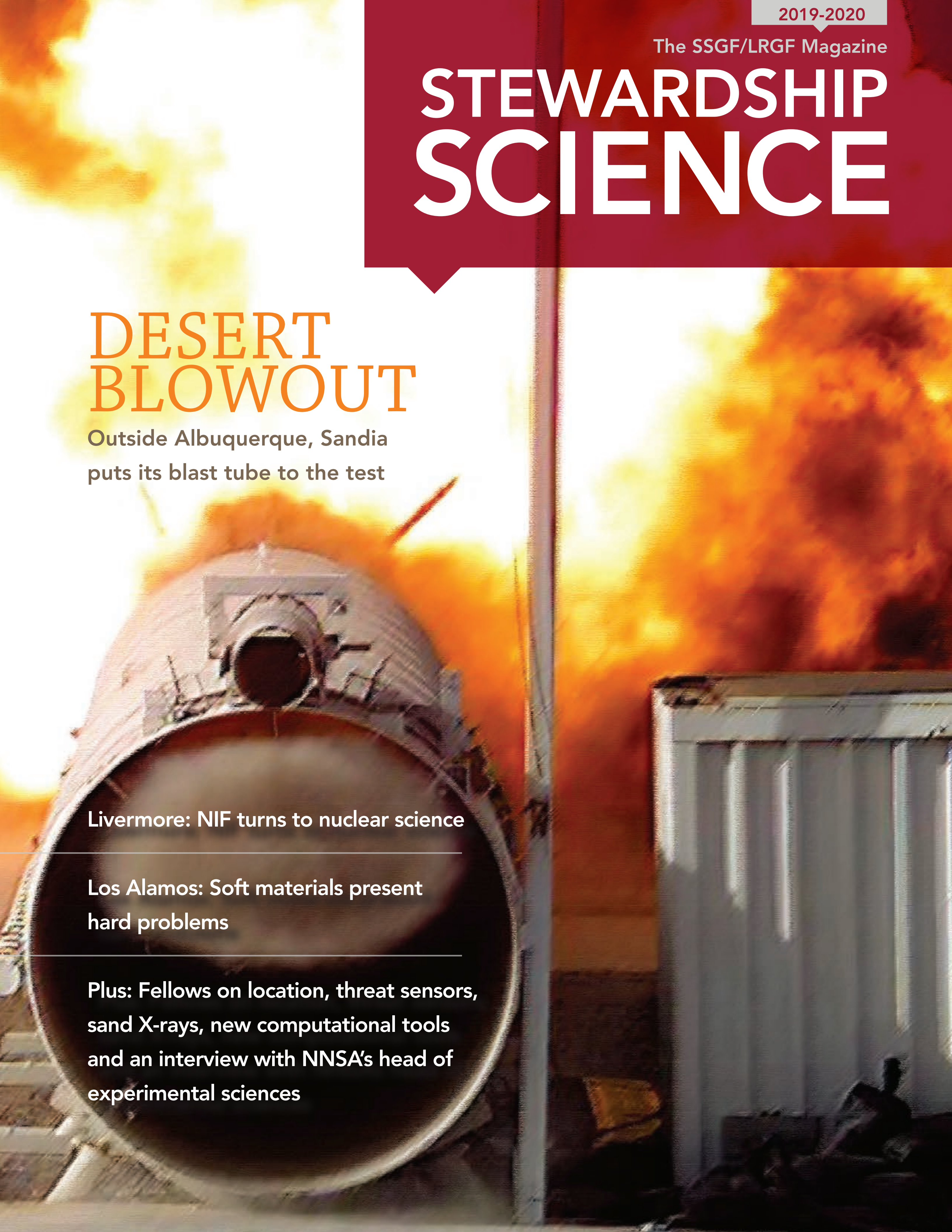
2019-2020

The SSGF/LRGF Magazine

STEWARDSHIP SCIENCE



DESERT BLOWOUT

Outside Albuquerque, Sandia puts its blast tube to the test

Livermore: NIF turns to nuclear science

Los Alamos: Soft materials present hard problems

Plus: Fellows on location, threat sensors, sand X-rays, new computational tools and an interview with NNSA's head of experimental sciences

ANNOUNCING THE 2019-20 INCOMING FELLOWS

DEPARTMENT OF ENERGY NATIONAL NUCLEAR SECURITY ADMINISTRATION

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The Department of Energy National Nuclear Security Administration **Stewardship Science Graduate Fellowship (DOE NNSA SSGF)** provides outstanding benefits and opportunities to students pursuing a Ph.D. in stewardship science-connected fields, including properties of materials under extreme conditions and hydrodynamics, nuclear science and high energy density physics. The program includes a 12-week research experience at Lawrence Livermore, Los Alamos or Sandia national laboratories.

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The Department of Energy National Nuclear Security Administration **Laboratory Residency Graduate Fellowship (DOE NNSA LRGF)** provides U.S. citizens entering their second (or later) year of doctoral studies with a unique option: pursuing research at NNSA facilities for extended periods. Candidates studying fields relevant to nuclear stockpile stewardship work in residence for at least two 12-week periods at Lawrence Livermore, Los Alamos or Sandia national laboratories or the Nevada National Security site.

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Images courtesy of Sandia National Laboratories (top) and Lawrence Livermore National Laboratory (bottom).

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LETTER FROM THE EDITORS

Milestones

WELCOME TO *STEWARDSHIP SCIENCE* MAGAZINE, our 10th issue. A milestone, to be sure, but by no means the only one.

You may have noticed our tagline has changed, reflecting the inclusion of the Laboratory Residency Graduate Fellowship, or DOE NNSA LRGF. It's the Department of Energy National Nuclear Security Administration's latest effort to replenish our nation's stockpile-stewardship research workforce. This summer also marks a milestone in the young program: By the time you read this, members of our first class, selected a year ago, will be deep into or will have completed their first residency at an NNSA lab. We hope to share their and subsequent classes' lab-research experiences in future issues.

You need not wait to hear from our final-year SSGF recipients, who over the next few pages describe their research and lab practicum experiences. Elsewhere you'll find in-depth tales of painstakingly planned and documented blasts, explosions and implosions, plus a fellow essay that was judged best among a record number of submissions in this year's SSGF Essay Slam. And we talk with Njema Frazier, who directs NNSA's Office of Experimental Programs and reminds us that it's "the people who bring new thoughts, new energy and new talent that will help us face challenges that emerge and will help us refine the excellence we must maintain."

– The Editors, *Stewardship Science: The SSGF/LRGF Magazine*

2019 2020

STEWARDSHIP SCIENCE

DEPARTMENTS

COVER

BOOM, BOOM, BOOM

A view from behind Sandia National Laboratories' blast tube, firing in the New Mexico desert. The tests are designed to show how nuclear weapons would fare in the shock wave of an enemy weapon and to validate computer models. The experiments are a major production, involving as many as 30 people and up to a month of preparation, safety evaluations and blasts that can be heard for miles. Read more on page 12.

SSGF LRGF

Stewardship Science: The SSGF/LRGF Magazine showcases researchers and graduate students at U.S. Department of Energy National Nuclear Security Administration (DOE NNSA) national laboratories. *Stewardship Science* is published annually by the Krell Institute for the NNSA Office of Defense Program's Stewardship Science Graduate Fellowship (SSGF) and its Laboratory Residency Graduate Fellowship (LRGF), both of which Krell manages for NNSA under cooperative agreement DE-NA0002135. Krell is a nonprofit organization serving the science, technology and education communities.

For additional information, please visit www.krellinst.org/ssgf, www.krellinst.org/lrgf or contact the Krell Institute 1609 Golden Aspen Dr., Suite 101 | Ames, IA 50010 | Attn: SSGF/LRGF | (515) 956-3696

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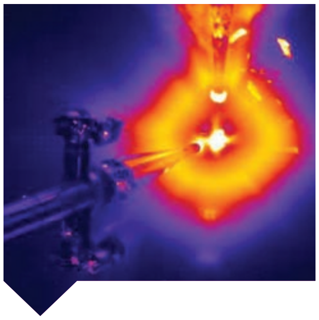
By Monte Basgall
Explosive tubes in the desert outside Albuquerque help Sandia researchers hone the science of "hostile blast-testing."

The author is a freelance writer and former reporter for the *Richmond Times-Dispatch, Miami Herald, Raleigh News & Observer* and Duke University's news office.



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Livermore scientists aim NIF's powerful lasers at the atomic nucleus to fine-tune stockpile stewardship models.

The writer is a contributing science editor for *Highlights for Children Inc.* and a freelance science writer and editor.

