Quarterly Highlights

Mission Agility | Technical Vitality | Workforce Development

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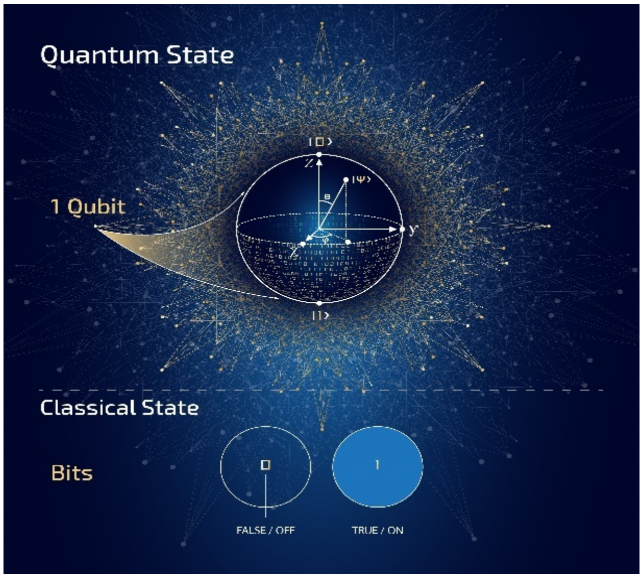
Sandia National Laboratories

HIGHLIGHTS

LDRD investments in quantum pave the way to Sandia leading one of five national research centers in quantum computing research

Sandia will serve as the leading partner in one of five national research centers for quantum information science established by DOE. The Quantum Systems Accelerator is a multidisciplinary team comprising dozens of researchers from 15 labs and universities. Together, they will collaborate to transform rudimentary quantum computers and related technologies into machines that perform valuable work for DOE and the nation. Such work could include advances in scientific computing, discoveries in fundamental physics and breakthrough research in materials and chemistry. A key focus for the initiative is to train the future workforce in the area since many are unaware of the possible connection to their future careers.

"The QSA combines Sandia's expertise in quantum fabrication, engineering and systems integration with Berkeley Lab's lead capabilities in quantum theory, design, and development and a team dedicated to meaningful impact for the emerging U.S. quantum industry," said Sandia's Rick Muller, deputy director of the Quantum Systems Accelerator.



Quantum Systems Accelerator center members are collaborating to fast track advances in information science and prepare the nation's workforce for a future quantum economy. Quantum bits of information have the potential to make powerful calculations that classical bits cannot. (Image by Michael Vittitow) Click the thumbnail for a high-resolution image.

Quantum computers and other devices operate using peculiar laws of physics — quantum mechanics — that affect matter at its tiniest scales. Sandia and its partners believe these machines would perform certain calculations much faster than normal computers if they could be made to run reliably.

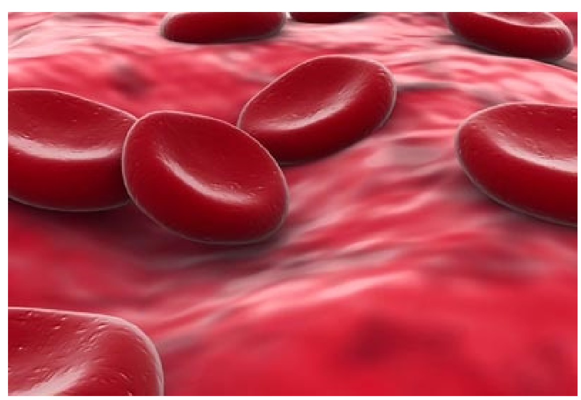
"The Sandia LDRD program can take major credit for this win," Muller said. "It's unlikely that without the intense and sustained support over more than 10 years that we would be here."

Total planned funding for the center is $115 million over five years, with $15 million in fiscal year 2020 dollars and out-year funding contingent on congressional appropriations. *(SAND2020-7621E)*

Sandia focuses on remote sensing of explosive fireballs

Sandia's new Grand Challenge LDRD project, *Light Speed: Accelerating Fundamental Predictions of Explosive Optical Emissions*, will accelerate and add critical physics to explosive fireball simulations while quantifying uncertainty. Faster and higher fidelity explosive signature predictions will advance the nation's ability to provide actionable information on accelerated timelines, responding to rapidly evolving and unpredictable nuclear threats. *(SAND2020-9845O)*

Scientists at Sandia develop artificial red blood cells that mimic natural ones while adding extra abilities



A group of collaborative researchers are focused on creating new and improved artificial red blood cells. Natural red blood cells (RBCs) are flexible, capable of transporting oxygen, and have long circulation times. The synthetic version developed by the team from Sandia, DOE's Office of Science (DOE SC), the Air Force Office of Scientific Research (AFOSR), the National Institutes of Health (NIH), and the National Natural Science Foundation of China (NSFC) is similar to natural ones but possess other features.

Scientists have created artificial RBCs before, but they only contained one or few key features of the natural cells. This version is the first to hold all the natural RBC properties and provide more.

The artificial cells were created by coating donated human RBCs with a thin layer of silica. Then, positively and negatively charged polymers were layered over the silica-RBCs. Once researchers carved away the silica, they produced flexible cell clones. The surface of the replicas was then coated by the researchers with membranes from organic RBCs.

The researchers then supplied the artificial cells with either hemoglobin, a toxin sensor, an anticancer drug, or magnetic nanoparticles to demonstrate that they could carry loads. They also established that the new RBCs could function as decoys for a bacterial toxin. In a clinical trial with mice, the synthetic RBCs lasted for more than 48 hours, with no observable toxicity. Moreover, the researchers say that future studies will explore the potential of artificial cells in medical applications, such as cancer therapy and toxin biosensing.

The research was funded by Sandia's LDRD Program, the DOE SC, AFOSR, NIH, and the NSFC. *(SAND2020-6217J)*

COVID-19 research and impacts at Sandia

Carboxylic acids as sanitizers

A Sandia Labs project demonstrated that carboxylic acids can be combined with a surfactant to create a disinfectant that neutralizes a surrogate for SARS-CoV-2. These mixtures are nontoxic and noncorrosive and are already used by some industries to kill bacteria. The research team tested several mixtures of levulinic acid and acetic acid (vinegar) and found both completely neutralized the bacteriophage used as a surrogate for COVID-19. The team hopes additional studies can be done to determine the minimum concentration of carboxylic acid needed in the mixtures to defeat viruses and to define the mechanism that makes the acids act as antivirals.

