser-based FA approaches.

Mitigation of Cyber Proliferation

200113 | Year 2 of 2

Principal Investigator: S. Elliott

This project developed technologies to understand the size, scope, and content of darknets and enable mitigation of cyber weapon proliferation in this space. The tools and techniques developed enable DOE/NNSA and other government agencies to curb the proliferation of malicious cyber tools and exploits.

Motion and Trajectory Algorithms for Visual Information Foraging in Intelligence Analysis Workflows

193424 | Year 3 of 3

Principal Investigator: L. A. McNamara

Eye tracking systems are not designed for capturing data about how people interact with information in real-world environments. This project developed a prototype system to collect and analyze gaze data in user-driven dynamic workflows. Products included algorithms and analysis techniques to explore the feasibility of capturing and automatically associating eye tracking data with geospatial content in a dynamic visual search task. We demonstrated the feasibility of automatically capturing, associating, and expressing gaze events in terms of geospatial image coordinates, even as the human "analyst" was given complete freedom to manipulate the stimulus image.

Multimodal Data Integration under Uncertainty

190991 | Year 3 of 3

Principal Investigator: D. J. Stracuzzi

This project developed methods for estimating the uncertainty associated with predictions made by machine learning and statistical models, focusing specifically on evaluating the uncertainty due to the measured observations and model structure. An important goal of the project was to provide information not available through traditional methods to model developers and national security decision makers. Results included demonstrations on imagery analysis, including integration of data from multiple sensor types, cybersecurity, and seismic data analysis. Many specific applications have been identified to benefit national security mission spaces, including defense, intelligence, homeland security, and the nuclear weapons life cycle.

Novel Approach for Uniform, Localized Die Thinning

200066 | Year 2 of 2

Principal Investigator: D. P. Adams

This project has utilized predictive finite element thermal model simulations, experimental studies of laser-solid interactions, and advanced microstructure characterization to identify novel laser etching methods that uniformly thin semiconductor substrates. The developed techniques should enable improved failure analysis of integrated circuits.

Persistent Tracking of Dismounts by Multichannel Radar

200065 | Year 2 of 3

Principal Investigator: D. L. Bickel

The purpose of this project is to develop a capability to track high value dismounts in all weather conditions using a radar system. This work extends previous work done for tracking high value vehicles. Successful completion of this research will lead to an important capability relevant to DOE intelligence, surveillance, and reconnaissance-related activities.

Predictable Lifetime Devices

209270 | Year 1 of 3

Principal Investigator: B. J. Kaehr

This project will develop humidity-sensitive electronic materials that can be integrated into devices to provide autonomous on/off functions in a predictable manner. This effort will deliver a key element that will advance the broader grand challenge for national security to design and develop components that function autonomously in response to environmental cues.

Random Laser Physical Unclonable Function

210212 | Year 1 of 1

Principal Investigator: D. Scrymgeour

We began basic research using an optical physical unclonable function (PUF) based on a random laser implementation. We grew multiple thin films for optical characterization and random lasing demonstrations. This new laser PUF concept will circumvent vulnerabilities in existing optical PUF designs. We made progress toward demonstrating and analyzing the technology which will enable a more secure optical PUF implementation for trusted systems that enable standoff authenticity/integrity checks and counterfeit detection.

Rapid Abstraction in Confined Environments (RACE)

200070 | Year 2 of 3

Principal Investigator: S. Buerger

This project will develop a perception capability to rapidly produce abstract representations of sensed objects, described both geometrically and semantically, to facilitate autonomous mission execution by unmanned systems in confined environments. This work will develop new multiphysics classification methods for perception with sparse training data; it will pioneer the active control of sensors to "close the loop" around classification uncertainty and provide key future technology to support NNSA missions.

Scalable, Targeted Code Analysis using API Abstraction

200059 | Year 2 of 2

Principal Investigator: D. Bueno

This project investigated abstraction as a means to prove that software behaves safely. Reduced-fidelity (abstracted) models of software enabled faster and more scalable algorithms. The goal of the project was to increase the speed of tasks, such as automated interface analysis and network protocol analysis through a novel approach to reasoning about computer programs. Automated software analysis is the new frontier of software assurance research for DOE missions.

Semi-Autonomous Methods for Rapid Prototyping of Software Defined Radio Frequency Counter-Unmanned Aerial System Techniques

209262 | Year 1 of 3

Principal Investigator: J. A. Gilbert

This project will demonstrate that advanced Counter-Unmanned Aerial Systems (CUAS) radio frequency (RF) effects need not be limited to the current static library-based models, and that required skilled operator input can be reduced. This is a significant advancement in the CUAS RF effect domain and enhances posture for these capabilities to be leveraged for critical asset/force protection applications.

Single Chip MEMS Ultrasonic Imaging System

209264 | Year 1 of 3

Principal Investigator: R. W. Reger

This project will develop fundamental acoustic modeling and experimental characterization to explore coupling of piezoelectric micromachined ultrasonic transducers (PMUT) to materials of varying acoustic impedance–from human tissue to structural materials. This project aims to create a novel monolithically integrated PMUT array on complementary metal-oxide-semiconductor electronics, enabling deployment of single chips for sub-surface imaging for a variety of national security applications.

Synthetic Aperture Radar Image Formation and Feedback to Navigation Subsystem in Global Position System Denied and Degraded Environments

209267 | Year 1 of 3

Principal Investigator: S. Jenkins

This project will develop method(s) to use synthetic aperture radar (SAR) measurements in aiding inertial navigation systems. The goal is to provide continuous SAR operation in degraded and denied global position system (GPS) environments and to leverage the SAR intelligence, surveillance and reconnaissance (ISR) instrument as an active alternate/aided airborne platform navigation system, for ISR and strike capabilities.

Tools and Techniques for PRESTIGE (PRactical Evaluation and Synthesis of Trust In Government systEms)

201939 | Year 2 of 3

Principal Investigator: B. K. Eames

This project will develop a practical approach to evaluate risk of development-time manipulation of microelectronics-based systems. The approach incorporates visual modeling of development processes and potential attacks against system development, coupled with a game theoretic analysis of attack viability. This quantitative risk assessment will facilitate making informed engineering tradeoff decisions, and reduce attack risk for multiple government programs.

Ultra Low Level Security Introspection of Computer Operating Systems

200069 | Year 2 of 3

Principal Investigator: R. E. Bell

This project will develop new tools to introspect low level x86 security features present in the desktop and server computing hardware that is ubiquitous throughout personal, commercial, and government sector. This project will use the created tools to explore the inner working of these features as well as their implications on the security of the entire system. The development of these tools will increase the understanding of poorly documented and underutilized low-level security features–allowing the Nation to better secure its computer systems. They may also enable the identification and understanding of future threats.

Unpowered, Stackable, Large Area Semiconductor Neutron Detector

209265 | Year 1 of 2

Principal Investigator: S. S. Chou

This project will develop organo-lead halide perovskite materials for neutron detection; in particular, the development of material processes, models and experiments to validate neutron-perovskite interactions within broad energy ranges and doses. If successful, we will have demonstrated the first solution processed, solid-state detector with potentially revolutionary form factors, thus improving our capability for nonproliferation and counter proliferation.

Waveform-Agile Multi-Channel Cognitive Digital Radar for Multi-Mission Intelligence Surveillance and Reconnaissance and Radio-Frequency-Enabled Cyber

200133 | Year 2 of 3

Principal Investigator: H. Loui

This project will develop a multi-mission digital radar architecture that simplifies and modularizes a radar's radio frequency frontend by replacing application-specific analog detection methodology with flexible and programmable digital signal processing. It enables advanced real-time multi-mission sensors that can send/receive/process arbitrary signals with large instantaneous bandwidth using multiple channels. Radars with these capabilities enable smarter sense, analyze, and respond cycles for DOE national security applications. This year, we have successfully obtained real-time digital-detection radar impulse response from a prototype and demonstrated multi-channel synchronization.

NUCLEAR DETERRENCE

Sandia's Nuclear Deterrence (ND) mission is to manage the nation's nuclear weapons stockpile, provide our customers with research, development, and testing services, and manufacture specialized non-nuclear products and components for national defense and security applications. The purpose of the ND Portfolio is to enable safe and secure deterrence through science, engineering, and management excellence. Our Investment Area focuses upon developing cutting-edge revolutionary technologies that enable our mission with maximum potential for eventual deployment. Our prime customer is the NNSA/DOE. Other customers include the Departments of Defense, Homeland Security, and other Federal agencies such as the US Strategic Command. Stakeholders include the Congress of the United States, the American people, the federal, state and local agencies that have regulatory authority over our work, and the communities in which we work.