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SOFT MATERIALS, EXTREME SHOCKS
By Sarah Webb
At Los Alamos, a team turns a gas gun from metals to polymers and foams in a search for sturdier soft stuff.

The author is senior science writer at the Krell Institute and a frequent contributor to *Stewardship Science*.

IMAGE CREDITS
Cover, Sandia National Laboratories (SNL); Pages 4-8 (portraits), Krell Institute; page 4, Michael P. Short; page 5, Lawrence Livermore National Laboratory (LLNL); page 7, Arianna Gleason; page 9, SNL; page 11, DOE/NNSA; pages 12, 13, SNL; pages 16-19, LLNL/ Damien Jemison (NIF interior); pages 21, 22, Los Alamos National Laboratory/University of Illinois (Eric Brown portrait); page 24, Erin Good.

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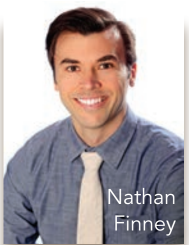
This year's four outgoing DOE National Nuclear Security Administration Stewardship Science Graduate Fellowship recipients share their research experiences.



TWISTED RESISTOR

Nathan Finney never expected to be a full-time researcher. By 2015, he'd spent several fulfilling years teaching physics, math, engineering, skateboarding, and art to kids in grades 7 through 12 at New York City's Columbia Secondary School. In the evenings, he took graduate-level science courses, and he spent summers working on research projects in the **Columbia University** laboratory of mechanical engineer James Hone.

Finney soon realized that a Ph.D. was an option. "It was a difficult decision. I was happy with my job," he recalls, but the opportunity to work in a top lab in an exciting, emerging field was too good to pass up.

At Columbia, Finney studies twistable electronics – layered nanoscale systems in which the electronic response changes as one sheet is rotated relative to the others. Until recently, however, researchers couldn't easily turn single atomic layers relative to each other within a device. "It's very difficult to do science where the twist angle between atomically thin crystals is your independent variable," Finney says.

Last year in the journal *Science,* Finney's Columbia colleagues described a three-layer device built with insulating boron nitride (BN) and conducting graphene, an atom-thick layer of bonded carbon, topped with a layer of BN shaped like a gear. Using the tip of an atomic-force microscope (AFM), they pushed this top disk relative to the slightly misaligned layers below and studied the device's electronic response. "The ability to dynamically rotate layered crystals in a single device opened the door to really understand complicated twistable systems," Finney says.

BN and graphene both have honeycomb-like hexagonal patterns or lattices of atoms that are almost the same size (2.5 and 2.46 Angstroms, respectively). Just as when light shines through two bigger, partly transparent geometric patterns, the combination at the nanoscale creates a larger interference pattern, known as a moiré superlattice. Finney has aligned the bottom two layers of BN and graphene and then rotated the top BN layer relative to the lower ones. That twisting alters the overall symmetry in the device and can tune its electronic response. When all three layers are perfectly aligned, the combined interference pattern enhances the bandgap of this system – the difference between two allowed ranges of electron energy in a solid – to 60 meV, more than half that of the semiconductor silicon. When the top layer is rotated 60 degrees, the gaps are suppressed to less than 20 meV, nudging the material toward metallic behavior.

This platform could eventually help researchers develop mechanically tunable devices that change their electrical properties when exposed to light in the far-infrared spectrum, Finney notes. These photodiodes could be useful for astronomy, medicine, and search and rescue. If researchers can swap an AFM tip's nudge for electromagnetic force, these tiny electronics could use their own feedback for real-time adjustments.

Finney completed his practicum in 2016 with Marcus Worsley at Lawrence Livermore National Laboratory, where he studied techniques for making graphene aerogels, which are low-density solids. He expects to graduate in 2020 and is exploring a range of postdoctoral research options.

FASTER MATERIALS TESTING

Cody Dennett now designs testing strategies at the **Massachusetts Institute of Technology** for materials used under extreme conditions, but carpentry and handyman work with his father in small-town Maine shaped his career path. "Those skills, building systems and testing things, have been almost as important as the technical education," he says. While a Cornell University undergraduate, he employed these abilities installing and evaluating a new system to measure how materials performed in the university's synchrotron X-ray source.

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Cody Dennett uses lasers to heat metal, exciting the samples and generating acoustic waves whose motions enable him to study the material's defects.

Lawrence Livermore National Laboratory physicists are developing an array of liquid scintillator cells to track with high precision neutron and gamma ray emissions from special nuclear materials, providing information about a radioactive source's elemental constituents, size, and configuration.

Sensing Threats Where They Are

In July 2010, a cargo ship pulled into Genoa, Italy, carrying a container holding two tons of scrap metal that were emitting torrents of radiation. Fearful that the box housed a dirty bomb, multiple government agencies spent three days determining the true source of the radiation: a nine-inch rod of cobalt-60 that likely came from a medical device or a machine used to sterilize food.

One day, customs officials will quickly and safely assess the danger such mystery objects present, thanks to a well-refined theory and the detectors that a team of Lawrence Livermore National Laboratory (LLNL) physicists is developing with support from the Department of Energy National Nuclear Security Administration's nonproliferation and counterterrorism offices.

"We want to be able to take an object that we already know is radioactive and determine its level of threat," says project leader and LLNL scientist Les Nakae, who stresses that his team's goal is assessment, not detection. "We're not going to be out searching the world for radioactive materials."

Special nuclear materials (SNM) – such as highly enriched uranium and plutonium-239 found in nuclear stockpiles – are unique among radioactive substances because they create self-perpetuating fission chain reactions and in turn emit bursts of neutrons and gamma rays. Precisely tracking the paths and timing of these bursts can provide a wealth of information about a radioactive source, including its elemental constituents, size, and configuration, all of which can be used to create a threat profile.

Nakae and his team have fine-tuned their method for analyzing SNM emissions – based on nuclear fission chain theory – for nearly two decades. They use Monte Carlo methods to exactly reproduce the various probabilities of observing specific fission chain signatures. Famed physicist Richard Feynman originally developed these methods to measure SNM criticality for the Manhattan Project. The mathematical structure employed in fission chain work anticipated methods Feynman applied in his Nobel Prize-winning research in quantum electrodynamics.

Beyond its theoretical work, the team has built prototypes of hardware capable of counting neutrons and gamma rays with nanosecond timing. These devices – liquid scintillator arrays – contain cells of liquid that light up as charged particles move through them. The arrays allow Nakae's team to test its theory across multiple time scales, since neutrons propagate through various materials within the arrays and induce interactions at different speeds.

The biggest advantages of liquid scintillator arrays are their nanosecond resolution and their sensitivity to both neutrons and gamma rays. Nakae says the arrays are so much faster and provide so much more detail than the thermal detectors they formerly used that they had to modify their fission chain theory to accommodate the extra information.

However, myriad disadvantages of scintillator arrays make it challenging to build field-ready versions. About the size of a footlocker, the arrays are much bulkier than thermal detectors. They also are filled with mineral oil that requires special handling and contain elaborate electronics that need a portable generator for power and must be recalibrated almost every time they are moved. "At the moment, we can run them fine in a lab or measuring facility," Nakae says, "but you can't just put them out in the street, turn them on, and expect them to work."

As if all these constraints aren't enough, the arrays produce a startling amount of data. "These things sample so quickly, we end up spending hours, days even, processing the data," Nakae says. "And that's just not appropriate for a real-time field operation."

To accelerate data analysis, Nakae's team is designing an intelligent onboard processor that can selectively sample the data. They're also working on displays so the devices can deliver results in intuitive graphics to non-specialist users.

Despite all of these challenges, Nakae says getting the arrays to work outside the lab – likely a multiyear effort – is worth it. "The quality and depth of information provided by these arrays more than justifies the level of effort."

Chris Palmer

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A senior-year course convinced Dennett that nuclear energy would be a key part of a sustainable energy mix. As he considered graduate studies, one of his professors told Dennett about the need for advanced materials that can withstand the extreme conditions in nuclear reactors.

Most operating nuclear plants in the United States were developed half a century ago. However, the high radiation, temperatures and pressures, plus the effects of corrosive fluids, stretch the ability of many materials to perform safely for decades. Most dramatically, years of service can alter the shape and length of stainless steel components by tens of percentage points. "Just from an engineering standpoint, that's hugely detrimental," Dennett says. Maintaining nuclear reactors requires understanding material degradation and employing materials immune to the most severe damage.

Testing materials in these extreme environments, however, is slow and costly. Researchers commonly expose substances to radiation, wait for any activated isotopes to dissipate, and destroy them to understand properties and performance. The process can take years. In his Ph.D. research with Michael Short at MIT, Dennett has developed a non-destructive approach that examines material performance in real time using ion beam irradiation, which blasts materials with charged particles. Researchers can now observe changes continuously, replacing months or years of testing with a single day of experiments. If scientists adopt this faster testing strategy, they could explore a larger range of new reactor materials.