Studying the viability of sterilizing masks with supercritical carbon dioxide

Researchers at Sandia Labs are testing the use of supercritical carbon dioxide (CO_2) to safely and reliably sterilize N95 masks and other critical medical supplies for reuse by health care workers on the front lines of the COVID-19 pandemic. Many conventional sterilization methods cannot be used because they degrade mask performance. Supercritical CO_2 is a solvent with the ability to penetrate microporous materials without leaving residue and alleviates the need to use harsher, more hazardous chemicals for sterilization. Supercritical CO_2 cleaning equipment is becoming increasingly popular as an eco-friendly alternative in the dry-cleaning industry and, if deemed an appropriate and effective solution, could be rapidly deployed at wide scale.

First lot of 100 pathogen management kits

Pathogen Management Kit

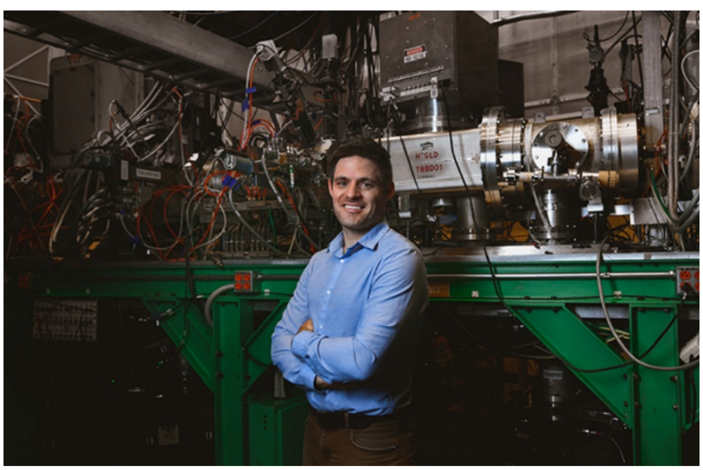
Sandia Labs has developed and produced a simple add-on kit (Pathogen Management Kit, or PMK) that can quickly add on to ventilators of all types to disinfect exhaled air to keep healthcare workers safe. The PMK design consists of a polished aluminum tube that amplifies energy from embedded UV light to decontaminate the exhaled breath by disabling pathogens that pass through. The PMK was developed, built, and tested to ensure sufficient exposure of the entrained pathogens to UV energy. Using a UV light source to kill pathogens, rather than a filter, eliminates the possibility of clogging that is commonly experienced with HEPA designs. The unit was tested with the Phillips Respironics V60; however, because the unit does not add any flow resistance, it could be retrofitted into other existing respiratory assistance devices. The design utilizes commonly sourced, commercially available, off the shelf parts, with only a few requiring custom manufacturing. To prove the effectiveness of the device, Sandia deployed UV exposure measurements coupled with light-propagation modeling to ensure the design had significant margin over what would be required to kill live coronavirus. Sandia's unique aerosol test facility also was used to ensure the design was safe and effective. *(SAND2020-6127W)*

Los Alamos NATIONAL LABORATORY EST. 1943

HIGHLIGHTS

Los Alamos LDRD researcher optimizes compact particle accelerator performance

The Laboratory has been awarded $200,000/year for three years in annual funding for advanced research projects in Particle Accelerator Science and Technology. This U.S. Department of Energy funding will support LDRD researcher Alexander Scheinker of the Low Level Radio Frequency Engineering group at Los Alamos National Laboratory in his development of advanced adaptive control systems for compact accelerators.



Scheinker at the low energy beam transport section of LANSCE where a continuous stream of protons is compressed into a train of discrete bunches five nanoseconds apart.

The Los Alamos Neutron Science Center (LANSCE) proton accelerator —as well as the Stanford Linear Accelerator Center (SLAC) electron accelerator in California and a swath of other accelerators around the world — stand to benefit as R&D engineer Scheinker develops new systems to speed their start-up — and to automatically improve and maintain their.

operating performance "Without the results (published papers and experimental results) from my LDRD projects, I don't think I would ever been part of this national initiative," said Scheinker.

Scheinker received reserve funding from LDRD in 2017 and 2018 that funded a majority of his work on adaptive control methods for accelerators. The LDRD program employs reserve funding for strategic initiatives to facilitate institutional agility when addressing time-urgent, national security challenges. Scheinker is also leading an LDRD Director's Initiative project which will conclude at the end of September 2020, "Adaptive Machine Learning for Advanced Diagnostics and Autonomous Control of Particle Accelerators." The Director's Initiative fosters growth in the Laboratory's strategic initiative to "advance accelerator science, engineering, and technology to enable future stewardship capabilities."

What's a compact accelerator good for? Mesoscale material science

In particular, the funded Los Alamos work is focused on compact accelerators for

Alex Scheinker at the great lookout at LANSCE that overlooks the truck route.

ultrafast electron diffraction (UED). The entire UED setup for this project is approximately 5 meters in length and therefore is considered to be compact compared to a machine such as LANSCE, which is closer to 1kilometer in length. "This project is important for maintaining LANL's lead role in adaptive machine learning for accelerator controls and diagnostics," Scheinker said.

Why? Compact accelerators such as high repetition rate UEDs can be used for preliminary dynamic material studies related to LANL's Dynamic Mesoscale Material Science Capability (DMMSC) project. (DMMSC will address the control of performance and production of materials at the mesoscale.) Also, the general algorithms that are developed here will directly inform both the performance and design of a future free electron laser (FEL), such as the matter-radiation interactions in extremes (MaRIE) FEL envisioned for the DMMSC project.

Machine learning advantage

The main goal of the Los Alamos work is to develop adaptive machine learning algorithms for non-invasive diagnostics and optimal feedback control of time-varying systems with un-modeled disturbances. Another goal is to develop an optimal design approach for new compact accelerators.

"In particular, we are focused on compact particle accelerators whose beams and components drift unpredictably with time," Scheinker said.