Targeting a 100X Reduction from Design to Analysis: An Agile Workflow for Stronglink Design

Project 200242, PI: James W. Foulk, III

Sandia researchers demonstrate a 100X reduction in time from design to analysis, by developing an agile workflow for stronglink design. A multi-disciplinary team, consisting of designers, researchers, code developers, and analysts, developed a new analysis workflow with a focus on 10-node composite tetrahedral elements, tetrahedral meshing, and contact. Long-standing barriers to productivity were removed to successfully reduce the time for design iteration by 100X. This was done by relieving engineers from the time-intensive burden of discretization and enabling an iterative process where computation is increasingly integral to design. The new tetrahedral workflow is illustrated on a prototypical assembly containing parts of significant geometric complexity. This work, not only provided the requisite technology, but also a teaming environment among people and products (Sierra/SM, Cubit) to overcome long-standing barriers and achieve a substantial reduction from design to analysis. Since the new analysis workflow was proven on the most geometrically complex components in the stockpile (stronglinks), these accomplishments have the potential to broadly impact the assessment and rapid qualification of components and systems through predictive simulation.
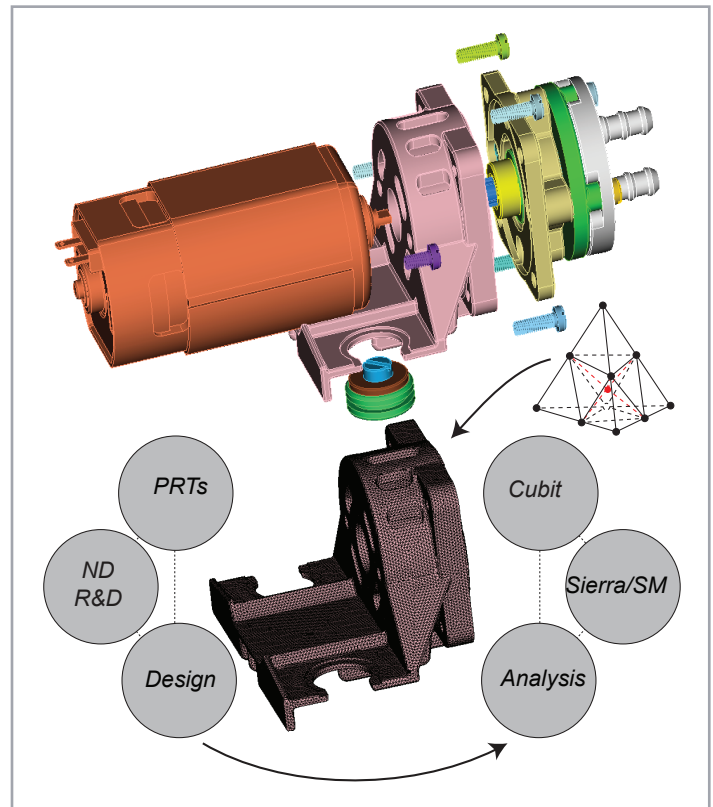
PROJECTS

A Silicon/III-V Photonics Platform for Optical Data Communications and High Functionality Photonics

200257 | Year 2 of 3

Principal Investigator: A. L. Lentine

The goal of this work is to develop a silicon/III-V photonics platform for optical data communications and high functionality photonics. The development of a platform that supports multiple concurrent optical busses with on-board optical processing, reconfigurable routing, and secure communications would have significant impacts to system agility and assurance for numerous national security applications.

AMPPED Components: Advanced Models of the Physics and Phenomena of Electrical Discharge

209241 | Year 1 of 3

Principal Investigator: P. G. Clem

In this project, we are focused on quantifying and modeling coupled plasma-surface feedback phenomena critical to electrical discharge processes. We are developing world-first secondary electron emission measurements of electrodes, photon energy spectra, and ion energy spectra during discharge. The quantities are being used in more advanced models of electrical discharge/breakdown. Physics-based knowledge of the surface role in discharge processes is a required step to enable quantitative design margins, assurance of safety architectures, and implementation of novel materials and technologies for nuclear deterrence, defense, and energy applications that require preventing or controlling electrical discharge.

Additively Manufactured Shock Absorbing Engineered Materials

193407 | Year 3 of 3

Principal Investigator: N. Leathe

This project focused on utilizing additive manufacturing for the development of shock absorbing materials to offer conformal protection in extreme shock events. This capability can facilitate safety enhancements in NNSA systems and in other areas ranging from aerospace and defense to the automotive industry. Additionally, this project furthered the development and calibration of computational models to predict material performance—enabling iterative design prior to product fabrication.

Advanced Positional Awareness Employing Xtremely Cold Atoms (APEX)

200256 | Year 2 of 3

Principal Investigator: G. Biedermann

This project will investigate a new approach to guiding matter waves for precision inertial measurements with atom interferometers. The guiding of matter waves holds promise for improved navigation and positional awareness for future DOE and DoD systems, but the realization has been challenging. By using a combination of theoretical modeling and experimentation, we will explore new techniques for this purpose. Specifically, we are exploring the possibility of guiding matter waves using the evanescent fields of nano-optical structures.

Agile Component Design through Integrated Diagnostics and Computational Optimization

200243 | Year 2 of 3

Principal Investigator: A. Grillet

This project will develop agile design tools for vacuum arc sources through model optimization and experimental discovery of the role of surface adsorbates on the initiation of electrical breakdown. Electrical breakdown is key to the operation of several nuclear weapon components but also a critical failure mechanism for others. The new agile design tools developed will enhance future stockpile modernization programs.

Bridging the Gap: Evaluating Compatibility and Reliability of Interfaces between Additively Manufactured and Conventional Gas Transfer System Components

191227 | Year 3 of 3

Principal Investigator: K. Allen

This project characterized the dynamic interfaces formed between machined additively manufactured (AM) surfaces and conventional hardware following explosive valve actuation and resistance forge welding, two gas transfer system processes with severe sliding contact environments. This characterization has aided in understanding the interactions at interfaces between AM and conventional parts and in assessing AM suitability for nuclear security applications.

Creating Robust and Secure Free-Space Optical Systems for Information and Power Transmission in Confined Environments

191234 | Year 3 of 3

Principal Investigator: P. C. Galambos

Our goal was establishing that the free-space-optics (FSO) transceiver we created worked with the Foundation Bus (FB) communications architecture in challenging environments. This goal was demonstrated by using our prototype FSO transceiver to send/receive FB messages. This impacts national security by demonstrating a robust, modular (no cables/connections), and electrically isolated link between subsystems for applications including nuclear weapons.

Dynamic Strain Aging in Additive Manufactured Alloys and Components

200248 | Year 2 of 3

Principal Investigator: B. R. Antoun

This project will expand the environmental and application space for additive manufactured parts by improving our fundamental understanding of microstructurally driven dynamic strain aging that negatively affects material response and Sandia's ability to model the material behavior correctly. The project will develop temporally extreme measurements and advanced microscopy methods focused on nuclear weapon abnormal environments, used to develop dislocation and physics-based modeling capability that bridges length scales from subgrain to continuum level.

Fabricating Bilayer Resistive Random-Access Memory for a Radiation Hard Nonvolatile Memory

209283 | Year 1 of 2

Principal Investigator: D. R. Hughart

This project will fabricate bilayer resistive random access memory (ReRAM) in order to be used in a radiation hard nonvolatile memory (NVM). A radiation hard NVM is useful for future nuclear deterrence applications like a field-programmable gate array, and has potential benefits like reducing design costs by enabling reprogramming on the fly and mitigating testing costs and risks of using commercial memory.

Fuze Positional Awareness and Jammer Resistance from Radar-Based Terrain Aiding

209284 | Year 1 of 3

Principal Investigator: G. R. Sloan

This project will develop viable, analysis/simulation-validated radar fuzing concepts to implement enhanced positional awareness for improved safety in weapon delivery systems. Specifically, the study will investigate the positional accuracy achievable from advanced altimetry for various terrain and trajectory scenarios. The potential impact is a revolutionary leap forward in weapon situational awareness, enabling significant enhancements in accuracy, safety, and overall system effectiveness.

Intrinsically Radiation Hard, High-Voltage, Solid State Switch

209281 | Year 1 of 3

Principal Investigator: G. Pickrell

This project will demonstrate a wide-bandgap III-Nitride high-voltage, high-current transistor switch prototype. The focus will be on a trench metal-insulator-semiconductor field-effect transistor. Key areas of research include epitaxial materials growth, design and fabrication of the insulating gate, and high-voltage edge termination. If successful, the prototype transistor will serve as a model for high-power switches applicable to NNSA's nuclear deterrence mission.

Investigation of 10-28 nm Commercial Integrated Circuits for use in Nuclear Weapon Radiation Environments

200260 | Year 2 of 3

Principal Investigator: N. A. Dodds

This project will investigate the response of 10-28 nanometer commercial integrated circuits to radiation environments that are of interest for national security applications. These advanced technologies have more processing power than older technology generations, but their reliability in radiation environments is not well understood. Experiments and simulations will characterize their reliability margins and give insight into the radiation-induced failure mechanisms.

Mechanical Communication using Piezoelectric-Magnetoelastic Transducers

201545 | Year 2 of 3

Principal Investigator: I. F. El-Kady

The proposed approach is a novel innovative concept for information transmission across barriers that has never been demonstrated before. Major fabrication and experimentation risks exist pertaining to mechanical impedance matching the actuated signals to the barrier material. First, unique electrical carrying data signals will be transduced into mechanical oscillations via piezoelectric/magnetoelastic actuation. Next, the mechanical signals will propagate through the exclusion barriers with high fidelity. Finally, the transmitted signals will be readout and re-transcribed through magnetoelastic/piezoelectric reverse actuation. Successful demonstration will lead to a new paradigm for safety, where a sensor validates the correct configuration of modules or improper assembly/damage.