One critical piece of this research has been designing and constructing the online ion beam irradiation test facility, a challenge smoothed by Dennett's fellowship. Materials scientist Khalid Hattar at Sandia National Laboratories in New Mexico learned of the research and asked Dennett if he'd like to build the proposed facility within Sandia's Ion Beam Laboratory. "Making that connection was really, really key to the work," he says.

Dennett spent his 2017 practicum at Sandia and has returned every few months to test materials. He and his Sandia colleagues are currently evaluating new alloys from other national laboratories, providing complementary results to other assay strategies. Dennett appreciates the national labs' collaborative environment and the dedicated staff that keep facilities he relies on running. After graduation, he hopes to broaden his work on testing materials as a postdoctoral associate at one of the DOE laboratories. In that environment, he says, "there's a lot of good work to be done that I think I can do quickly."

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Shocked Sand Under the X-ray

The substances Arianna Gleason examines are as common as sand but nonetheless yield interesting discoveries as she refines X-ray instruments that could reveal properties of more unusual materials.

Gleason is a scientist at California's SLAC National Accelerator Laboratory, which she joined as a Los Alamos National Laboratory Reines Distinguished Postdoctoral Fellow with an aim to connect the facilities for stockpile stewardship research. She now is a Los Alamos guest scientist and a Stanford University adjunct professor.

Gleason's main tool is SLAC's Linac Coherent Light Source (LCLS), which accelerates electrons to produce bright, brief X-ray pulses that capture the fast, tiny interactions of atoms and molecules. Recent experiments have focused on silicon dioxide, the main mineral in sand, glass, and quartz. The second-most abundant material on Earth's surface, scientists have often squeezed it to see how high pressures change its crystalline structure. "It's a good testbed material to make sure we understand how we orchestrate ***in situ*** time-resolved measurements" of structural changes under pressure.

Her experiments focus on the mesoscale, which is the space between atomic structure and bulk material properties. Her work addresses how grains that compose solids form and how grain boundaries influence large-scale performance. The results feed into mathematical models that researchers use to engineer new materials.

What's more, such models can calculate aging's effects, such as embrittlement and void development, on nuclear stockpile materials.

"We have to benchmark our models with experiments that are at the appropriate time scale, length scale and strain rates – *in situ* measurements" capturing behavior as the materials change.

Tests on benign samples such as silicates also answer questions about the physics of Earth's geology. "You get to do really exciting geoscience, but you're also building up this materials genome, this broader understanding of materials properties at extremes."

In a 2017 *Nature Communications* paper, Gleason and her collaborators described using the LCLS's Matter in Extreme Conditions end-station to recreate the tremendous fast shock of a meteorite hitting Earth or another planet. Such impacts transform silicon dioxide to a diaplectic glass, in which the crystals dissolve into a disordered state of variable density without melting.

Arianna Gleason makes final adjustments to detector positions inside the Matter in Extreme Conditions target chamber at the SLAC Linear Accelerator Laboratory.

In the experiment, a high-intensity laser blasted a plastic film, sending a shockwave toward a pure silicon dioxide target. The LCLS's bright, trillionths-of-a-second X-ray pulses struck the material as it was shocked and diffracted into patterns the scientists studied to learn how the sample's atomic structure changed over time.

The data revealed that the transition from quartz to diaplectic glass occurred in a mere 2.4 nanoseconds and at a pressure of 33.6 gigapascals – approximately the pressure found around 300 miles below Earth's surface. When the initial shock hit, the sample's crystalline structure changed to stishovite, a denser form of the mineral. But when the pressure released, it became diaplectic glass.

"For the first time we witnessed the transformation mechanism" from a sample at ambient conditions to stishovite to glass, Gleason says. The pressure at which the transformation occurred was lower than that predicted from analyzing impact-formed glass at craters. This means previous calculations had overestimated how big the space rocks had to be to compress silicates into glass.

Beyond the geophysical data, the experiment demonstrates the *in situ* X-ray diffraction method's capability. "Maybe there's some unique phase of a metal or an alloy that has unusual strength and ductility," Gleason says. "We could use this platform to examine those properties."

Scientists from SLAC, LANL, and other institutions contributed to the project, including Department of Energy National Nuclear Security Administration Stewardship Science Graduate Fellowship alumnus Rick Kraus at Lawrence Livermore National Laboratory, who helped analyze shock velocity and pressure data.

More recently, Gleason and Stanford graduate student Shaughnessy Brennan Brown performed similar laser-driven compression experiments but added a second instrument to capture *in situ* images of shocked silicon. As before, an X-ray diffraction beam tracked structural changes, but a second beam perpendicular to the shock also captured X-ray images of the material as the shock hit.

Such visualizations can help scientists make fewer assumptions about the process and map critical points in the transformation, Gleason says. "A lot of folks at Los Alamos and other labs are very interested in developing this."

Thomas R. O'Donnell

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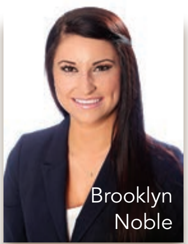
SKIMMING SURFACES



Brooklyn Noble had an early passion for science, encouraged in part by her mother. They were together a few years ago when Noble realized a childhood dream: touring the CERN supercollider in Switzerland. Her mother, Noble says, "is not a scientist, but she loved it because I loved it."

Noble first learned about tribology – the study of wear, friction and lubrication – in a **University of Utah** undergraduate course with her future Ph.D. advisor, Bart Raeymaekers. Much of how materials interact with their environment depends on their surfaces. Researchers might find that a material has interesting bulk properties, such as conductivity, formability, or stiffness, but wears easily, she notes. Adding a surface coating could make that material more durable without altering other desired features.

Noble soon became fascinated with understanding surfaces and how they could be changed. As an undergraduate, she worked with Raeymaekers to study ultrathin lubricating films in collaboration with computer hard disk-drive maker Western Digital. Hard drives require atomically smooth surfaces, a quality that involves this type of exact engineering.

As a Ph.D. student, Noble has focused on broader tribology questions. She uses molecular dynamics computer simulations to calculate materials' atomic-level surface properties and study how they interact with their environments. "My day-to-day question is digging deeper: well, why did that happen?" she says.

Tribology is filled with conflicting results, in which one group's observations seem at odds with another's. Noble thinks these apparent discrepancies are linked to design differences, such as the temperature or scale of the experiments, rather than errors. She focuses on explaining what's happening at an atomic level.

In a recent paper in the journal *Nanotechnology*, Noble recounts modeling nanoscale surface textures and how polymer-based liquids spread across those textures, describing the roles of pressure and how polymer molecules tangle with each other.

These fundamental insights could help with various precision design problems. In addition to hard drives, ultrathin polymer films could coat medical devices, preventing bacteria from sticking to them and growing. If researchers could design strong, atomically thin coatings that resist wear, they could develop and build nanoscale motors.

For her 2016 practicum at Lawrence Livermore National Laboratory, Noble took her molecular dynamics simulations skills and applied them to a different problem: understanding strongly coupled plasmas. These dense ionized gas clouds – found in astrophysical bodies and inertial confinement fusion experiments – transport energy differently from other plasma types. Noble used molecular dynamics to model the flow behavior, or viscosity, in these systems.

Noble enjoyed the teamwork at Livermore and would like to work at a national lab after graduation. "All the resources there were incredible. The supercomputers, the environment, and the people were really amazing," she says.

GRASPING A BLAST

Christopher Miller enjoys digging into classical properties of materials, such as how they deform and resist fracture. For his Ph.D. research with Min Zhou at the **Georgia Institute of Technology**, he has examined the structural mechanics of highly energetic materials, such as explosives. A better understanding of how they respond to impacts – from the molecular level to the macroscale – can prevent accidental detonations.

Miller is most interested in what happens at the mesoscale level – the interaction of energetic crystals the size of sand grains. Because that scale, measured in microns, bridges the gap between molecular dynamics and bulk material response, his work incorporates chemistry, materials science, solid mechanics and wave propagation.

As shock waves spread through energetic composites, the materials deform and crack. Those physical changes generate heat, which starts chemical chain reactions. Testing these processes experimentally is time-consuming and expensive, Miller says, and researchers can't record many of the physical changes at the explosive's center, which are essential to understanding how it detonates. High-performance computing is invaluable to overcome these challenges and to study existing explosives and develop new ones. Miller says he "can run 1,000 simulations overnight of some of these impact tests rather than an experiment that takes multiple hours to set up."