"The UED that we are working with is a high repetition rate machine at Lawrence Berkeley National Laboratory, in which a pulsed laser is used to emit electrons out of a metal target via the photoelectric effect 1 million times per second, with each electron bunch containing roughly 1 million electrons and with bunches being as short as 1 femtosecond (1 fs = 10^-15 s)," Scheinker explained.

"A resonant radio frequency accelerating cavity, technology very similar to what we use at LANSCE to accelerate protons, is then used to accelerate those electrons up to energies of approximately 1 million electron volts (MeV) within a very short distance by using accelerating electric fields with gradients of greater than 20 million volts per meter," he said.

The extremely short and closely spaced energetic electron bunches are then used to make movies of dynamic phenomenon in materials at fs resolution. This is done by creating electron diffraction patterns that map out the arrangement of atoms in materials to see details including defects and their effects, and track electronic and superconducting properties in exotic materials. The project is focused on developing an adaptive machine learning (ML) approach that uses all of the components and diagnostics of the compact UED simultaneously to automatically optimize properties of the beam, including reducing jitter in the arrival time of the electron bunches, which becomes very important in such precisely timed dynamic experiments when dealing with such short and closely spaced electron bunches.

Scheinker operating a new digital electromagnetic field controller at LANSCE.

About the accelerator stewardship projects

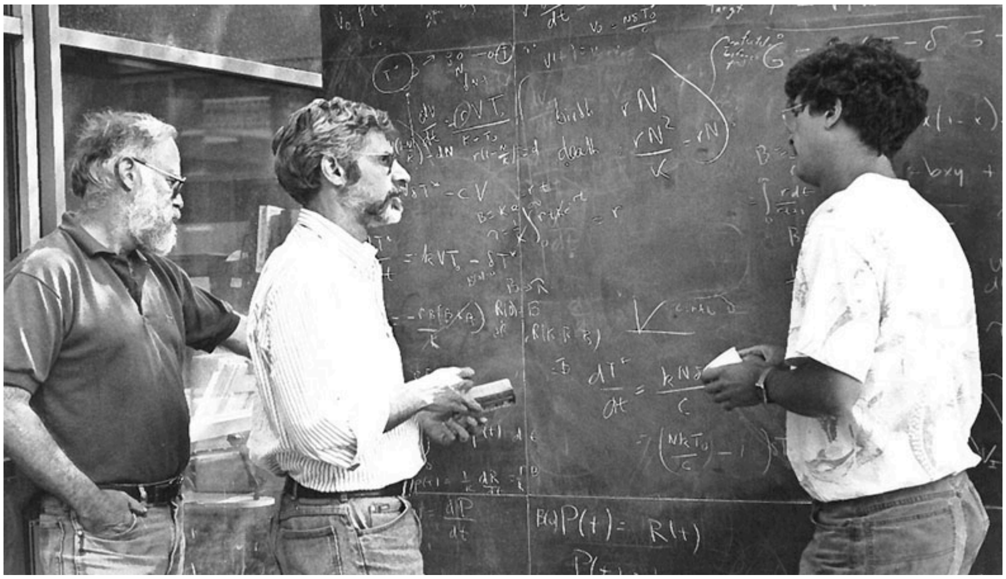
The Los Alamos effort is one of 12 research projects involving scientists at 23 U.S. institutions, including eight universities, 10 national laboratories and five companies, which are working together to solve some of the most challenging problems in medical, industrial, and security applications of accelerator technology.

The projects were selected by competitive peer review under the DOE Funding Opportunity Announcement for Research Opportunities in Accelerator Stewardship, sponsored by the Office of High Energy Physics (HEP) within DOE's Office of Science. *(LA-UR-20-27274)*

Los Alamos LDRD researcher using mathematical modeling to battle viruses like COVID-19

Using a science still in its infancy, Perelson applies mathematical models to advance medicine. Today, he's battling hepatitis B and COVID-19.

LDRD researcher Alan S. Perelson of the Theoretical Biology and Biophysics group at Los Alamos National Laboratory leans back on a chair and reviews his work. In front of him is a computer screen that displays part of his latest computer model, one designed to ascertain key characteristics of a virus and its detrimental effects on the human body.



Perelson began doing research with LDRD funding as early as 1995. Since then, he has led and participated in several LDRD projects that focused on viruses including HIV, H1NI, and now COVID-19. Now a Los Alamos National Laboratory Senior Fellow, his ongoing work helps establish the fields of theoretical immunology and viral dynamics.

Behind Perelson, scribbled all over a chalkboard, are complex mathematical equations designed to calculate predictions related to viral load (a numerical expression of the quantity of virus in a given volume).

He's looking into drug effectiveness designed to treat patients infected with a virus and how often a virus is likely to mutate. Long before battling viruses that cause diseases like AIDS or hepatitis C, Perelson was a student at the Massachusetts Institute of Technology (MIT), where he started off studying life sciences. In 1967, Perelson graduated from MIT with BS degrees in both Life Sciences and Electrical Engineering. In 1972, he graduated from the University of California at Berkeley with a doctorate in Biophysics. Perelson then worked as an acting assistant professor at Berkeley. At the University of Minnesota, Perelson worked as a postdoc in chemical engineering.

"I studied how chemical reactions could lead to pattern formations — trying to determine things like 'how do zebras get stripes,'" he says.

While at the University of Minnesota, Perelson was contacted by George Bell**,** a senior physicist at Los Alamos National Laboratory who was interested in developing a new theoretical biology group at the Lab. Perelson became one of the founding members of a new Theoretical Biology and Biophysics group at Los Alamos.

Except for a brief stint as assistant professor of medicine at Brown University, Perelson has been with the Theoretical Division since 1974, developing models of the immune system and infectious disease.