Miniature Accelerometers with Sub-Microsecond Timescales for Characterization of Structural Dynamics

209280 | Year 1 of 3

Principal Investigator: K. M. Casper

We will develop integrated chip-scale accelerometers that improve temporal (x100) and spatial (x25) resolution in comparison to current technologies, to increase the accuracy of environmental specifications for weapon components. These sensors could be embedded into a future system for surveillance and monitoring. This technology will enhance our nation's capabilities to design safe and reliable components and provide system assurance.

Modular Optical Bus Fabrication by Additive Manufacturing and Heterogeneous Integration

209282 | Year 1 of 3

Principal Investigator: D. K. Serkland

This project will develop novel additive manufacturing and heterogeneous integration technologies to fabricate millimeter-scale optical transceivers for multichannel fiber optic data communications. Transparent microlenses will be fabricated using high-resolution additive manufacturing processes and printed together with transceiver housings to assure accurate optical alignment.

Multi-Material Additive Manufacturing for Trusted Ceramic Packages with Embedded Capacitors

191232 | Year 3 of 3

Principal Investigator: S. S. Mani

This project developed and investigated methods to fabricate custom multi-material electronic packages that include capacitive, conductive, and insulative materials. Direct write additive manufacturing (AM) using multiple materials offered the ability to create novel structures and apply materials in an atypical fashion onto traditional and nontraditional surfaces and provided significant innovation opportunities for nuclear weapon and other national security applications.

Nanocomposite Films with Tunable Physical Properties as Robust Corrosion Barriers

200241 | Year 2 of 3

Principal Investigator: E. J. Schindelholz

This project will develop a new class of low-cost conformal corrosion barrier coatings via layer-by-layer (LBL) technology with coating architecture adaptable to chemical/physical function requirements. We will test the hypothesis that LBL nanocomposites impart exceptional corrosion resistance through charge transfer and mass transport inhibition. Success will provide an implementable pathway to increase assurance for nuclear stockpile materials and components.

Nondestructive Evaluation for Encapsulated Component Qualification

200254 | Year 2 of 3

Principal Investigator: A. L. Dagel

This project will develop a new nondestructive inspection technique with high sensitivity for low density materials. Foams, fillers, and epoxies serve important roles in preventing critical failure modes in nuclear weapons components due to effects such as thermal fluctuations, shock, or high voltage discharge. This project will enable nondestructive inspection for defects including voids, delamination, and inhomogeneities in these materials.

Rectenna Thermal Power Supply

200245 | Year 2 of 3

Principal Investigator: P. Davids

The purpose of our research is to design, fabricate, and demonstrate a new thermal power supply based on direct rectification of infrared radiation from a thermal source. This new form of radiative thermoelectric transduction represents a radical departure from conductive heat transfer and conversion for thermal power supplies and could dramatically reduce cost, improve safety, and provide an alternative source of power for nuclear weapon applications.

Sandia Heterogeneous Architecture of Disaggregated Electronics (SHADE): Advanced Packaging to Increase Radiation Hardened Capabilities and Trust

209286 | Year 1 of 2

Principal Investigator: C. Michael

This project will design and simulate a compelling future capability to advance the flexible Sandia heterogeneous architecture of disaggregated electronics (SHADE) for advanced defense microsystems that leverages leading-edge commercial processes while addressing strategic weapons requirements. Intimate trusted assembly of diverse technologies offers a flexible and sustainable path to achieving superior military electronics while maintaining the highest trust and survivability. The project will explore subtle challenges associated with tight integration of very different technologies and work towards a standardized plug-and-play interface.

Slurry-Processing Enabled Development of Thin, Large Surface Area, Non-Cylindrical Thermal Batteries for High Power Applications

209285 | Year 1 of 3

Principal Investigator: E. Allcorn

This project will develop a large area, low-profile, and non-cylindrical thermal battery cell facilitated by a unique slurry-processed binder chemistry and realized through an additive manufacturing fabrication approach. Realization of previously unattainable geometries will enable a new paradigm for weapon system designs in which the power source is a modular, instead of fixed, design aspect of a weapon system.

Targeting a 100X Reduction from Design to Analysis: An Agile Workflow for Stronglink Design

200242 | Year 2 of 2

Principal Investigator: J. W. Foulk, III

Previously, the model development and analysis of a stronglink design, dominated by mesh generation, frequently took six months (a stronglink is a nuclear weapon safety component). We developed new capabilities in higher-order tetrahedral elements, meshing, and contact that reduced design iteration by two orders of magnitude. Those methods were implemented in Sandia's production codes, Sierra/SM and Cubit. Through our work over two years, we have taken a significant step towards relieving engineers from the time-intensive burden of discretization. Needs can be met in multiple days, not multiple months. Designers can readily form and test hypotheses to realize affordability, agility, and assurance for new stronglink designs.

Grand Challenges are bold, game-changing ideas with the potential for enormous impact to the security of the nation through transformational 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 missions and programs. These projects result in a long-term science, technology and engineering 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.

Changing the Engineering Design and Qualification Paradigm in Component Design and Manufacturing (Born Qualified)
Project 191144, PI: R. Allen Roach

Born Qualified developed several capabilities to revolutionize design and manufacturing by combining additive manufacturing techniques with deep materials and process understanding. We made significant breakthroughs in processes, diagnostics, modeling and simulation, data analysis, and optimization techniques. These capabilities are the first step to transform qualification paradigms for materials, designs, and ultimately components for multiple national security applications including nuclear weapon systems. With these capabilities, margins to requirements, limits of physics, and process uncertainties will be known at birth, and product changes can be swiftly propagated through the design-manufacture-sustainment chain to assess impacts and revolutionize product realization.

Overview of our multiscale, multi-physics approach to elucidate the Process-Structure-Property-Performance connectivity critical to predict performance probabilistically, to optimally control the manufacturing process, and to implement accelerated cycles of learning.

LDRD

PROJECTS

Changing the Engineering Design and Qualification Paradigm in Component Design and Manufacturing (Born Qualified)

191144 | Year 3 of 3

Principal Investigator: R. A. Roach

This project developed several capabilities to revolutionize design and manufacturing by combining additive manufacturing techniques with deep materials and process understanding. We made significant breakthroughs in processes, diagnostics, modeling and simulation, data analysis, and optimization techniques. These capabilities are the first step to transform qualification paradigms for materials, designs, and ultimately components for multiple national security applications including nuclear weapon systems. With these capabilities, margins to requirements, limits of physics, and process uncertainties will be known at birth, and product changes can be swiftly propagated through the design-manufacture-sustainment chain to assess impacts and revolutionize product realization.

EMP-Resilient Electric Grid for National Security

209239 | Year 1 of 3

Principal Investigator: O. Lavrova

This project pioneers a comprehensive approach to defending the electrical grid against an electromagnetic pulse (EMP) from a high-altitude nuclear detonation or a geomagnetic disturbance (solar storm). The primary task, vulnerability assessment, identifies component and system vulnerabilities and provides quantitative hardness-level requirements through modeling and Sandia-unique testing facilities. The Material and Device Innovation subtask investigates EMP surge arrestors and "smart" transformer oil additives while the Grid-Scale Assessment subtask develops scalable approaches to grid-scale probabilistic outages models.

Enabling Modular Architectures with Radiation Hard Bus-Based Power Delivery

200184 | Year 2 of 3

Principal Investigator: J. C. Neely

This project will develop a new radiation hard power distribution and conversion architecture for select space and defense applications. Developing radiation hard power conversion components and circuits that also support superior efficiency and power density capabilities will greatly enhance the nation's ability to iterate and optimize systems that are constrained by volume, weight, and radiation environment specifications. This architecture will also be a candidate method of standardizing component interconnects so as to reduce the time and cost to perform system design upgrades.

NanoCRISPR: A Revolutionary Therapeutic Platform for Rapidly Countering Emerging and Genetically Enhanced Biological Threats

190245 | Year 3 of 3

Principal Investigator: D. Y. Sasaki

The goal of this project was to develop a rapid, cost-effective therapeutic approach for biological pathogens (e.g., Ebola, Zika, Burkholderia) based on the recently discovered Clustered Regularly Interspaced Short Palindromic Repeats (CRISPR) gene-editing technology and Sandia-developed nanoparticle technology for efficacious in vivo delivery. This project addressed a critical national security need for a method to produce countermeasures against biological warfare agents for which effective therapeutics do not exist and against new agents that might appear in the future.

Smart Sensor Technologies

189614 | Year 3 of 3

Principal Investigator: D. W. Peters

Sensing is vital for many tactical and strategic applications—alerting warfighters or decision makers to the occurrence of an event. For infrared sensing, a critical tool for national security, the physical sensor is the limiting factor in improving data delivery, as current infrared detectors approach their noise floor. We address this need—offering fast, agile spectral bandwidth control, while simultaneously offering increased signal to noise well beyond the current limit.