A range of physical processes occur as an explosion begins: pores collapse, materials deform, and friction between grains generates heat. Modeling these systems requires simulating each of these

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Computing at the Vanguard

Sandia National Laboratories computational scientists are testing Astra, one of the first supercomputers that uses ARM processors found in smartphones and cars. It's the first project in the Vanguard program, which aims to expand the large-scale computer architectures available for the Department of Energy National Nuclear Security Administration (DOE NNSA).

Vanguard falls between small testbed systems and the full-scale production supercomputers that stockpile stewardship has relied on since U.S. nuclear weapon explosive testing ended a quarter-century ago. These large-scale hardware systems run codes to model complex scenarios in chemistry, physics, materials science and engineering. To support these efforts, computational scientists at Sandia and the other NNSA national security laboratories – Lawrence Livermore and Los Alamos – need new hardware like Astra's.

Investigating new computer equipment on this scale can involve risks, says James Laros, Vanguard project lead at Sandia's site in Albuquerque, New Mexico. A technology that shows promise on a handful of nodes might not work the same at scale. Vanguard enables researchers to test production codes on sufficiently large prototypes without the immediate pressure to support day-to-day operations. Laros and colleagues began testing the first 64-bit ARM technology in small testbed systems in 2014. ARM processors are ubiquitous in consumer electronics, Laros notes, but until recently haven't performed well enough to compete with the workhorse IBM or Intel CPUs in today's largest computers.

A newer family of ARM processors is more powerful and offers other advantages, including better memory bandwidth. "We have really twice as many memory channels on the ARM chip as we have on some of our production server-class processors in our other systems," says Simon Hammond, a Sandia research scientist. Many of the NNSA applications require integrating data from various parts of the hardware, he notes. Twice the memory channels could at least double the speed at which hardware access those various data components.

The Astra planning started in June 2017, as Laros and his team worked with vendors on an ARM-based approach. In fall 2018, the team started its initial assessment of Astra's performance and accuracy, using unclassified codes as benchmarks. Eventually, they'll directly compare Astra's performance on NNSA's classified codes and the overall user experience with the same metrics on existing production systems.

The prototype system allows the team to focus on analyzing and improving Astra's performance and on whether they can boost efficiency and accuracy. "What do we need to do to the environment to make the applications run on this pathway?" Hammond asks. "It's a perfect combination of still trying to solve the hard problems with real applications but not being under the gun to do it really, really quickly."

Throughout Astra's development and optimization, the Vanguard team has collaborated with Westwind Computer Products and Hewlett Packard Enterprise. Hammond compares these architectures to stacked plates whose base includes layers from suppliers that map some of the basic structure and primitive functions into the system. "So it's important that we get those base plates really done well," he says. "Above that then there's a load of other plates, and that's the bit where the DOE and the teams here at Sandia and (Los Alamos and Livermore) will add all their value in their applications."

Laros expects Vanguard will go beyond examining processors to, for example, testing advanced network technologies. "Just like memory bandwidth can be a bottleneck, networks can also be a bottleneck because our applications run on thousands to tens of thousands of nodes in cooperation."

The Vanguard program won't solve all the challenges inherent with large-scale computer platforms, Laros says, but it will create a path for testing ARM and other new technologies and comparing their performance to current computer architectures. If someone wants to propose a future ARM-based production system, his team will know whether it's viable after testing Astra.

Sarah Webb

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processes, weighing their effects, and matching those combinations with experimental results. "One of the largest unsolved questions of the shock physics community is how relatively important each of these effects are," Miller says.

At Georgia Tech, he and his colleagues use an algorithm called Cohesive Dynamics for Explosives (CODEX) to study explosive grain structure, examining how embedded aluminum shavings can stabilize the materials by improving their structural integrity and making them less likely to detonate. "As the stress wave propagates through the material, tiny aluminum particles help to redistribute the pressure," he says.

Miller's also worked with other codes in practicums at two national laboratories. With Laurence Fried at Lawrence Livermore National Laboratory in 2016, Miller used the ALE3D code to model the effects of friction within explosives. In 2018, he and Cole Yarrington used Sandia National Laboratories' CTH code to incorporate the effects of holes and pores on explosives at the mesoscale. The codes have various tradeoffs in time versus accuracy and in how well they can scale up for larger simulations, Miller notes. "This is a research problem that will require a number of codes to fully answer. I can examine each physical process using the best possible tool for the job."

Miller would like to integrate results from various simulations and codes to answer important questions and make predictions. For example, he's observed that smaller individual grains within explosives make the materials more sensitive, primarily because of the increased surface area. He's also examining how the aluminum shavings desensitize explosives without compromising power. "They don't react in initiation, but when the explosive detonates, they'll go."

CONVERSATION

Njema Frazier directs the Office of Experimental Sciences in the National Nuclear Security Administration. She previously worked with the Advanced Simulation and Computing Program and led the Office of Inertial Confinement Fusion. She is a Leadership Ambassador for the OneDOE Campaign as well as for the Department of Energy's (DOE's) Minorities in Energy Initiative. She co-founded the POWER (Professional Opportunities for Women at Energy Realized) Employee Resource Group at DOE. Dr. Frazier is a theoretical nuclear physicist with master's and doctoral degrees from Michigan State University and a bachelor's degree from Carnegie Mellon University.

Embracing New Approaches

Give us an idea of what you do.

I'm responsible for a suite of experimental facilities that provide the science basis for ensuring the U.S. nuclear weapons stockpile is safe, secure, and reliable while sustaining our weapons-testing moratorium. This includes research in nuclear physics, plasma physics, materials science, chemistry, metallurgy, and other subjects using light sources, gas guns, lasers, particle accelerators, and similar devices. Our team works with other federal agencies and employs academic alliances and industrial partnerships to accomplish our mission.

What challenges does stockpile stewardship face in the coming years?

They aren't much different from the ones we've confronted in the past: maintaining a rigorous scientific base upon which to make some really high-consequence decisions. Because we must certify to the president every year that we have a safe, secure, and effective stockpile, we must ensure that conclusion is rooted in the strongest evidence possible. That's an enduring and pervasive challenge we face, so we need the best equipment, best minds, best plans, and best management.

If the challenges have changed little, do you follow the same course or are there new frontiers the NNSA will explore to address them?

The way we do business can be informed by new ideas and approaches – new architectures, new technologies, new ways of learning. For example, we could bring in machine learning for uncertainty quantification or traditional business practices to make sure we're streamlining the process and have improvement procedures. There's a stable base of knowledge upon which you need to be flexible, you need to be in tune, and you need to be aware to incorporate improvements into operating these programs. We want to think about whether we can build facilities in a new way, store data in a new way, or use computational science in new ways. It's those types of emerging areas we want to be sure we can incorporate into the program and into the science we do.

How does the DOE NNSA SSGF fit into that mission?

In a couple of ways. Much of its research is relevant to what we do, so the papers, the journals, and the poster sessions the program produces looking at these key areas comprise a base level of knowledge for us. The other is workforce development. We cultivate people who are not only trained in specific scientific areas and understand the phenomena, but also think about things scientifically, challenge assumptions, and develop hypotheses to unravel what we don't know. Those are all things that are invaluable to us. It really is the people who bring new thoughts, new energy, and new talent that will help us face challenges that emerge and will help us refine the excellence we must maintain.

You're an advocate for a diverse workforce at DOE. What progress have you seen in this area and what more can be done?

Progress has been made, particularly in the representation of women within the NNSA. That took deliberate effort. If it was naturally going to happen, it probably would have already. Underrepresented minorities – blacks, Hispanics, people who have come back from continuing education, veterans – those are where we want to make sure we don't lose focus. There are DOE offices set up that address that and they really try to give high visibility to various programs, but a lot of work still needs to be done – especially in scientific areas. I hope it stays on everyone's mind to provide opportunities – not just at the upper echelon, but to a broader range of academic institutions, companies, and other organizations and groups. We should consider how we can partner with those institutions, such as adopting a school, because everybody doesn't have equal resources or entrée into fellowships, centers or other programs. We must ensure we're not just working with the same 10 universities or 10 groups or 10 associations.

What would you tell a student considering research in stewardship science?

I would tell her or him what I tell all students deciding on an area of study: If you have a passion for it, if you're curious about it, you should pursue the most challenging problems that can make the most impact. That's an intersection that stands out in stewardship science. Not every field has both of those elements.

TOTALLY TUBULAR

SANDIA NATIONAL LABORATORIES PRODUCES EARTH-RATTLING EXPLOSIONS IN CAVERNOUS CYLINDERS TO LEARN HOW OUTER-SPACE BLASTS MAY AFFECT NUCLEAR WARHEADS.