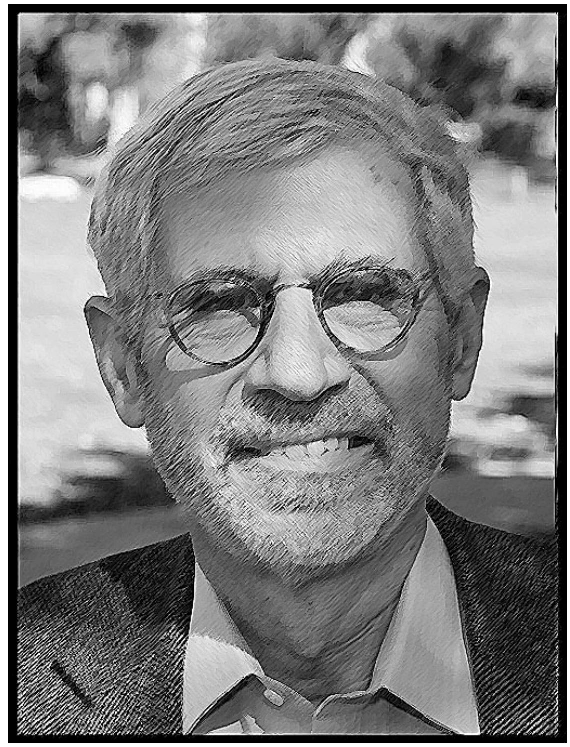
"Modeling infectious diseases is a key element of immunology. However, such models are much more practical than theoretical. These models can influence how medical personnel subsequently treat those who are infected," said Perelson.

Read more about LDRD and Perelson's response to COVID-19

Because LDRD is a proving ground for new concepts, it positions the Laboratory to respond in times of crisis. As part of the Complex-wide effort related to the COVID-19 outbreak, LDRD at Los Alamos reviewed 42 proposals as part of a quick-turnaround call and has used the available funds to select those best suited to address the COVID-19 crisis, as well as the inevitable next pandemic.

Perelson is a co-investigator on one such selected project. "I am trying right now to learn as much as I can about COVID-19. I am building models of how the virus infects cells and replicates, just as I have for other viruses," Perelson said. "My early work is aimed at examining how drug therapy might be used to prevent people from being infected or to decrease the amount of virus they can spread."

France, with other European institutions, is implementing a randomized clinical trial in 62 hospitalized patients. Through a collaboration with French researchers and Certara Integrated Drug Development of New Jersey, Perelson contributed to "Timing of antiviral treatment initiation is critical to reduce SARS-1 Cov-2 viral load," an unpublished manuscript



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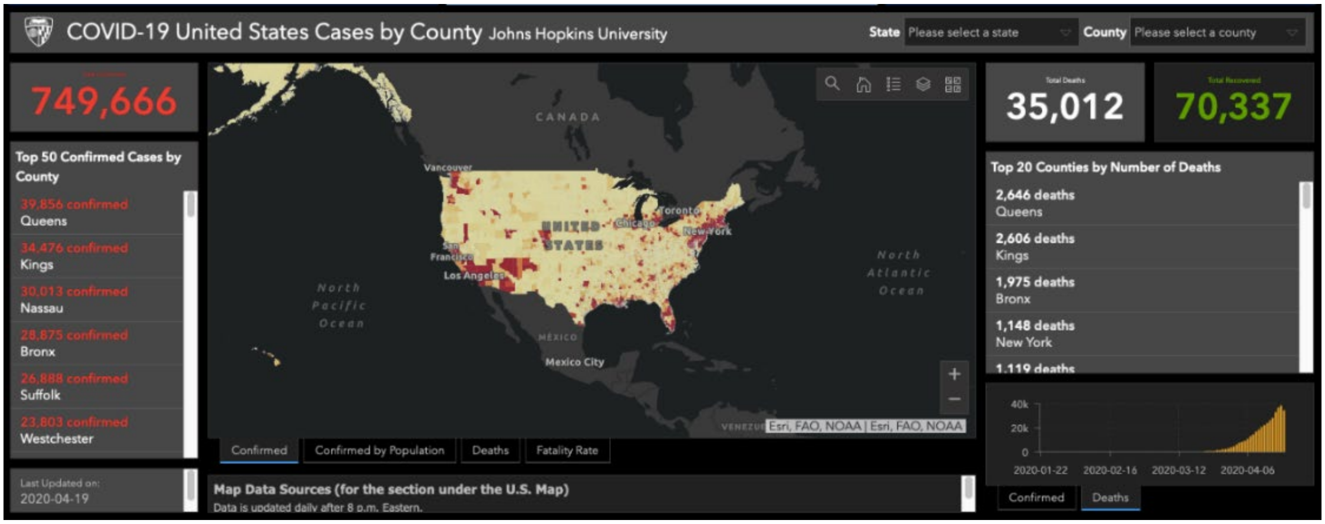
(preprint) posted on April 7 by medRxiv.A science still in its infancy

Perelson says that the science of mathematical models as applied to medicine is still in its infancy.

"Unlike physics models where there's a history of how to describe concepts like gravitation and magnetism developed over a number of centuries, we are still in the infancy of coming up with fundamental equations that describe biological phenomena," says Perelson. "We've slowly built up models that have been extremely successful in describing biological characteristics, such as viral dynamics and equations that show the networks of infections."

In 2017, Alan earned the American Physical Society's Max Delbruck Prize in Biological Physics. He received this prize in part, "For profound contributions to theoretical immunology, which bring insight and save lives."



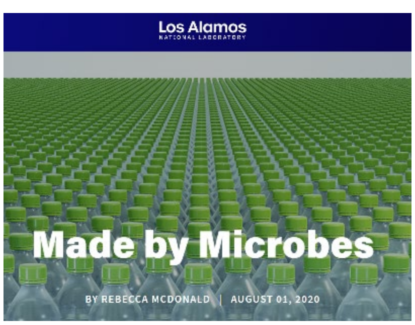
Perelson and his colleagues are building models of how COVID-19 spreads in a given population. Other colleagues are studying the genetic sequencing of the virus to understand how quickly it evolves.

In 2014, Perelson was named to the Thomson Reuters list of "The World's Most Influential Scientific Minds." At the time he said, "It is an honor to have the value of my work recognized and to be included in this list. However, the real success in my area of modeling infectious disease only comes when the work has an impact on treating diseases such as HIV, influenza and hepatitis, and ultimately in saving lives."

Despite receiving such prestigious awards, Perelson says that his greatest reward is watching as new therapies and vaccines are distributed so that humanity can continue to thrive in an ever-challenging world.