Strategic Inertial Guidance with MAtterwaves (SIGMA)

209238 | Year 1 of 3

Principal Investigator: G. Biedermann

We propose to develop the world's first low-SWaP (size, weight, and power) inertial sensor based on atom-interferometer (AI) technology. To accomplish this goal, we must research a variety of technologies such as photonic systems and vacuum packaging that can enable miniaturization of an AI device and expand its dynamic range. This system will form the foundation of future low-SWaP strategic-grade inertial measurement units for national security applications.

Towards Predictive Plasma Science and Engineering through Revolutionary Multi-Scale Algorithms and Models

209240 | Year 1 of 3

Principal Investigator: G. R. Laity

This project will develop advanced multiscale computational plasma physics models, surface physics theory, and supporting experimentation enabling significant improvement in computational efficiency and fidelity for plasma physics simulation. This will enable a revolutionary plasma engineering capability impacting pulsed power accelerators, select nuclear weapon components, radiation effects qualification, reentry vehicle plasma sheaths, high-power electromagnetic diodes, and high energy density science.

AUTONOMY FOR HYPERSONICS (A4H)

Mission Campaigns

Mission Campaign Investment Areas provide an agile, strategic process to bridge ST&E and mission and move intentionally from idea to impact. Each Mission Campaign Investment Area (IA) combines strong leadership and coordination with a guiding roadmap to develop key capabilities and overcome high-risk technical hurdles. The goal is to build an innovative portfolio of LDRD projects that tackle future national security mission needs. The Autonomy for Hypersonics Investment Area, the first Mission Campaign, was started in the middle of FY 2018.

Autonomy for Hypersonics

The Autonomy for Hypersonics Investment Area seeks the research and development of autonomous system technologies that will significantly enhance the warfighting utility of hypersonic flight systems. This IA seeks transformative research that will: 1) enable autonomous mission planning for rapid response to time-sensitive threats, and 2) provide highly maneuvering hypersonic flight vehicles that intelligently navigate, guide, and control themselves and home-in on targets.

Robust, Rapid, Autonomous Mission Planning for Hypersonic Flight Vehicles

Project 211826, PI: Julie Parish

The extreme aero-thermal environments associated with hypersonic flight create unique obstacles for mission planning and real-time decision making. To address these concerns, this project is developing a Re-entry Analysis Program To Optimize Roll (RAPTOR) algorithm. This algorithm leverages a large flight point matrix built using the Sandia Automated Ballistic Reentry Evaluation (SABRE) code suite, which performs detailed three-dimensional heating and thermal responses for advanced geometries. During mission planning (or potentially even during flight), the integrated heating at key points on the vehicle is calculated; these results are analyzed to determine when a guidance and control action must be taken to mitigate excessive heat loads. This work is foundational to developing feasible trajectories and defining constraints for optimization and solution evaluation. Automating this part of the trajectory generation process will help address the problem of quality 'big data' for consumption by machine learning algorithms

PROJECTS

Convex Optimization using Geometric Programming on Field-Programmable Gate Arrays

212042 | Year 1 of 2

Principal Investigator: M. J. Grant

This project will develop a new fundamental understanding of the use of convex optimization algorithms with field-programmable gate arrays that may enable real-time rapid trajectory generation on board hypersonic flight vehicles. The use of geometric programming, a specific form of convex optimization, is expected to significantly reduce or eliminate the computationally intensive iteration commonly associated with trajectory generation algorithms. Understanding the hardware and software interaction will significantly impact our nation's ability to develop autonomous hypersonic boost-glide flight vehicles that successfully operate within highly dynamic, contested environments.

Multi-Fidelity Toolkit

212091 | Year 1 of 2

Principal Investigator: R. M. Wagnild

This project will develop a multi-fidelity computational toolkit to predict quantities of interest for hypersonic vehicle trajectory design and mission planning for national security. The toolkit will automate meshing and data reduction, and provide optimal sampling of parameter space and parallelization of the vehicle characterization, filling a void that exists in the physics-based mod/sim capability required for rapid trajectory generation.

Optimal Elevon Control Allocation and Fault Detection/Recovery for Hypersonic Flight Vehicles

212080 | Year 1 of 2

Principal Investigator: D. M. Kozlowski

We will develop an optimized control allocation method that can be combined with existing model reference dynamic inversion control techniques to improve performance of hypersonic glide airframes for national security missions. Understanding the control allocation problem under all conditions of hypersonic flight will enable advanced algorithms to autonomously address catastrophic issues such as actuator failure and recovery for over-actuated vehicles.

Perception-Based Navigation Algorithms for Hypersonic Vehicles

212093 | Year 1 of 1

Principal Investigator: J. S. Jones

Navigation aiding algorithms will be developed for a hypersonic flight vehicle of the future that perceives its surroundings viewing both natural and man-made features and intelligently fusing these data to estimate its location without the need of the global positioning system (GPS). The project will quantify the potential for this navigation method and determine limitations and recommendations for further research.

Rapid Estimation for Hypersonic Engagements

211884 | Year 1 of 2

Principal Investigator: L. A. Jones

This project will develop new, rapid, estimation algorithms for use in missile defense against hypersonic threats. Rapid estimation algorithms are being developed for: 1) hypersonic threat tracking for defensive fire control, 2) hypersonic threat flight prediction for defensive fire control, and 3) relative navigation for interceptor homing on hypersonic threats. This work is significant because algorithms from other types of engagements, such as air-to-air engagements and ballistic missile defense engagements, are inadequate in hypersonic engagements. The results from this work with contribute to the development of missile defense solutions for hypersonic threats.

Robust, Rapid, Autonomous Mission Planning for Hypersonic Flight Vehicles

211826 | Year 1 of 2

Principal Investigator: J. M. Parish

This project will integrate high-fidelity hypersonic vehicle models with scalable, parallel stochastic optimization tools to rapidly generate robust trajectories. This new capability will enable warfighters to quickly plan complex missions with a high level of mission assurance. Foundational algorithm development work will capture impacts of models, uncertainties, computational complexity, memory, and human-machine interfaces; these will inform hardware requirements for deployable systems.

Synthetic Aperture Radar for Autonomous Hypersonic Mission Terminal Guidance

212081 | Year 1 of 2

Principal Investigator: T. Burkhard

Future hypersonic vehicle missions will require real-time terminal autonomous guidance capability to ensure success against adversarial countermeasures and "fleeting targets." We will test the performance limits of current technology and develop an autonomous real-time, automatic target recognition algorithm that will operate with forward-squinted synthetic aperture radar data that is capable of detecting, locating, and classifying the target of interest to ensure mission success.

Synthetic High Forward Squint Synthetic Aperture Radar Images using Generative Adversarial Networks

212040 | Year 1 of 2

Principal Investigator: J. J. Coon

This project will train a generative adversarial network (GAN) to generate high fidelity simulated synthetic aperture radar (SAR) images. The ability to generate these SAR images is critical for developing automated target recognition (ATR) systems for hypersonic weapons platforms in cases where little SAR data currently exists and new data is difficult and expensive to obtain.

Using Generative Models to Generate Hypersonic Boost-Glide Vehicle Trajectories

212018 | Year 1 of 2

Principal Investigator: M. R. Sena

This project will create new capabilities for generating synthetic flight trajectories. These synthetic trajectories can train and validate neural networks for rapid hypersonic boost-glide vehicle (HBGV) flight planning. We hypothesize that a properly designed and trained neural network can quickly generate initial vehicle trajectories and enable the vehicle to react intelligently to dynamic environments and emerging threats that may arise mid flight.

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 four times each year. A small amount of funding (≤ $100K) 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.

Coupled Magnetic Spin Dynamics and Molecular Dynamics in a Massively Parallel Framework

Project 211666, PI: Julien Tranchida

While used broadly in both research and everyday life, our understanding of magnetic materials at the nanoscale remains severely limited. Sandia researchers have made a significant leap forward by combining, in a computationally efficient way, different numerical methodologies within Sandia's code LAMMPS. This effort led to a massively parallel framework to study the interplay between microstructure and magnetic properties of materials at previously unreachable accuracy and scale. Research groups at Sandia are planning to use this tool to better understand a broad range of magnetic phenomena. These include magneto-elasticity, phase transitions, irradiation damage, and the effects of strong laser pulses on magnetic materials. A series of publications is planned in the *Journal of Computational Physics*[1].

Schematic overview of the multiscale framework bridging between ab-initio and device-level atomistic magnetic simulations. On the left, zoom-in on experimental observations. The middle and right images represent the numerical approach embedded in LAMMPS.

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[1] J Tranchida, SJ Plimpton, P Thibaudeau, and AP Thompson. "Massively parallel symplectic algorithm for coupled magnetic spin dynamics and molecular dynamics." *Journal of Computational Physics*, 372:406-425, 2018.

PROJECTS

EXPLORATORY EXPRESS

PROJECTS (continued)

Additively Manufactured Transparent Optical Glass

209911 | Year 1 of 1

Principal Investigator: J. Choi

This project explored methods to additively manufacture transparent optical glass materials, expanding the understanding of glass printing. We successfully printed and sintered silica samples with the desired transparency and printed and sintered borosilicate glass samples with varying degrees of transparency. The processing knowledge gained as a result of this project provide the necessary background to re-evaluate and optimize the printing of borosilicate glass in the future. Once further developed, the technology may support on-demand fabrication of custom optics with tunable material properties for use in harsh environments relevant to national security applications.