BY MONTE BASGALL

Sandia National Laboratories' blast tube.

When Sandia National Laboratories loads more than 100 pounds of bulk explosives into one of its blast tubes outside Albuquerque, New Mexico, lab officials put out an advance media alert. That's because, depending on the weather, the blast can be heard nine miles away in the city's business district.

Up close, firing one of these 12-foot-diameter by 120-foot-long tubular steel facilities is an impressive national stockpile security exercise. Roaring flames erupt after a NASA-like countdown. Then, in an instant, a potentially supersonic pressure wave pushes a heavily-instrumented mock nuclear warhead.

Experts conduct follow-up analyses after each blast tube test series, gathering vital physical evidence for something that has only been computer-modeled – and never, thankfully, actually happened. The government needs to know whether a U.S. nuclear weapon could weather an attempted enemy interception as it re-approaches Earth's atmosphere en route to a target.

"That's why Sandia developed these back in the late 1950s," says Nathan Glenn, test director and a mechanical engineer with a graduate degree in energetic materials.

Glenn describes such exercises as hostile blast-testing, a scenario in which adversaries attempt to damage or destroy a weapons system. "We want to understand what that does to our weapon. We want to have some certainty that it can survive that event and still detonate."

The studies he directs are not responses to a specific threat, he notes, but rather to improve how warheads may respond to dangers and to improve associated computer modeling.

Of course the United States already knows plenty about how its missiles behave. "We'll do flight tests," Glenn says. "We'll send them up and then bring them back in." But a successful flight test cannot demonstrate what might happen in a hostile blast environment at the edge of space. That's what Sandia's blast tubes try to evaluate. "If another weapon went off beside it, it would create a blast wave, and that is what we're simulating. That blast environment could be from another nuke or a conventional weapon." Surprisingly, the difference between a chemical or a nuclear explosion can be subtle.

At Sandia, this energy is provided by C-4 type explosives molded into flat sheets with a rubberizing agent and then hung inside a blast tube. "We can go up to 300-pound charges," Glenn says. "That's a lot of explosives."

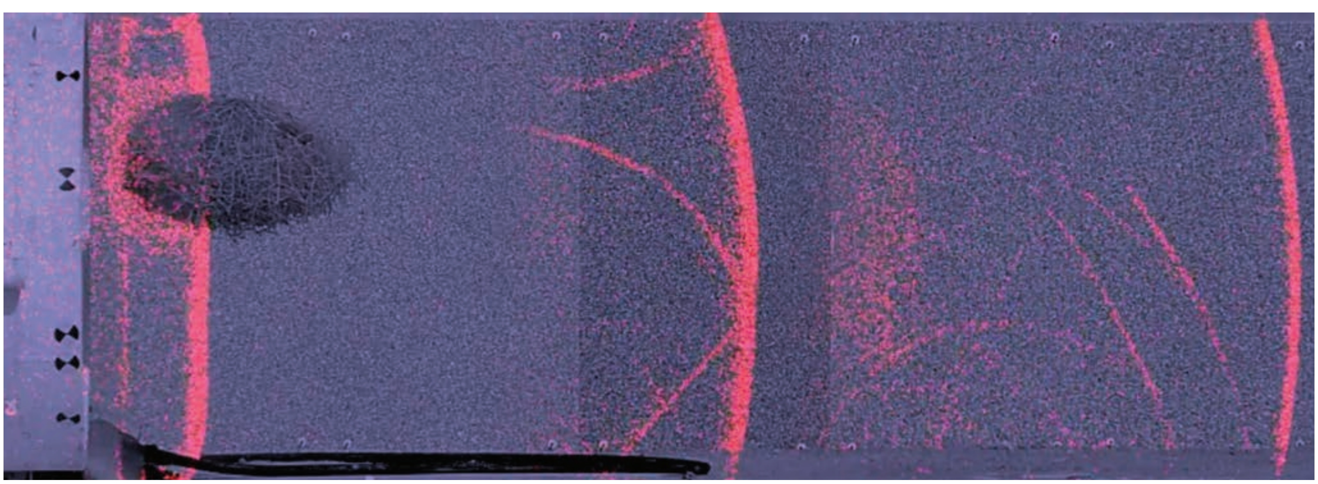
The shock tube's clients, which include the U.S. Department of Defense and units within Sandia, begin the process by asking Glenn to create a blast wave of specific strength. A typical request may be 100 pounds per square inch peak pressure, 30-millisecond pulse duration, he says.

The experiments are labor-intensive, requiring up to 30 people to devise those extreme conditions in a series that lasts about a month, including safety and environmental-impact evaluations.

Meanwhile, the researchers gather the right blast tube parts from collections stored at Sandia's 13,740-acre complex or imported from other facilities. They can also roll new tubes made of different grades of steel.

"In the late 1960s and early '70s, Sandia had five blast tubes in operation at the same time," Glenn notes. "We also do blast-effect studies on structures, aircraft components, buildings and trees."

His team consults Sandia's own shock physics code to estimate the proper explosive size, then double-checks whether that much charge will create a shock wave of the desired strength by conducting up to five live shots in a tube with 12 pressure-detecting transducers.



A wavefront image taken at 35,000 frames per second to analyze blast wave dynamics invisible to the eye. Such images help Sandia researchers determine how well nuclear weapons could survive a shock wave.

Attention then shifts to mockups of nuclear warheads, also called test units. They are hung inside a blast tube with detachable Kevlar ropes in front of the explosive, a placement that allows the blast's shock wave to push the test unit into an unrestricted, free-fall trajectory.

The Sandia team typically conducts two more live firings to confirm the pressure wave is loading the test unit correctly. It's common for them to subject additional test units to two trajectory shots and three or four calibration shots before switching to a higher-fidelity representation of an actual nuclear weapon – minus, he emphasizes, nuclear material.

That final unit is laden with strain gauges, accelerometers and pressure transducers to detect how the blast wave has affected all parts of the mock warhead's structure.

The test ends once the blast wave sweeps over the high-fidelity mockup, Glenn says. Then the focus shifts to the crucial test unit's welfare. "We want to catch it safely and softly" because "we want to be able to differentiate damage that happens during the blast event from what happens when it lands," keeping the latter to a minimum.

Test units usually fly no more than 30 feet from a blast tube's end before reaching a 10-by-40-foot catch pit. For lower-pressure shots, thousands of foam blocks topped with cargo nets soften a test unit's landing. Those subjected to stronger blast waves settle onto gym mats stacked like a pole-vaulting pit, anchored with nylon straps.

"All of our tests are really very harsh and dangerous environments, and they're very short events of only milliseconds," notes Anthony Tanbakuchi, a Sandia optical engineer.

Because its firings are over too quickly for human senses to register unaided, Tanbakuchi's Photometrics Group drastically slows down what blast tube video browsers see and hear.

With customized cameras that can log and manipulate 25,000 images each second, his group can also track the diameter of a pressure wave inside the tube and how it interacts with the test unit, Tanbakuchi adds.

"We're looking for the speed of the wave, the width of the wave, and then, as it moves across the unit, how it starts to deform and change," he says. "After (the wave) has passed the test unit we also want to see how that test unit moves through space."

The researchers can eavesdrop on all of this with a high-speed digital photography technique – called synthetic schlieren imaging – that reveals tiny background wobbles invisible to the unaided eye. *Schlieren* is a German word for "streak."

When a blast tube fires and dragon-like flames erupt from its gaping exit, a single high-speed photograph won't reveal much of anything about what is transpiring inside, Tanbakuchi explains. Despite appearances, the air is clear inside, and the effects are subtle.

The wobbles are due to tiny changes in the index of refraction, a measurement of how light propagates through materials.

His group is particularly interested in how the index is altered wherever the air is subtly squeezed by explosion-induced pressure waves.

'What's really unique at Sandia is we do this integrated engineering, modeling and testing.'

On digital equipment like that which the Photometric Group uses, the wobbles are visible only at the sub-pixel range, a tiny unit of programmable color on computer displays. The team can amplify the digital signals and color the wobbles red. "And the more it wobbles, the more we color it red." As a result, researchers can see and track the pressure waves as diagonal red streaks on their computer displays.

Tanbakuchi also developed special image stabilization algorithms to address unavoidable obstructive vibrations. "The problem is we have a very large explosive close to our camera system," he says. So "at the same time this pressure wave is moving across the test unit, the cameras are getting shaken like crazy."

His solution is to harness synthetic schlieren as a sub-pixel image-stabilizer. His algorithms can recover the tiny motion behind the massive camera movement the explosion causes. "It looks like the cameras aren't getting shocked at all."