"As we learn more and more about how the human immune system reacts to these viral invaders, we will modify these models so that we can more accurately predict the effects such viruses have on the human body," Perelson says. *(LA-UR-20-27274)*

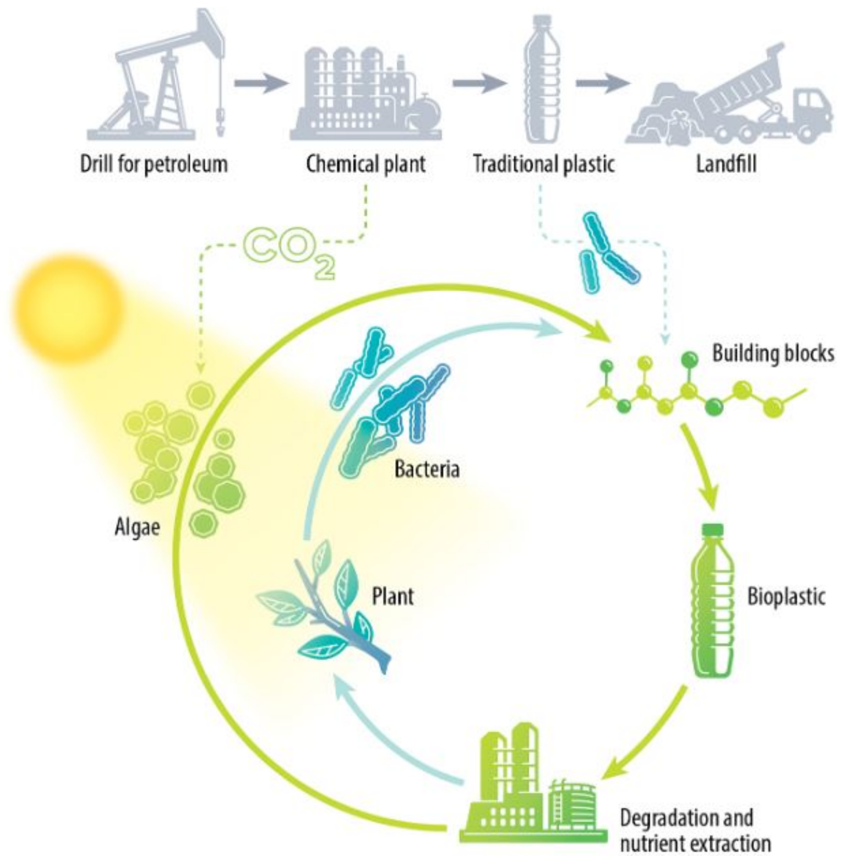
New plastics are needed to help the planet, and Los Alamos LDRD researchers are leading essential efforts



Interested in this topic? Click the image to read more.

Plastics made from petroleum are a mainstay in our daily lives, but the environmental problems they create are driving an urgent search for bio-based alternatives. LDRD researchers are looking to more environmentally friendly resources— such as bacteria and algae. The goal is this: the plastics of the future will be bio-based, biodegradable, and of course, perfectly designed for every imaginable need.

In 2018, LDRD Researcher Babetta Marrone convened a multi-disciplinary team of scientists at Los Alamos, and that team was selected to explore this challenge in a project called BioManIAC (BioManufacturing with Intelligent Adaptive Control). Inspired by MANIAC, the pioneering first computer at Los Alamos, Marrone and her team are using biology, chemistry, and machine learning to create a process for finding entirely new plastics. Their goal is to identify monomer building blocks that are made using photosynthetic microbes such as algae and that readily return to the ecosystem as the plastic degrades, eliminating the need to collect and recycle waste materials. Microalgae are an attractive bio-feedstock for industrial applications because of their rapid growth and higher productivity-per-unit-land-area than any plant system. Marrone's LDRD team is well positioned to revolutionize the field of plastics and to solve the global plastic pollution problem. The chemical knowledge base and systemic approach developed by this LDRD project can be adapted for applications in medicine, agriculture, 3D printing, and more.



Research in bio-related materials is one of the fastest growing interdisciplinary research areas globally. Plastics made from petroleum in a traditional "linear" economy (top row) are mostly sent to landfills and are slow to degrade in the environment. In a more circular "bioeconomy," proposed by Marrone and her team, products do not become waste but rather feed back into the system to become something else, or the same thing again

"By harnessing the rich and vast landscape of algae biology and polymer chemistry, we will create a framework from which to design a new generation of biopolymers that serve as the basis for revolutionary new bioplastics," LDRD researcher Babetta Marrone.

(LA-UR-20-24819)

SDRD SITE-DIRECTED RESEARCH & DEVELOPMENT

HIGHLIGHTS

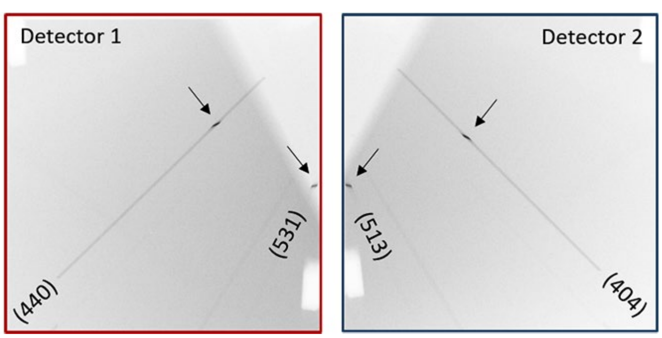
NNSS develops novel x-ray polarizing beam splitter for plasma diagnostics

The x-ray polarizing beam splitter (XRPBS) is a compact x-ray optical component that uses a perfect crystal to split an incident x-ray beam into two beams with mutually orthogonal linear polarizations. The two outgoing beams emerge in directions perpendicular to each other and to the direction of the incoming beam. This spatial separation enables using x-ray detectors that are the most appropriate for the actual measurement.

The XRPBS with silicon diode detectors installed on a goniometer for synchrotron measurements.