Adjoint-Based Calibration of Plasticity Model Parameters from Digital Image Correlation Data

212582 | Year 1 of 1

Principal Investigator: D. T. Seidl

Sandia relies on large deformation numerical simulations to predict weapon performance in extreme environments. Their quality depends heavily upon accurately calibrated models of plastically deforming materials. Thus, model calibration algorithms have a considerable impact on confidence in weapon system simulations that are critical to national security. We developed an adjoint-based model parameter calibration algorithm and evaluated it on synthetic full-field displacement data. We found that it out-performed state-of-the-art finite difference-based approaches by a significant margin.

Bioenergy Fuels Biodefense Research: Discovering New Antibiotics from Algal-Bacterial Production Ponds

212585 | Year 1 of 1

Principal Investigator: C. L. Fisher

Antibiotic resistance (both natural and engineered) is a national security and biodefense concern. Identifying novel chemicals with novel mechanisms of activity that are active against human pathogenic strains will promote national security by enhancing the country's ability to combat natural antibiotic resistance and bioweapons agents with engineered antibiotic resistance. Algae production ponds contain a rich, unstudied, microbial and chemical diversity and constitute a promising source of antibiotic and antifungal chemicals. The goal of this project was to identify antibiotic and/or antifungal activity from wastewater collected from algae production pond samples. We successfully found antibiotic or antifungal activities present in 25 chemical mixtures of the 75 algae-bacterial samples that were screened.

Chance-Constrained Optimization for Critical Infrastructure Protection

210602 | Year 1 of 1

Principal Investigator: B. Singh

Stochastic optimization deals with making highly reliable decisions under uncertainty. Chance constraints are a crucial tool of stochastic optimization to develop mathematical optimization models; they form the backbone of many important national security data science applications. In this investigative study, we 1) developed new algorithms to approximate chance-constrained optimization models, 2) demonstrated an application of chance-constraints to a national security problem, and 3) investigated related stochastic optimization problems. We believe our work is a stepping stone for new research in stochastic optimization as well as securing critical infrastructures against unforeseen attacks.

Characterizing the Spatiotemporal Evolution of Xenobiotic Degrading Microbes

209228 | Year 1 of 1

Principal Investigator: G. Bachand

In the course of this project, we developed an understanding of the spatiotemporal dynamics microbial consortia evolved to degrade recalcitrant xenobiotics (i.e., synthetic materials such as plastics). The mixed fungal-bacterial community efficiently degraded resorcinol (a toxic phenolic resin) as the sole carbon and energy source. A novel understanding directed evolution of microbial communities for xenobiotic degradation was established in this project, with direct impacts on DOE's mission in novel bioremediation approaches for contaminated environmental sites, and enhanced our ability to predict the aging and reliability of synthetic materials used for a broad range of national security applications.

Chemo-Mechanical Controls on Induced Seismicity

209697 | Year 1 of 1

Principal Investigator: R. C. Choens

Induced seismicity associated with wastewater disposal from unconventional reservoirs is creating unprecedented seismic hazards in the midcontinent US. Events are occurring near critical infrastructure, threatening energy security. The proposed research was a novel approach to the problem of induced seismicity, coupling chemical and mechanical effects in fault reactivation. We conducted experiments on laumontite, a common alteration product observed in fault and fracture systems. Our experiments demonstrated that chemical reactions between laumontite and wastewater chemistries would not affect stress distributions along faults, but fault strength changes associated with reactions could trigger seismicity.

Computational and Experimental Characterization of Intermediate Amorphous Phases in Geological Materials

210592 | Year 1 of 1

Principal Investigator: J. Rimsza

Engineered barriers are employed in underground nuclear waste repositories to minimize actinide solubilities. During hydration, the microstructure of multiphase oxides used as barriers can evolve, altering the effectiveness of the barrier. Experimental and computational nuclear magnetic resonance (NMR) spectroscopy was employed to identify and separate overlapping chemical environments in these multiphase oxides, and unexpected secondary impurity phases were detected. This provides the basis for further investigations into the role of secondary phases on the effectiveness of engineered barriers and developed capabilities to analyze disordered materials, providing a link between computational and experimental characterization methodologies.

Conversion of Plastic Work into Heat: A Full-Field Study of Thermomechanical Coupling

209695 | Year 1 of 1

Principal Investigator: A. Jones

This project provided an unprecedented full-field understanding of the conversion of plastic work (work due to the plastic deformation of a material) into heat using advanced diagnostics (digital image correlation combined with infrared imaging). This understanding was envisioned as a catalyst for reformulating the prevalent simplistic model, which will ultimately transform Sandia's ability to design for and predict thermomechanical behavior, impacting national security applications including nuclear weapon assessments of accident scenarios. Synchronized deformation and thermal measurements were successfully delivered, characterizing a mission relevant material and laying the groundwork for understanding the complex interplay between temperature, strain, and strain rate in failure of metals.

Coupled Magnetic Spin Dynamics and Molecular Dynamics in a Massively Parallel Framework

211666 | Year 1 of 1

Principal Investigator: J. G. Tranchida

This work developed computational capabilities to address a key modeling deficiency in understanding the structure-property relationship in magnetic functional materials, and is enabling simulations of coupled magnetic and mechanic phenomena with previously unachievable fidelity and scale. Deeper understanding of these phenomena will allow prediction and exploitation of advanced functional materials in national security applications including remote sensing, quantum computing, or energy conversion.

Deformation and Fracture in Complex-Shaped Energetic Particles

211664 | Year 1 of 1

Principal Investigator: M. A. Cooper

We developed a new technical basis of the mechanics of energetic materials at the particle scale. Despite energetic powders being in most Sandia nonnuclear explosive components, we previously lacked any fundamental understanding of quasi-static mechanical behavior at the particle level. We advanced nanoindentation methods for application to films and single particles of energetic materials with complex shapes, and collected discovery data that elucidated particle strength, elastic and plastic deformation, and fracture phenomena. The experimental data were distilled into relationships of particle deformation and fracture suitable for use in predictive particle-level simulations of compaction processes. This technical basis has enabled new engineered powders and manufacturing technologies.

Determining Saturation Velocity for AlGaN Alloys to Justify Investment in RF Transistors

209700 | Year 1 of 1

Principal Investigator: B. A. Klein

This project sought to measure the saturation velocity (vsat) of AlGaN High Electron Mobility Transistors (HEMT), which was previously unreported. This work was used to determine if AlGaN's experimental vsat metric lived up to its predicted value, and was used to determine if further investment in AlGaN HEMTs for radio frequency (RF) communication, and radar applications was merited. Our team measured a saturation velocity of 3.8×106 cm/s, a value that shows AlGaN devices can meet or exceed the Johnson figure of merit of GaN, supporting predictions of higher output power achievable through Al-rich AlGaN. The maturation of this technology could lead to differentiating national security capability for radars.

Developing an Inductively Driven Transmission Line to Power X-Pinch Radiation Sources on Z

211669 | Year 1 of 1

Principal Investigator: C. E. Myers

X-pinch radiation sources would provide transformative x-ray radiography and diffraction capabilities to the inertial confinement fusion and dynamic materials properties programs at the Z Pulsed Power Facility, thereby benefitting nuclear deterrence. This project successfully demonstrated that inductively driven transmission lines (IDTLs) can generate the 100+ kA of electrical current that x-pinches require without perturbing the power flow to the primary Z load. Additionally, short-circuit IDTLs were deployed as low-noise, self-common-mode-rejecting load current monitors. Finally, several higher-voltage IDTLs were designed and fabricated to serve as the next step toward developing an IDTL-driven x-pinch capability for Z.

Development of Metal Hydride Nano-Inks for Multi-Materials Production

211660 | Year 1 of 1

Principal Investigator: T. J. Boyle

The goal of this project was to develop metal hydride nano-inks that can be transformed after deposition into alternative materials (oxide, sulfides, nitrides). A variety of metal hydrides (titanium, erbium, and lithium aluminum) were successfully synthesized as stable inks that were inkjet printed into specific traces that were readily converted to alternative materials (metals, oxides) through select processing, without loss of the original trace geometry. Stable reactive nano-inks for 3D additive manufacturing (AM) production are of interest for national security (neutron generators, energetic materials, glass-to-metal seals, quasi-metal applications, sensor applications, power sources), environmental protection, and commercial products.

Digitally Designed Porous Media to Control Capillary Imbibition and Release under Mechanical Deformation

211663 | Year 1 of 1

Principal Investigator: B. J. Kaehr

The ability to print devices using roll-to-roll approaches can impact long-standing national security needs for rapid prototyping/production of customizable electronics with flexible form factors (e.g., environmental sensors, component interconnects). This project examined the ability of architected 3D micro-porous stamps with designed mechanical deformations (i.e., mechanical metamaterials) to tackle current limitations for high-speed/high-resolution printing technologies such as flexography. Using this approach, we determined key properties of porous media that influence print fidelity and film uniformity. Overall, this work provides a foundation to apply precision fluid mechanics to improve the performance and reliability of printed devices that can quickly address complex and emerging national security challenges.