The Photometrics Group's cameras are bunkered about 150 feet away from the blast tubes. To minimize distortions, glass does not shield their lenses; instead, they look out through small holes in protective half-inch steel-plate walls.

One camera is typically aimed from the side of the blast tube's entrance to capture the wave-front imaging, Tanbakuchi says.

Another looks up the barrel to view the moving test unit. A third provides an overhead view of how the test unit falls once the shock wave hits it.

At the same time, physical data from the blast tube's and test unit's large array of detectors are carefully monitored by another data acquisition system 100 and 200 feet from the blast tube's end, in a so-called blast-hardened trailer with thick steel walls.

"What's really unique at Sandia is we do this integrated engineering, modeling and testing," Tanbakuchi notes. "After the tests, we fuse all this data together so, as a complete team of modelers, engineers and testers, we can pull out data and better inform the models and inform the engineering."

That means Tanbakuchi's group can superpose visual and instrumental data, allowing the entire blast tube team to review, Glenn says, a "whole video of the event. It's amazing."

Glenn says the goals of Sandia's blast tube testing are actually two-pronged. One is to see the effects on the weapons system components and assess how the system responds. That might provide engineers clues for buttressing missiles. The second: providing Sandia modelers with data to verify their calculations. Each blast tube test can provide only one or two data points of such backup, he notes, but it's cheaper to start with models and conduct expensive blast tube testing to calibrate them.

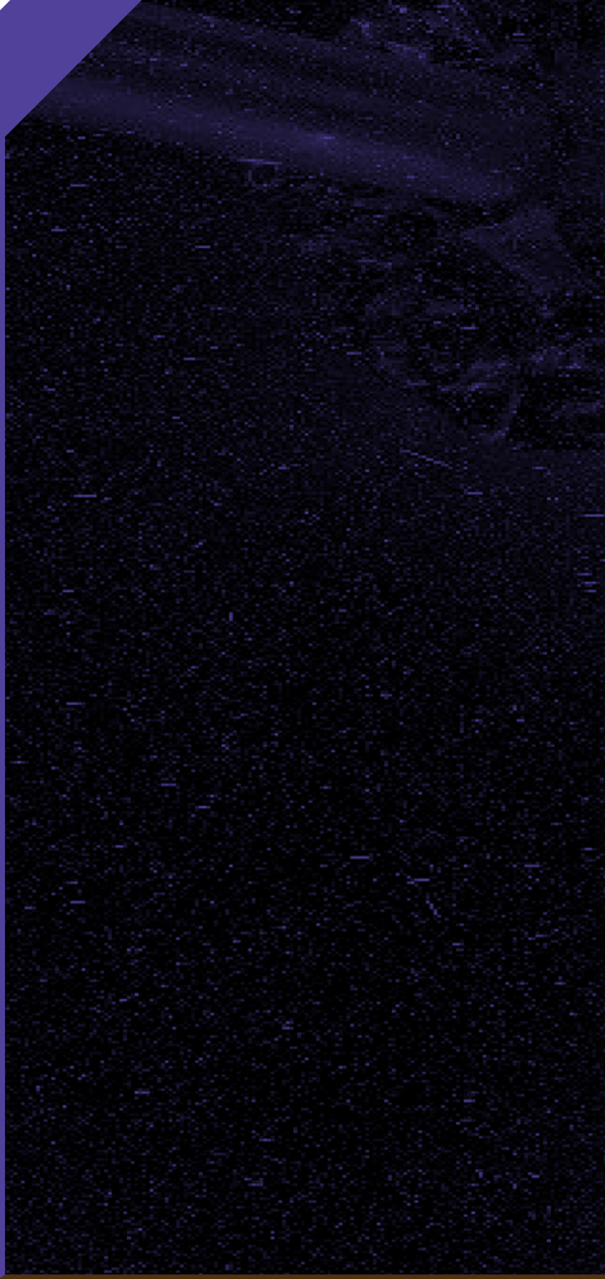
To provide such verification, Glenn describes how Sandia modelers would subject new blast tube shock-wave information to four different simulation codes, written in parallel so they can be processed in one of Sandia's supercomputers "for days or weeks, depending on what we're trying to make them do."

The team frequently uses two supercomputers: Pecos, which has 19,712 cores and can process a peak 410 trillion floating-point operations per second, and the newer Cayenne, with 40,392 cores and a peak performance of 1.3 quadrillion FLOPS.

CTH, the lab's shock physics code, yields a shock-wave pressure history that can be fed into a computational fluid dynamics (CFD) code. The CFD output can augment a structural response program that will tell Glenn's team how everything inside the blast wave is moving. Finally, they can plug the data into flight dynamics software that predicts how far the test unit will travel.

One vital interval that cannot be evaluated using a blast tube is a missile's actual atmospheric reentry. That's the unstable minutes when its nose cone heats up and sheds material. "There is spin," he says. "There is deceleration."

Though blast tubes can separately evaluate reentry effects – speed changes, spin rate, vibration, heating and the like – "the combination of those must be simulated by modelers."



INVENTIVE EXPERIMENTS YIELD NUCLEAR NUGGETS OF INTEREST IN MONITORING FALLOUT AND SHARPENING STOCKPILE STEWARDSHIP MODELS.

HOT PLATE

BY ANDY BOYLES

It was September 7, 2015.

Experiment Day. Dawn Shaughnessy and the colleagues she leads in Lawrence Livermore National Laboratory's Nuclear and Radiochemistry Group knew the results could either justify or dash a concept for generating high-value data for their national security research. "If that had been a null result, probably we would not have been able to move forward with anything else," Shaughnessy says.

On that day, Livermore research scientist Narek Gharibyan waited inside the National Ignition Facility (NIF) – home of the world's most powerful laser system. One part of the facility is the target bay, a roughly cylindrical structure with an interior space more than 15 meters in diameter and nearly 26 meters tall, divided into seven floors. It houses the target chamber, a 10-meter-diameter sphere standing on massive metal supports. Inside, 192 lasers would soon converge to trigger a brief, intense nuclear fusion reaction.

Shaughnessy sat in a car, waiting to take Gharibyan and the device they had designed for the experiment across the Livermore campus to a laboratory where another colleague, radiochemist Ken Moody, stood by to analyze results the moment they arrived.

The team had one main worry. They had spent years developing new diagnostic platforms – collectors – to capture bits of debris from nuclear reactions at NIF. Would this collector catch enough of the type of debris they sought?

The National Ignition Facility (right) and a look inside at its laser bay.

At last, the NIF technicians were ready and initiated the laser shot that triggered the reaction. That burst of nuclear fusion is the same melding of atomic nuclei that takes place in the sun, in experimental fusion machines and in thermonuclear weapons. Livermore scientists use NIF to study a range of subjects, including the promise of nuclear fusion energy.

But this experiment was about something else. It took advantage of NIF's ability to unleash high-energy neutrons. At the center of the lasers' focus sat a tiny metal container called a hohlraum, and inside it was a minute capsule filled with hydrogen isotopes that would fuse in the nuclear reaction. For the first time, uranium had been incorporated into the capsule's thin plastic wall. Fifty centimeters away, the team's new collector was held in place on the end of a large boom extending into the chamber. The plan was for the fusion reaction's neutrons to split uranium atoms. Then the passive witness plates on the collector would catch debris from the capsule, including the uranium fission products zirconium, molybdenum and tellurium, as well as activated uranium.

There was some tension. "We thought maybe we wouldn't see anything," Shaughnessy recalls.

Another pause after the shot demanded still more patience. The neutrons had contaminated equipment and surfaces throughout the target bay, making them radioactive. After about two hours, Gharibyan was able to enter and stand outside a roped-off central area as safety-suited technicians removed the collector. One held it up. Even from a distance, Gharibyan could see that the flat, round surface was peppered with debris. "I basically started taking pictures and sending them to the rest of the group," he says.

Once the collector was bagged and sealed in a tough plastic carrying case, Gharibyan and Shaughnessy took it to the radiochemistry laboratory. Moody put the witness plates on a radiation counter. "They had fission products on them," Shaughnessy says. "I think I shrieked in delight."

Since then, the team has developed a range of devices that induce neutrons to bombard various materials, capturing data on nuclear reactions relevant to two national security concerns. First is nuclear forensic analysis of fallout after a nuclear device is detonated, either in a weapons test or in warfare. After the complex reactions in a detonation, the soil and structures throughout the area are radioactive. Shaughnessy and her colleagues want to understand the process in enough detail to describe the event and the weapon that caused it. "Hopefully, that's a scenario we never have to truly exercise," Shaughnessy says. "But we have to be ready for a case where someone potentially detonates a nuclear explosive. The role of the national labs would be to actually figure out what went into the device and to provide important information to the government."