Traditionally, the x-ray polarization degree is measured using either a pair of crystal spectrometers oriented for mutually perpendicular reflections, or a single crystal in different orientations over successive exposures. Both methods are problematic for spatially extended, short-lived sources. But using a single-crystal XRPBS improves the accuracy by enabling measurements of both polarization components simultaneously with the same crystal. This method provides more accurate results because the XRPBS ensures that the polarized x-rays are emitted from the same region of the x-ray source, follow the same path from the source to the crystal, and are diffracted at the same location in the crystal. In this situation the polarization degree measured is characteristic of the source or any objects traversed by the x-rays on their path from the source to the crystal.

Analyzing the linear polarization of the x-rays provides information about the x-ray source or about the materials the incoming x-rays interacted with. For example, the polarization of the spectrum emitted by a plasma can be used to detect or measure plasma anisotropies generated by macroscopic electric and magnetic fields or charged particle beams.



Pair of Cu spectra from a Manson source, recorded with a Ge crystal XRPBS. The arrows point to the Cu Kβ line diffracted by the {440} polarizing planes (along the detectors' diagonals highlighted by the bremsstrahlung continuum spectrum), as well as by other internal planes {531}.

Using an XRPBS for plasma polarization spectroscopy (also known in this setup as single-crystal x-ray spectropolarimetry) extends the applicability of this diagnostic technique to high energy density laboratory plasmas that are large and irreproducible.

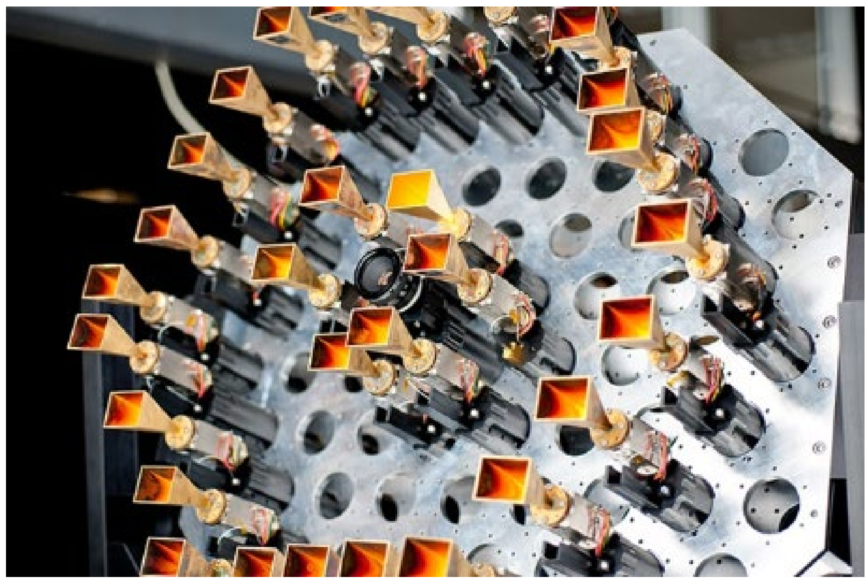
The XRPBS is most impactful on the x-ray polarization spectroscopy of laboratory and astrophysical plasmas, where it can greatly improve measurement accuracy, decrease instrument size, reduce measurement time, and simplify the alignment process. In a different type of application, the XRPBS can be used at synchrotrons and x-ray free electron lasers for in situ beam monitoring, for beam multiplexing to enable beam sharing, or as a component of delay lines for beam characterization or pump-probe experiments.

For additional information, see Wallace, M. S., R. Presura, S. Haque, I. Pohl, P. Lake, and M. Wu, "Cubic crystals in an x-ray polarization-splitting geometry," *Rev. Sci. Instrum.* 91 (2020) 023105.

(DOE/NV/03624--0856)

NNSS advances in millimeter-wave imaging for fireball characterization

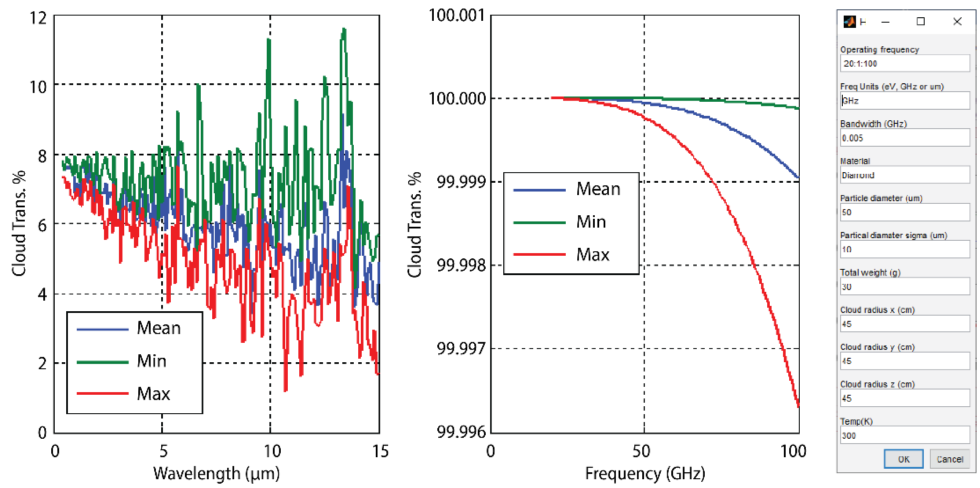
Nuclear nonproliferation programs increasingly focus on understanding how high explosives (HE) particulates and case fragments produce signatures and observables indicative of potential proliferation activities. Unlike optical sensing modalities, millimeter-wave (mmW, 60–100 GHz) imaging can see through the soot, smoke obscurants, and metal fragments generated at early times in HE test events.



The PSI mmW imager developed by AFRL and operating at 77 GHz, for use on our mmW experiments.