Dissipative Nonlinear Topology Characterization

210579 | Year 1 of 1

Principal Investigator: N. Leathe

This project developed a new, fundamental understanding of dissipative lattices to optimize performance in extreme environments. It built off the commonly accepted honeycomb material to include additional methods of energy dissipation such as Coulombic friction and pneumatic damping. This research has potential to impact a breadth of Sandia's national security applications.

Efficient Generalizable Deep Learning

212581 | Year 1 of 1

Principal Investigator: T. A. Catanach

Deep learning extracts patterns from data to make predictions. Popular approaches identify models and validate their prediction generalizability using additional data. This approach is challenging when datasets are limited and often can inadequately capture uncertainty yielding inaccurate predictions. This project demonstrated that we can use Stochastic Hessian projection to assess generalizability for deep learning. We developed a metric that explicitly predicts how well a model will perform on new data without needing additional hold-out data. Using this metric during training can improve predictions when data are scarce and understanding prediction variability is critical. Generalizable deep learning can improve modeling tools for national security applications like cybersecurity and autonomy.

Engineering Microbial Assassins to Target Bacterial Pathogens

201876 | Year 2 of 2

Principal Investigator: A. Ruffing

Antibiotic resistant bacteria pose an increasing threat to public health and may be used as agents of bioterrorism. We proposed a novel method for killing pathogenic bacteria by engineering programmable and autonomous microbial assassins with contact dependent inhibition (CDI) systems. We successfully demonstrated targeted killing of an E. coli target strain using an engineered E. coli assassin strain expressing a CDI system. We also developed a vector for CDI expression in an Agrobacterium strain; however, expression of the CDI operon was toxic in this strain. Further development of microbial assassins may provide a versatile and modular tool for treatment and decontamination of bacterial pathogens.

Fabrication of Position Controlled Si/SiGe Quantum Dots for Integrated Optical Sources and Beyond

210567 | Year 1 of 1

Principal Investigator: K. R. Sapkota

This project explored the recently discovered phenomena of enhanced germanium diffusion along an oxidizing silicon/silicon dioxide interface and how this process can be controlled to create novel silicon/silicon germanium (Si/SiGe) nanostructures. We successfully demonstrated enhanced germanium diffusion in vertical Si/SiGe nanopillars leading to encapsulated Si nanodisks for the first time. Such nanostructures could lead to novel device architectures and device fabrication methods with relevance to mission-related areas such as Beyond Moore's Law and quantum computing.

Feasibility of Single-Sided 3D Elemental Imaging

209699 | Year 1 of 1

Principal Investigator: M. Sweany

This project intended to demonstrate feasibility of single-sided 3D imaging and elemental identification of non-nuclear materials. We aimed to determine if we could reconstruct an object's position and elemental constituents. We expected to confirm the expected signal for carbon and oxygen, proving feasibility to extrapolate to other elements. If successful, this technique would apply to munitions remediation, emergency response, and border security. Our results suggest that, in order for this technique to be feasible, significant background reduction is necessary. Associated-particle imaging would allow one to ignore neutrons from the deuterium-tritium (DT) source that did not interact with the sample of interest, which overwhelms those that do interact with the sample.

High-Resolution Raman Measurements of Gradients at Interfaces

211658 | Year 1 of 1

Principal Investigator: R. S. Barlow

High-resolution Raman spectra of a gaseous fluoroketone ($C_6F_{12}O$) were measured over the temperature range 300K to 700K and spatially resolved measurements of fluoroketone, carbon dioxide (CO_2) and nitrogen (N_2) in the gas phase boundary layer above a liquid surface were obtained using a modular imaging spectrometer developed specifically for this project. This project demonstrated the feasibility of applying laser Raman scattering for quantitative investigations of high-pressure gas-liquid interfaces, which is an emerging area of fundamental interface science with potential to impact liquid fuel injection technologies for improved efficiency of advanced, high-pressure engines for transportation and propulsion (a DOE energy security mission).

Hole Spin Qubits in Germanium

209680 | Year 1 of 1

Principal Investigator: D. Luhman

The goal of this project was to develop and demonstrate a new qubit using a novel, yet highly relevant, material system. The concept of the new qubit utilizes the spin of holes in strained germanium quantum wells. This system potentially overcomes many of the challenges with current semiconductor qubit systems and has the potential to be high impact in the quantum information field. Through the course of this project, we developed and demonstrated a quantum dot platform in the material system, which is a critical step toward a qubit demonstration.

Improved Wave Energy Production Forecasts for Smart Grid Integration

210648 | Year 1 of 1

Principal Investigator: A. R. Dallman

This project developed and assessed a wave modeling framework with real-time data assimilation capabilities for wave energy converter power prediction. This is a significant advancement in proving the methodologies needed to implement power from wave energy converters successfully into a smart grid, increasing energy resiliency. The outcome of this project aligns with DOE's energy security mission.

Infrared Characterization of Anisotropic Materials through Plasmonic Coupling

211656 | Year 1 of 1

Principal Investigator: M. Goldflam

We demonstrated a method for examining optical phenomena in high-index of refraction birefringent infrared-active materials and applied it to new infrared detector materials. Specifically, we developed a procedure for optically probing both in-plane and out-of-plane optical properties of these types of materials, which is difficult to do with preexisting techniques. Layered materials have been being heavily examined for applications including optical detector and tunable filter technologies and a deeper understanding of these materials is required. These results will directly impact infrared detector technologies impacting space-based imaging and defense capabilities.

Lattice-Matched, Low Dislocation Density AlGaN Epitaxy via High Temperature Annealing of Sputtered ScAlN Thin Films

209229 | Year 1 of 1

Principal Investigator: A. A. Allerman

Typically, Aluminum Gallium Nitride (AlGaN) films exhibit large dislocations densities that are detrimental for device performance and represent a major hurdle for the realization of AlGaN-based devices. This project addressed the use of lattice-matched Scandium Aluminum Nitride (ScAlN) buffer layers for the mitigation of material defects in AlGaN films. We successfully reduced the defect density of ScAlN films on sapphire substrates but encountered rough surface morphologies. Overcoming high defect density is important to demonstrating of state-of-the-art, ultrawide bandgap AlGaN materials that would enable new device architectures with radiation hardness and high voltage/power handling at reduced size, weight, and power for NNSA applications.

Leveraging Intrinsic Principal Directions for Multi-Fidelity Uncertainty Quantification

211665 | Year 1 of 1

Principal Investigator: G. Geraci

Uncertainty quantification (UQ) is pivotal for predictive computational analysis, and multi-fidelity techniques are critical enablers for high-fidelity simulations. In this project, we proposed to combine dimension reduction and multi-fidelity techniques to obtain an efficient strategy particularly suited for computationally intensive national security applications. Dimension reduction was used to identify a subspace where the correlation between models is maximized. By providing a shared space between input, this approach allows correlating models with dissimilar parametrization. The performance of this strategy was demonstrated on problems ranging from analytical verification tests up to challenging computational fluid dynamics applications. This approach is expected to impact Sandia's ability to perform UQ through its implementation in Dakota.

Low Probability Events and High False Alarms: How Low do False Alarm Rates Need to Be?

210588 | Year 1 of 1

Principal Investigator: J. W. Wheeler

We determined how different false alarm rates impact threat detection when threats occur very rarely—a common occurrence in many national security domains. We know that low target/high false alarm situations have low detection rates, but previously did not understand the detection performance curve with different false alarm rates. This study informed future research that could fundamentally change how the nuisance/false alarm problem is viewed.

Low Temperature Hermetic Valves for Swallowable Sample Collection Capsules

211655 | Year 1 of 1

Principal Investigator: P. R. Miller

This project investigated a low power hermetically sealable valve as the essential component of a swallowable sample collection capsule for studying the brain-gut axis. This physiological system plays a role in a multitude of global security and war fighter health issues, such as post traumatic stress syndrome (PTSD) and sepsis.

Machine Learning of Signal Patterns for Protocol Informatics

211671 | Year 1 of 1

Principal Investigator: J. Galasso

This research applied Natural Language Processing (NLP) machine language techniques to hierarchical structures within radio frequency (RF) signals for the purpose of signal characterization in the same way that NLP is used to analyze language. This novel approach was able to identify related patterns within unknown signals that were not identified during the current manual and time-consuming examination. This signal characterization information is useful to protect the security of critical communication systems against a variety of attack vectors.

Mechanical Interfacial Control of Li-Metal Anodes

210568 | Year 1 of 1

Principal Investigator: K. L. Jungjohann

This project designed and tested an electrochemical cell with control over the contact pressure on electrode surfaces during charge cycling. Testing of lithium-metal anodes within this configuration found that different constant contact pressures dictated the lithium morphology and anode performance. Low contact pressure resulted in mossy dendritic lithium deposits (known to cause fires), where too high of contact pressure resulted in compact lithium metal with short-circuiting. In terms of DOE's Secure and Sustainable Energy Future mission, understanding the impact of mechanical contact pressure on the performance of lithium metal anodes could be a solution for rechargeable high energy density and high power energy storage applications.