Stockpile stewardship is the other national security concern. Today, scientists use computer simulations to help ensure the nation's existing nuclear devices would perform as intended if they were ever needed. But before the United States stopped traditional testing in the 1990s, scientists gathered extensive data about the reactions taking place. For example, the yttrium they added to nuclear devices played no role in the explosion, but the proportion converted from yttrium-89 to yttrium-88 during detonation gave clues about reactions that had occurred. Computer models demand ever greater details about these reactions.

NIF offers unique opportunities. In its experimental plasma, nuclei undergo a rapid-fire onslaught of neutrons, and a single nucleus can transform multiple times, shedding energy and particles as it changes identity again and again. Knowledge of those reactions would improve accuracy in computer models. "That's our main goal with the NIF radiochemistry – to try to measure some of these missing reactions so that others can use that data in their codes," Shaughnessy says.

Nuclear scientists refer to this information as reaction cross sections, the odds that an isotope will react with a neutron in some way, such as capturing the neutron and gaining its heft or splitting and releasing huge amounts of energy. Gharibyan says an isotope's cross section, based on the energy level of the neutron, is vital to knowing the production rate of a radioactive isotope, or radionuclide. "The cross section is a fundamental parameter that you need," he says. At NIF, the Nuclear and Radiochemistry Group can measure key reactions of isotopes when they are subjected to high-energy neutrons of 14 megaelectron volts (MeV).

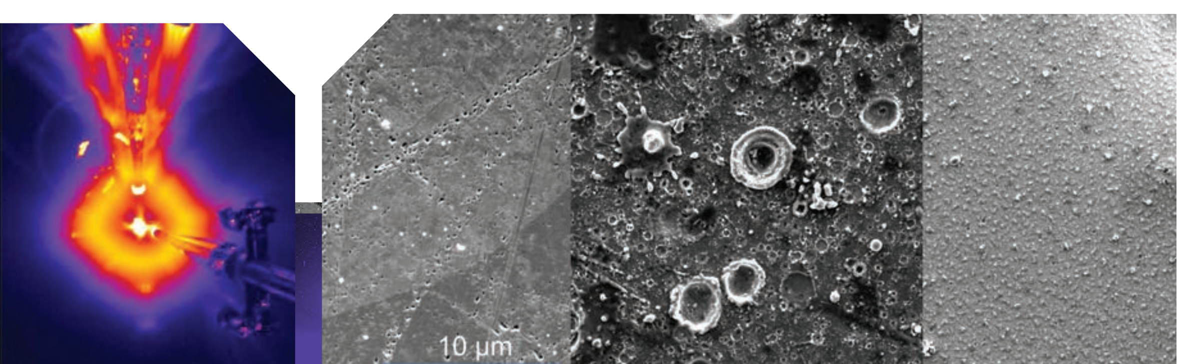
That energy level is important. Gharibyan says 14 MeV is the neutron energy in a thermonuclear device. As NIF shots approached that level, the research team was already providing radiochemistry diagnostics to support the facility's efforts to develop fusion as a power source. "From there we started developing different platforms to do different experiments at NIF that were unique to the facility, that you couldn't otherwise do at other facilities."

Their first platform, simply called Solid Radiochemistry, had a tapered metal tube whose tip pointed at the site of the impending nuclear reaction. Arranged around it, 50 centimeters away from the reaction, sat four round witness disks. After a few successful uses, including the one that day in 2015, the team realized it needed to capture debris from a larger area. The next platform – dubbed the Vast Area Detection for Experimental Radiochemistry (VADER) by *Star Wars* fan Shaughnessy – spanned a greater area but also relied on a long, tapered tube. The researchers realized they were losing some of the debris they sought because the X-ray and laser energies were ablating material off the tube, creating a cloud of detritus that shadowed the witness plate. Their current research workhorse is the Large Area Solid Radiochemistry (LASR) Collector, which is basically a single, large witness disk with no central tube. To capture debris during a shot, the physicists mount a foil of vanadium or some other metal that will release the fragments in later chemical treatments.

To refine their collectors, the team snagged and studied debris from standard NIF shots. In every experiment, a laser is amplified and split into 192 beams, each powered up to 20,000 joules. Banks of mirrors focus the beams into the ends of the hohlraum, which is about the size and shape of a pencil eraser. The sides of the hohlraum convert the laser energy into X-rays that meet at its center, crushing a plastic capsule, about 2 millimeters in diameter, containing a mix of the hydrogen isotopes deuterium and tritium. The intense pressure on the capsule forces the hydrogen nuclei to fuse. The laser and X-rays destroy the hohlraum and capsule, and the reaction releases energy and a short, intense burst of neutrons.

To convert laser energy into X-rays, the hohlraum must be made of a dense metal, typically gold, with certain properties. Sometimes, for an even greater conversion, it's lined with uranium. In those cases, experiments could be done as ride-alongs on other researchers' shots. For example, the group determined the cross section for gold at 14 MeV, then showed that the ratio of two gold radionuclides gives a glimpse into how long the nuclear fuel was confined during the fusion reaction.

Debris collection during a shot using a uranium-lined hohlraum found xenon radionuclides, telltale products of uranium fission, demonstrating that the system allows for experiments that reveal fission details useful in nuclear forensic analysis. The LASR collector could not capture xenon, however, since the element is an inert gas, so the team developed another system called the Radiochemical Analysis of Gaseous Samples (RAGS).



A laser shot (far left) with the team's first device. Passive debris collectors (near right) before a shot (left panel); a polar sample, with a high density of craters and large splats (middle); and an equatorial sample (right), with fewer craters but some large debris particles.

To launch experiments on other materials of interest, the group had to surmount another challenge: how to introduce them into the capsule. For the early proof-of-concept experiment in 2015, it was relatively easy. As General Atomics and Affiliated Companies made the capsule off-site, a source of uranium-238 was heated nearby so the isotope was deposited, or sputtered, into the forming capsule. That placed the uranium in the middle of the action during the shot.

For other elements, such as yttrium and beryllium, the challenge is greater because the materials are unavailable in amounts large enough to allow sputtering. On one hand, the small, intense burst of neutrons enables the team to discover cross sections with as little as 10^{13} to 10^{16} atoms of material. On the other hand, the team needed new ways to manipulate such small amounts.

CLEVER DOPING

The Nuclear and Radiochemistry Group at Lawrence Livermore National Laboratory is exploiting the National Ignition Facility's powerful neutron yield to probe the secrets of the stars. A collaboration with astrophysicists at Notre Dame University is using capsules doped by John Despotopulos (see main article) to study the transformation of carbon-13 into beryllium-10, a surrogate for future experiments involving boron. By doping a capsule with beryllium-7 and beryllium-10, the team showed that the ratio of the two isotopes that came out of a shot is the same as the ratio inside. With that knowledge, they experimented with a capsule that had carbon-13 sputtered into the capsule wall and beryllium-7 doped onto the inner surface. The shot was done in November 2018 and the data is under analysis. If all went well, the shot generated neutrons that converted carbon-13 to beryllium-10, and the known amount of beryllium-7 will reveal how much beryllium-10 was made.

Staff scientist John Despotopulos is developing a novel solution: adding a small amount to, or doping, the fuel capsule's inner surface. It's a tough job, partly because the shell is only 2 millimeters in diameter or smaller and the injection aperture is a mere 50 microns across. "I use micro-injection needles, fundamentally (in-vitro fertilization) technology, to inject the solution through the fill hole to the inner surface of the capsule," Despotopulos says.

Even the chemistry has been challenging. The first time he successfully introduced material into a capsule, contaminants plugged the injection site. That would not do, because the neutron-producing hydrogen isotopes had to be injected next. "It was kind of, 'Yay, we finally did it,'" Despotopulos says, "but at the same time now here's a number of other issues that we have to solve going forward." He turned to ultra-pure reagents and to miniaturizing everything, including the volumes of materials. Smaller amounts meant less contamination and less plugging of the injection site.