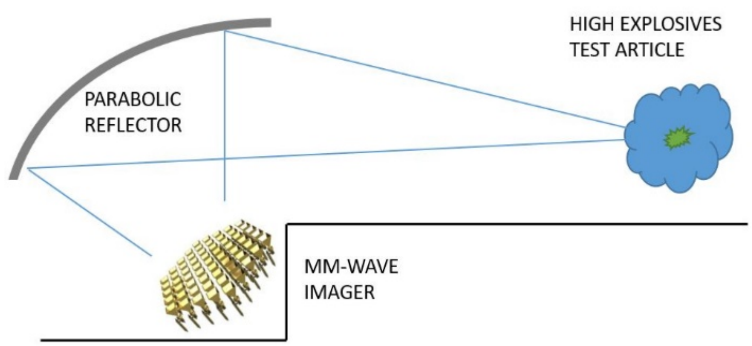
This 3-year SDRD project is developing a mmW imaging diagnostic to determine important fireball and case fracture parameters that could provide a new way to track early time movement of larger fragments and refractory components at shell break-up, increasing understanding of large-scale HE packages. Measuring passive mmW emissions and active attenuation through the detonation cloud, we can estimate particle size distribution, density, emissivity, and temperature. This work may lead to a new diagnostic capability at the Nevada National Security Site (NNSS) Big Explosives Experimental Facility (BEEF).

In this project, NNSS is partnering with the Air Force Research Lab (AFRL), using their millimeter-wave imaging system, originally designed for GPS-denied navigation applications. The project began by developing both Rayleigh and Mie scattering models to estimate mmW attenuation through particle clouds with selectable parameters for mass loading and particle cloud size. Expanding on this base, the modeling capabilities were extended to include a mmW sensor model capable of predicting scene and target irradiance as well as signal-to-noise and contrast-to-noise ratios applicable to the AFRL sensor system. The model can also simulate the Mie model- based target reflectivity, emissivity, and environmental attenuation parameters. Preliminary modeling of the AFRL sensor system to assess its ability to detect fragments within a cloud show good model agreement with AFRL's preliminary observational data on extended sources, although more rigorous verification will continue. The second-year efforts have included the development of extensive model capability improvements including performance predictions for the Phase Sensitive Innovations (PSI) system in a variety of environments, and a full dispersion model for determination of dielectric constant at a range of frequencies. The dispersion model in conjunction with the Mie model allows comparison of attenuation through a cloud for different frequencies or wavelengths and has been extended to handle UV/Vis/IR cases.



Output of the attenuation model at UV/Vis/IR (left) and for mmW (center) for diamond dust in the shock tube overpressure system. The menu on the right are the input parameters for the mmW case. The model allows us to determine how well we can see larger debris and discharges in the cloud.

The model verification work resulted in a new controlled particle and mass loading test apparatus installed in a dedicated anechoic chamber. This new shock tube overpressure system at the NNSS Special Technologies Laboratory (STL) will provide test and evaluation capabilities for both model verification and sensor performance testing, and is expected to be complete early in the first quarter of FY 2021. Preparations for mmW testing on large scale HE test events in the third year are underway with new designs recently completed for reduced focal distance imaging with the PSI system. The off-axis parabolic reflector design is based on a Herschelian telescope, and will provide both reduced focal distance for the distributed aperture imager as well as blast and fragment protection for the imaging hardware. *(DOE/NV/03624--0873)*



The reflector design models predict a spatial resolution of 2 cm on target at a range of 10 m (2 mrad), with a total field of regard on the order of 2 m. Coordination with AFRL's High Explosives Research and Development facility for participation in upcoming test events is expected to yield multiple test opportunities in the final year of the project.

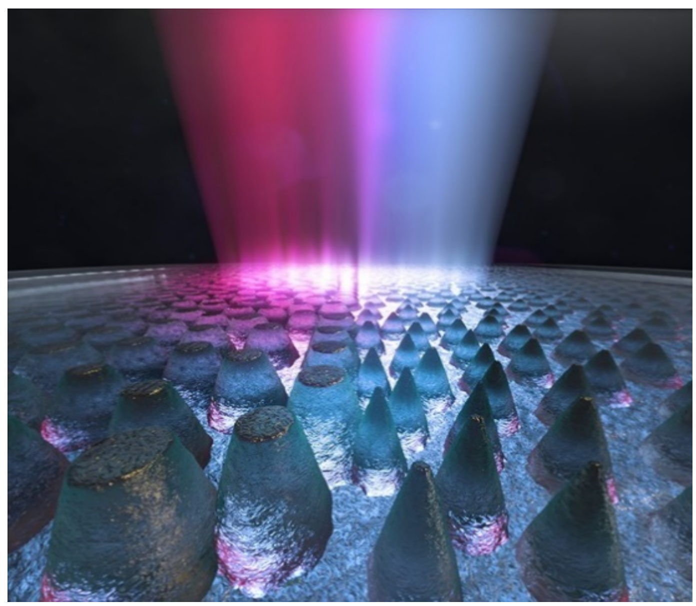
Livermore develops antireflective metasurface for laser optics

LLNL scientists developed a new method to add an antireflective metasurface (ARMS) layer on laser optics glass that significantly increases durability. The technique represents a substantial advancement, offering high flexibility in tailoring optical reflection properties that could benefit a wide range of lasers and imaging optics.

The technique transforms the optic's surface into a structured metasurface that is engineered for the desired wavelengths. In addition, the ARMS layered structure does not exacerbate the growth of damage normally caused by high-power laser light.

These metasurfaces show great promise to expand the applications of high-power lasers, including compact particle and x-ray sources, renewable energy, directed energy, and fundamental light–matter interaction exploration.

During the LDRD-funded project, the team explored ways to create an antireflective metasurface for optics without adding different materials to the glass or introducing potential defects that could diminish performance and durability. An anti-reflective layer is one of the most critical components of a laser optics system. The layer can help maximize energy transmission and help protect the system from damaging stray or deflected light.



An artist's rendering of cone-shaped nanostructures that can be created using an antireflective metasurface technique developed at LLNL, which enables more durable and flexible imaging optics.