Modeling Charged Defects in Non-Cubic Semiconductors for Radiation Effects Studies in Next-Generation Electronic Materials

212587 | Year 1 of 1

Principal Investigator: P. A. Schultz

The project extended predictive capabilities for modeling defects (e.g., for radiation effects assessments) to semiconductors with non-cubic crystal structures. The project generalized treatment of electrostatics boundary conditions to more complex materials, solving a fundamental impediment to achieving predictive accuracy (as obtained for silicon and III-V defect simulations) in next-generation electronic materials used in national security missions (SiC, GaN, Ga2O3, etc.).

Nanomagnet-Based Physically Unclonable Functions

209678 | Year 1 of 1

Principal Investigator: T. Lu

We studied the randomness of polarization of magnetically hard Samarium-Cobalt nanomagnets for developing physically unclonable functions (PUFs), which find applications in national security areas such as improved hardware security, product authentication, and secure communication. Two device fabrication paths were developed for creating Samarium-Cobalt nanomagnet arrays. Magnetic force microscopy measurements showed that, while some systemic bias exists in the polarization direction of a nanomagnet array, randomness can be observed with a nanomagnet spacing of ~500 nm, demonstrating the feasibility of using hard nanomagnets as PUFs.

Neural Networks as Surrogates of Nonlinear High-Dimensional Parameter-to-Prediction Maps

212725 | Year 1 of 1

Principal Investigator: M. Perego

We built surrogate models based on recurrent neural networks, multi-layer perceptron (MLP) and on the more established polynomial chaos expansion (PCE) approach, for approximating nonlinear parameter-to-prediction maps of expensive computational dynamical models. As an exemplar application, we targeted the problem of computing sea-level projections due to changes in the total mass of ice sheets, which is of interest for national security and to DOE earth system modeling efforts. In our simplified numerical experiments, PCE surrogates provided the best results in term of accuracy and cost. The accuracy of PCE surrogates deteriorated as the number of parameters increased, whereas MLP results were almost independent of the number of parameters.

New High-Resolution Electron Scattering Capability

212041 | Year 1 of 1

Principal Investigator: J. H. Frank

This project developed a new capability for studying collisions of electrons and molecules with unprecedented accuracy by combining high electron-energy resolution with velocity mapped imaging of electrons. Development of this capability will significantly enhance DOE/NNSA's ability to model plasmas relevant to atmospheric re-entry and neutron generation for weapons systems and provide fundamental understanding of electron-driven chemistry important to solar energy conversion.

Non-Contact Measurements of Density and Thermal Conductivity for Organic Thin Films such as Thin Film Explosives

210566 | Year 1 of 1

Principal Investigator: E. Ziade

This project developed a novel measurement capability for nanoscale research. The apparatus built in this project was used to measure the density of micrometer-thick films that are representative of thin-film explosives. The uncertainty in the measured results was lower than current state-of-the-art technology for density measurement of similar films. Future work could include model validation of thin film detonation phenomena.

Rechargeable Thermal Batteries with Novel Lithium-Boron (Li-B) Anodes

210594 | Year 1 of 1

Principal Investigator: M. P. Karulkar

This project demonstrated a rechargeable thermal battery chemistry based on a lithium-boron (Li-B) anode and an iron disulfide (FeS2) cathode. We confirmed that recharge rate strongly affects rechargeable capacity, and determined 470° C operation was preferable to 525° C. The system needs further optimization to mitigate capacity loss between cycles. In demonstrating our chemistry proof of concept, we achieved an important step towards realizing a rechargeable thermal battery. Such a battery could be tested before use to buy down risk, and enable rapid product realization by testing and fielding the same unit. It could also enable new use cases in the field.

Renewable Hydrogen Production via Thermochemical/Electrochemical Coupling

204724 | Year 2 of 2

Principal Investigator: A. Ambrosini

The individual components of a coupled electrochemical/thermochemical reactor that can renewably produce hydrogen from steam utilizing solar energy were demonstrated. The process, which employs a proton conducting membrane to separate hydrogen in situ, provides a pathway to a game-changing process of performing thermochemistry at lower temperatures, eliminating the need for expensive, high temperature-stable construction materials. The result is an efficient, carbon-free, solar-to-hydrogen process that will decrease production costs compared to current methods and enable scale-up to industrially relevant plant sizes. The domestic production of hydrogen from renewable, non-fossil fuel resources will enhance and secure America's energy and transportation future.

Seismic Phase Identification with Speech Recognition Algorithms

209745 | Year 1 of 1

Principal Investigator: T. J. Draelos

This project explored a new automated seismic phase identification technique using a merged deep neural network with spectrograms from extracted waveforms and scalar measurements of signal detections as input. A network trained on data from an International Monitoring Station designated MKAR resulted in 95.6% class average accuracy on First-P versus non-First-P phase classification, suggesting a potential significant impact on the reduction of false and missed events in a seismic signal processing pipeline. MKAR is a primary seismic monitoring station in support of the Comprehensive Test Ban Treaty (CTBT). Based on the project results, future work should focus on sequence learning methods applied to seismic phases.

Solution of the Generalized Linear Boltzmann Equation for Transport in Stochastic Media

212586 | Year 1 of 1

Principal Investigator: A. L. Frankel

This project explored the solution of the Generalized Linear Boltzmann Equation for solving transport in arbitrary stochastic media. This method improved the accuracy and efficiency of radiation transport calculations, with applications in DOE/NNSA mission areas such as climate modeling, plasmas, inertial fusion, combustion, radiation environments, and nuclear systems where accurate transport solutions in random or heterogeneous media are critical. The results proved that an accurate solver using this approach can be developed and is faster than sampling approaches. Additional work was performed to develop convenient approximations for common stochastic media that make using this methodology easier and more readily applied to the mission space.

Switchable Energetic Materials for Enhanced Safety and Security

209899 | Year 1 of 1

Principal Investigator: J. D. Olles

"Switchable" energetic materials, in which the state can be changed on-demand from a safe, highly insensitive form to a more sensitive one in which detonation can be initiated, have been shown to be feasible. These materials carry the promise of significant improvements in safety and security, and for enabling novel applications. Here we demonstrated proof of concept of a new technique for switching energetic materials from a safe to reactive state on useful (short) timescales. We showed that it is possible to control the state and, thus, reactivity of certain energetic materials through a unique prescribed input stimulus.

Testing the Possibility of Magnetic Contrast Imaging based on Circular and Linear Dichroism using Photoemission Electron Microscopy

206536 | Year 2 of 2

Principal Investigator: T. Ohta

The purpose of this project was to demonstrate proof-of-concept magnetic imaging based on magnetic circular dichroism (MCD) photoemission electron microscopy (PEEM) using a pulsed laser with a wavelength of 213 nm. We developed the laser setup for dichroic imaging using circular and linearly polarized laser coupled to PEEM, and demonstrated preliminary magnetic imaging of cobalt surface magnetic domains formed on polycrystalline nickel films. The knowledge of magnetic domain behaviors is one of the fundamental aspects for materials and nanoscience research, and is an important factor for controlling variability of magnetic materials for real-world applications.

Three-Dimensional Imaging through Shock-Waves at Ultra-High Speed

211659 | Year 1 of 1

Principal Investigator: Y. C. Mazumdar

Shock waves greatly obscure imaging in hypersonic or explosive environments. Here, we developed a new ultra-high-speed phase-conjugate digital in-line holography (PCDIH) technique for canceling shock wave distortions. Where previous implementations were limited to 10 to 20 Hz video rates, we utilized pulse-burst lasers and ultra-high-speed cameras for imaging at up to 2 to 5 MHz (million-frames-per-second), which demonstrated a speed increase of five orders-of-magnitude. This diagnostic was applied to studying laser-spark plasma-generated shock waves and explosively generated hypersonic fragments. Results showed a significant decrease in imaging distortions. In addition, this diagnostic enabled 3D, time-resolved object tracking through shock wave distortions in extreme environments relevant to national security applications.

Topological Spin Transistor

211668 | Year 1 of 1

Principal Investigator: W. Pan

We fabricated topological field effect transistors in topological materials of $ZrTe5$ and observed robust topological surface states against gate bias in these transistors. We further studied spin valve devices in tellurium thin films and demonstrated spin-polarized electronic transport in these thin films. The results obtained in this project have important implications to topological spintronic applications, and pave the way for future novel electronic functionalities that promise to extend and expand current information, sensing, and energy technologies far beyond the capabilities of silicon–thereby enhancing national security.

Topology Optimization for Nonlinear Transient Applications using a Minimally Invasive Approach

212660 | Year 1 of 1

Principal Investigator: J. Robbins

This project created and demonstrated a viable method that can use Sandia's existing analysis codes (e.g., Sierra, Alegra, the CTH hydro code) with minimal modification to generate objective function gradients for optimization-based design in transient, nonlinear, coupled physics applications. The resulting capability will be a valuable resource for meeting diverse engineering challenges for nuclear deterrence and other national security applications.

Total Ionizing Dose Response of Dielectrically Isolated FinFETs for Future Strategic Electronics Capability

209679 | Year 1 of 1

Principal Investigator: M. P. King

In this work, we have studied the total ionizing dose (TID) response of fully dielectrically isolated FinFETs (Fin field-effect transistors), fabricated on bulk wafers, using experiments and simulations. From our results, we have determined FinFETs fabricated using bottom oxidation through shallow-trench (BOTS) isolation (called BOTS-FinFETs) are an attractive candidate for strategically radiation hardened (SRH) microelectronics. This technology shows promise for robust operation and can enable gains in radiation hardness, power, performance, and reliability.

Using Analog SONOS for Energy Efficient Computing

210649 | Year 1 of 1

Principal Investigator: S. Agarwal

We showed that an accelerator based on floating-gate SONOS (silicon-oxygen-nitrogen-oxygen-silicon) transistors can train neural networks to ideal accuracies that match those of floating point digital weights on a handwritten digit dataset by using multiple devices to represent a weight or within 1% of ideal accuracy when using a single device. A neural training accelerator core based on SONOS with a single device per weight would increase energy efficiency by 120-fold, operate 2.1 times faster, and require 5 times lower area than an optimized system based on conventional transistors. Building such an accelerator would improve our nation's ability to analyze data for many applications including cybersecurity and geospatial analysis.

Visualizing Clustering and Uncertainty Analysis with Multivariate Longitudinal Data

209227 | Year 1 of 1

Principal Investigator: M. G. Chen

This project developed new methods for visualizing the clustering and uncertainty results of applying probabilistic clustering methods to multivariate time-dependent data, which can be used in a wide array of applicable areas. Developed methods provided clustering uncertainty for each data point relative to each data point's position in assigned clusters. This additional information over existing global quantitative cluster evaluation measures allowed assessment of the quality of analysis results from the implemented model. Decision makers could assess how confident they should be in the results presented to them. These benefits were demonstrated in imagery analysis, and can be realized in other national security applications such as video and cyberattack analysis.

Zeptocalorimetry

210569 | Year 1 of 1

Principal Investigator: C. T. Harris

In this project, we developed an ultrasensitive calorimeter for detecting zeptojoule energy dissipation events in very low power logic switches for reversible computing technologies. Sandia is actively pursuing research in ultra low power switching for future computing needs. However, no means exist for measuring and validating ultra low power logic switches. The research conducted fills a relevant technical void.

Unpublished Summaries

For information on the following FY 2018 LDRD Projects, please contact the LDRD Office:
Laboratory Directed Research and Development
Sandia National Laboratories
Albuquerque, NM 87185-0359

Project	Title
190971	Green Monopropellant System Design and Characterization for Threat Signature Analyses
190974	Optical Technology
190989	Creating Data for Validating Machine Learning Methods
190997	Assessment of Non-Traditional Phenomenologies for Proliferation Detection
191005	Development and Demonstration of Alternative Precision Navigation Capabilities in GPS-Denied Environments
191229	Advanced Neutron Generator
191239	Adjoint-Based Methods for Optimization and Uncertainty Quantification in Particle Transport
200013	Exploring Active Metal Spectroscopic Emissions in Explosive Detonations for Improved Weapon Discrimination
200018	Assessment of Post-Quantum Cryptographic Algorithms
200019	Featureless Radio-Frequency/Microwave Structures
200058	Landscape Monitoring using High-Resolution Remotely Sensed Imagery
200061	Ionospheric Impacts on Space-Based Radars: Characterization and Mitigation
200068	Understanding the Scientific Basis Behind Assumptions in Aerothermal Modeling
200115	Low-Cost, Large Area Neutron Sensor
200227	Additional Processing of Commercial Fin Field Effect Transistor Devices and Their Radiation Properties
200253	Novel Materials to Enable Future Weapon Architectures
209203	Finite Set Statistics Based Distributed Optimal Control for Space Surveillance
209204	Miniaturized Explosive Test for Optical Emission Diagnostics
209207	Quantum-Enhanced Imaging System (QEIS) with Unprecedented Resolution
209209	Intelligent Customized Spot Shielding for Microelectronics in Space Applications
209211	Emulating Genome Security Risks in Realistic Genomics Data Ecosystems
209212	Data Enrichment for Improved Intelligence Value and Situational Awareness
209258	Micro-Detonic Effects on Single Crystalline Materials
209259	Suitability of Advanced Antenna Window Materials for Extreme Re-entry Environments
209260	Modeling Complex Relationships in Large-Scale Data using Hypergraphs
209268	Novel Applications of Near-Field Scanning Optical Microscopy
209693	Novel Analysis Techniques for Field Programmable Gate Array (FPGA) Battery-Backed Random Access Memory (BBRAM)
210908	Tunneling Injection Into Electron Beam Photoresist
212224	Data Analytics in Commercial National Security Applications
212226	Development and Characterization of a Novel Supervisory Control and Data Acquisition/Industrial Control Systems Threat Model
212229	Proof of Principle Demonstration of Particle Beams to Disable Triggering Circuits

Awards & Recognitions

Award Description	LDRD Contribution
R&D 100 Award, *R&D Magazine*: Detergent-Assisted Fabrication of Multifunctional Nanomaterials: *Hongyou Fan*	Project 191194, "Cooperative Self-Assembly for Structure and Morphology Control of Energetic Materials"
R&D 100 Award, *R&D Magazine*: LAMMPS: Atomistic Simulation of Materials: *Aidan Thompson*	Project 52532, "Modeling Biomembranes," and others
R&D 100 Award, *R&D Magazine*: Large Field-of-View Bench Top 3-D X-Ray Phase Contrast Imaging System: *Amber Dagel*	Project 200254, "Non-Destructive Evaluation for Encapsulated Component Qualification"
R&D 100 Award, *R&D Magazine*: SWiCK Zoom: *David Wick*	Project 117843, "Determination and Optimization of Spatial Samples for Distributed Measurements," and others
2018 DOE Early Career Award: *Eric Cyr*	Project 209240, "Towards Predictive Plasma Science and Engineering through Revolutionary Multi-Scale Algorithms and Models"
The American Academy of Arts and Sciences Fellow: *Jeff Brinker*	Project 190245, "NanoCRISPR: A Revolutionary Therapeutic Platform for Rapidly Countering Emerging and Genetically Enhanced Biological Threats", and many others
American Physical Society Fellow: *Thomas Mattsson*	Project 105979, "Expansion of QMD Materials Modeling to Surface Phenomena of Importance to Electrical Breakdown in Pulsed Power Systems," and others
American Physical Society Fellow: *Alec Talin*	Project 180898, "Molecule@MOF: A New Class of Metal Organic Framework Optoelectronic Materials," and others
Asian American Engineer of the Year: *Hy Tran*	Project 117843, "Determination and Optimization of Spatial Samples for Distributed Measurements"
Rising Research Award, SPIE**:** *Amber Dagel*	Project 200254, "Non-Destructive Evaluation for Encapsulated Component Qualification"
2018 Women of Color Career Achievement Award: *Rekha Rao*	Project 190245, "NanoCRISPR: A Revolutionary Therapeutic Platform for Rapidly Countering Emerging and Genetically Enhanced Biological Threats," and others
William Robert Marshall Award, 2017 ILASS American Conference: *Daniel Guildenbecher*	Project 190222, "Explosive Challenge: Revolutionizing Spatial and Temporal Blast Characterization"
Award of Excellence, NNSA's Defense Programs: *George Laity, et al*	Project 209240, "Towards Predictive Plasma Science and Engineering through Revolutionary Multi-Scale Algorithms and Models"

Award Description	LDRD Contribution
Fellow of the Society of Industrial and Applied Mathematics: *John Shadid*	Project 209240, "Towards Predictive Plasma Science and Engineering through Revolutionary Multi-Scale Algorithms and Models"
Innovation and Creativity Award, NEES II Energy Storage Workshop: *Yiyang Li*	Project 209249, "An Interfacial Synaptic Transistor for Fast Neuromorphic Computing"
Best Talk, NMAVS Symposium and Exhibition: *Giovanni Esteves, et al*	Project 191198, "Scandium Aluminum Nitride for Advanced Piezoelectric Sensors, Actuators, and Filters"
2018 SAE World Congress Outstanding Oral Presentation Award: *Scott Skeen*	Project 191017, "A Fundamental Study on the Physicochemical Process of Soot Particle Inception"
Best Poster Award, QNDE Conference: *Joseph Bishop*	Project 200175, "Residual Stress Inversion using Ultrasonic Surface Waves, X-Ray Diffraction, and Sacrificial Material"
Best Poster Award, Rio Grande Symposium on Advanced Materials: *Craig Stewart*	Project 191051, "Water Treatment System for Resilient Energy Production"
Best Poster Award, Rio Grande Symposium on Advanced Materials: *Mary Louise Gucik*	Project 199992, "Multi-Level Memory Algorithmics for Large, Sparse Problems"

The following peer-reviewed publications, published in Fiscal Year 2017, are attributed to the active and completed LDRD projects. The publication metrics for Fiscal Year 2018 will be reported in the 2019 Annual Report because publications take as long as one year to appear in databases used to compile this list. This one-year latency, therefore, ensures the completeness of the publications list reported.

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ABSTRACT

This report summarizes progress from the Laboratory Directed Research and Development (LDRD) program during fiscal year 2018. In addition to the programmatic overview, the report includes progress reports from 371 individual R&D projects in 16 categories.

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