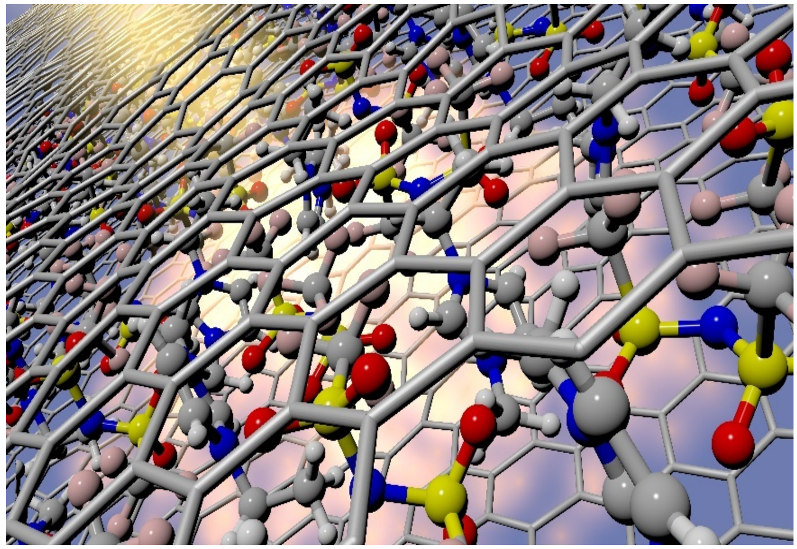
Currently, the two main types of antireflective coatings are a sol-gel coating layer, which is primarily used for fused silica substrates (with limitations such as frequency bandwidth, uniformity, and environmental stability), and multi-dielectric coatings (which have a lower laser damage performance). However, the coatings can become a source of failure for laser systems due to laser-induced damage.

"The strength of this new method is that we are etching directly into the substrate so that the antireflective layer is basically a reforming of the topography of the glass," said LLNL scientist Nathan Ray. "We haven't added any material to the optic, and it's easy to implement."

The research was funded by LLNL's LDRD program, and findings were published in *Optica*. *(LLNL-WEB-811142)*

Livermore investigators dive into the structure of molten salts in tight spaces

A special class of molten salts, known as room-temperature ionic liquids (ILs), promise far greater electrochemical performance compared to conventional aqueous solutions due to a suite of novel, tunable properties. Over the past two decades, ILs have been explored as a way to improve a range of technologies, including energy storage and conversion, catalysis, and electroplating of metals and semiconductors.



Artist rendering of experimental work at LLNL aimed at investigating the electrochemical stability of spatially confined ionic liquids. The illustration depicts the synchrotron X-ray beam impinging on ionic liquid molecules confined within a graphitic carbon slit-pore. X-ray scattering in the background reveals new details regarding their structure under nanoconfinement, which were validated by simulations.

A prime example of where ILs can make their mark is in carbon-based supercapacitors that store electrical energy at the nanoporous electrode-electrolyte interface. How ILs assemble at this interface governs the amount of energy stored and the charging and discharging rates in devices.

However, comprehensive structural insights have been slow to evolve because electrolyte behavior at interfaces and under confinement is challenging to resolve. This is especially true for ILs, which exhibit bulky, flexible, and widely varying molecular configurations.

During an LDRD-funded research project, LLNL scientists coupled X-ray experiments with high-fidelity simulations to investigate a widely used family of ILs confined in carbon nanopores typically used in supercapacitors. The work represents the first study that combines first-principles molecular dynamics and X-ray scattering to analyze spatially confined ILs, enabling new insights into exotic properties that only occur within these exceptionally small spaces.

The team experimentally detected extreme disruption in the structure of the ILs, which was uniquely predicted and explained by their simulations. They also demonstrated how deviations from typical liquid behavior depended heavily on the relative sizes of the ions and pores. Finally, despite significant deviations in structure under confinement, the study indicates that the superior electrochemical stability of ILs remains intact, which is important for maintaining the performance of energy storage devices.

A key part of the project’s success involves the integration between quantum-mechanical simulations, tailored nanomaterials synthesis, and advanced X-ray characterization. “This powerful combination of techniques offers a far more complete understanding of ILs structure in extremely narrow porous carbons,” said LLNL scientist Tuan Anh Pham.

LLNL researchers synthetically tuned the pore sizes within high-surface-area nanoporous carbon aerogels. This novel capability enabled the team to use synchrotron X-rays to probe various confined states of the ionic liquids and piece together a more comprehensive picture of the effects of confinement on structure. According to Eric Meshot, LLNL scientist and the principal investigator on the project, "We were able to uncover some key fundamental insights that have important practical implications for energy storage devices."

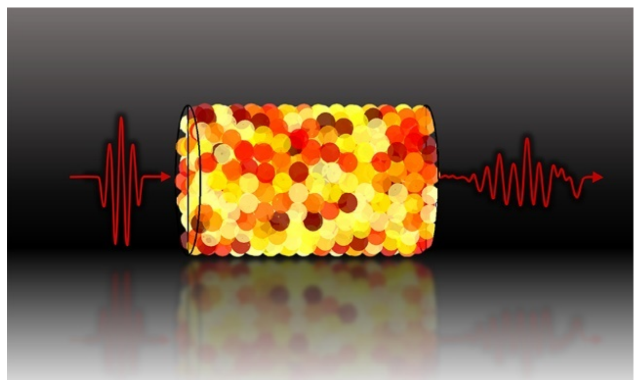
The research was funded by LLNL's LDRD program, and findings were published in the *Journal of Physical Chemistry Letters*. (*LLNL-WEB-458451*)

Livermore researchers catch a wave to study granular material properties

Stress wave propagation through granular material plays a key role in detecting the magnitude of earthquakes, locating oil and gas reservoirs, designing acoustic insulation, and designing materials for compacting powders.

A team of LLNL researchers studied the time- and frequency-domain features of wave propagation in randomly packed grainy materials to better understand the fundamental mechanisms controlling wave velocities, dispersion, and attenuation.

The scientists used X-ray measurements and analyses to show that velocity scaling and dispersion in wave transmission is based on grainy particle arrangements and inter-particle forces, while reduction of wave intensity is caused primarily by grainy particle arrangements alone.



This illustration depicts the experimental work done to measure ultrasound propagation in granular materials. The image is a combination of two sets of data from X-ray scans of single crystal sapphire spheres. The combination and colorization of the data shows the distribution of stresses for each grain under load.

The experiments, along with the supporting simulations, provided insight regarding why wave speeds in granular materials change as a function of pressure. They also quantified the effects of particle-scale phenomena on macroscopic wave behavior. Understanding these relationships enables design of wave-damping materials and non-destructive testing technologies.

The research was funded by LLNL's LDRD program, and findings were published in the *Proceedings of the National Academy of Sciences*. (*LLNL-WEB-458451*)

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