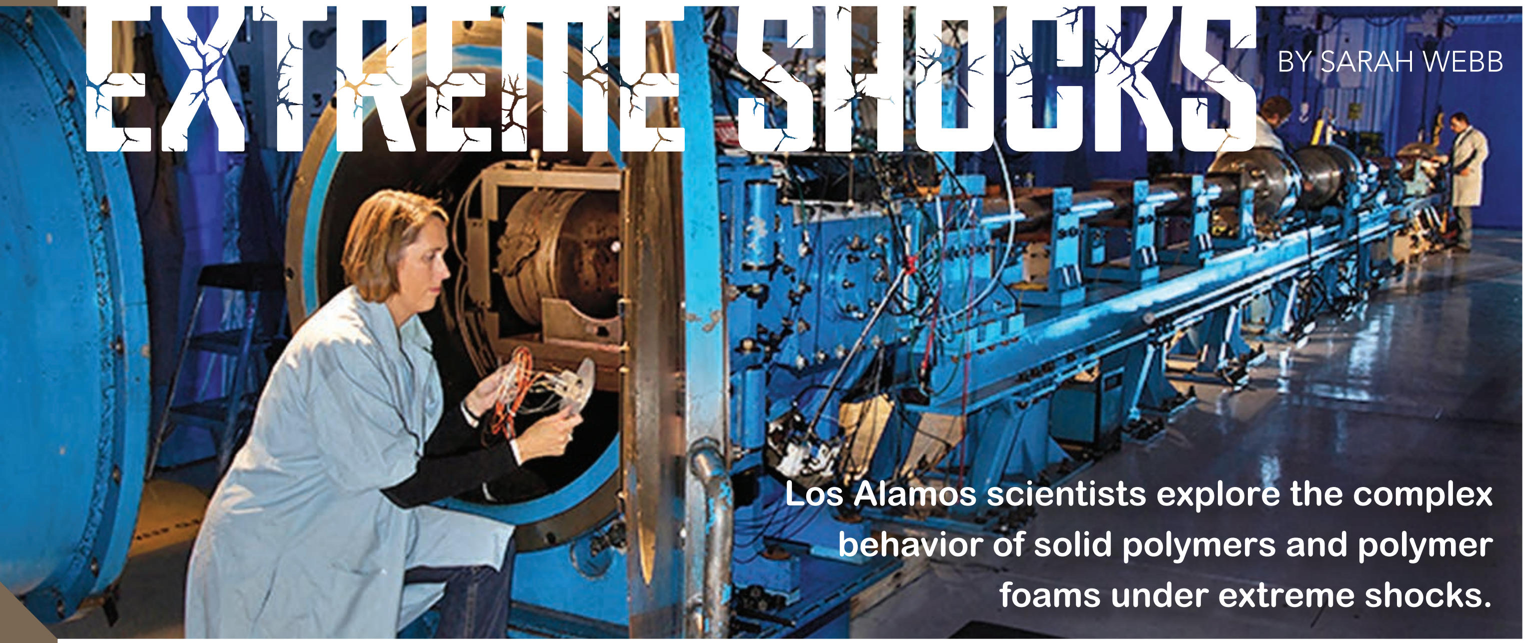
The group has experimented with capsules doped with different isotopes. Yttrium, the historic reaction marker used in 20th century nuclear tests, is an important one. The scientists plan to use a capsule doped with yttrium-89 in a shot this fall, presumably producing yttrium-88. Then, working to capture the multi-hit bombardment of nuclei in a nuclear device, they intend to dope a capsule with yttrium-88 and subject it to a second round of neutrons. The isotope's cross section was measured only once or twice before. "When this was done then, at an accelerator facility, the targets were highly radioactive and difficult to manipulate," Despotopulos says. "Basically in today's culture, you'd never be able to make one of those targets again."

The measurement can be done with the small amounts possible at NIF, but the experiment still will be a special challenge because yttrium-88 has a half-life of about 105 days. Once a sample is made, possibly at an accelerator, the team will have only two months or so to purify it, inject it into a capsule and deliver it in time for a dedicated NIF shot.

The payoff from such an experiment would be substantial. A more detailed understanding of the reactions that result in various end products would let scientists reconstruct the fine details of tests done decades ago. "If we get to that, and that's probably going to be a couple of years, that would be really, really awesome," Shaughnessy says. "That's like the drop-the-mic reaction. If we show that that worked and we get a number out of that, I think it would show that we could do any of these types of reactions."

Soft Materials, EXTREME SHOCKS

BY SARAH WEBB



Los Alamos scientists explore the complex behavior of solid polymers and polymer foams under extreme shocks.

Dana Dattelbaum prepares for a gas-gun shot.

A smooth-bore gas gun more than 80 feet long dominates a room with heavy steel doors shielding scientists in a separate control room. As the shot's countdown approaches, a firing technician and researchers fielding the day's experiment check off a list of diagnostics. Valves open and close; the countdown begins. Then, satisfaction: A projectile zips through the barrel and slams into a catch system at its terminus.

Los Alamos National Laboratory researchers use this gun, and others like it, to launch projectiles at dizzying speeds – several kilometers per second – toward sample test materials that range from explosives to polymers to metals. These research guns – and the diagnostic suites attached to them – are powerful, sophisticated instruments for generating and analyzing shock waves and their effects in materials. The researchers use a range of techniques to monitor what's happening inside, including physical tracers such as embedded gauges or fiber gratings. They can also measure light and X-rays moving through these complex systems on the order of millionths or billionths of seconds.

Historically, the bulk of shock wave research has focused on metals. But Los Alamos' Dana Dattelbaum examines the effects of shock wave compression on organic materials – explosives, solid polymers and polymer foams. Such measurements help researchers understand the performance and chemical stability of these materials for basic science, defense research and stockpile stewardship. Under these extreme conditions, organic materials don't behave like metals. Their physical properties alter, including their viscoelasticity and how their atoms compact. They also can chemically react.

"Comparatively less is known about how polymers evolve in these extreme environments," says Dattelbaum, program manager in the Explosive Science and Shock Physics Division at Los Alamos. "What we're after is a more accurate description of how polymers behave."

Shock testing at Los Alamos dates back to the lab's roots, from the years immediately after the Manhattan Project, division leader Eric Brown notes. Researchers initially developed tools like gas guns for studying nuclear weapon materials, primarily metals. In the 1970s and '80s, researchers at Los Alamos and other Department of Energy National Nuclear Security Administration (DOE NNSA) labs also tested other materials, such as polymers and high-energy explosives. Although metals show relatively consistent, ideal behavior in a shock front, Brown says, polymers, explosives and other organic materials are more complicated.

These materials respond in various ways to the high pressures and temperatures shock wave compression produces. Metal atoms have high masses and often pack together in regular crystalline patterns, creating ordered structures. Shock damage can melt metals, but they remain chemically intact while possibly changing the phase, or the arrangement, of the atoms.

By contrast, polymers are made of softer stuff. These long, repeating chains of atoms – primarily carbon, hydrogen, oxygen and nitrogen – are far more heterogeneous. They can be twisted, packed and folded, forming materials that are stiff and glass-like or flexible and rubbery. Under high temperatures and pressures, they chemically decompose into simpler molecules, an irreversible process. Models must capture this one-way trajectory. In that way, the chemistry is more like that of high explosives, which are also organic materials. But polymers are not reactive enough to release the extreme energy that fuels powerful detonation waves in explosives.

After subjecting polymer materials to extreme shocks, Dattelbaum and her team measure how wave velocities change and other responses. Joshua Coe, a Los Alamos theoretical physicist, uses those experimental data – and other information, when available – to develop an equation of state (EOS), a mathematical relationship that describes the pressure, volume and temperature interaction in these materials. They map the shock locus as a Hugoniot, a graph that plots pressure and how the material compresses. Researchers incorporate EOS models into larger hydrodynamic computational simulations that examine the fluid dynamics of polymers in context. That work is important for a basic science understanding of materials, but also for a range of practical applications: stockpile stewardship and national defense, such as in conventional weapons and body armor.

Researchers used to treat polymers in hydrodynamic simulation like metals, modeling EOS transitions as reversible. “That’s not right,” Coe says. Using reversible polymer transitions in these calculations “can produce some pretty serious artifacts” that diminish the simulations’ accuracy, he says. For example, weapons simulations that don’t include appropriate models might not account properly for double shocks, or the speed at which release waves travel back through a material, Dattelbaum says.

Studies of extreme shocks in solid polymers dating back to the 1970s showed these materials have a distinct transition in their Hugoniots – at around 20 GPa, nearly 200,000 times the pressure of Earth’s atmosphere. These transitions presumably represent the point when the polymer samples decompose. It’s impossible to get detailed chemical information about samples *in situ*, as they’re shocked. These transitions happen within tens of nanoseconds.

Dattelbaum’s team has done further work to explore and describe details of solid polymer behavior, studying a range of materials including epoxy, polyethylene, polyurethane and polysulfone. They’ve shown that simple polymers, such as polyethylene, with less branching off the central chain, show smaller Hugoniot transitions than more complex polymers such as polysulfone. The simpler polymer is more organized structurally to begin with.

The shock wave profiles measured in these experiments only hint at the polymers’ chemical reactions. In the absence of more detailed chemistry data, Dattelbaum, Coe and their colleagues assume that these materials react completely and produce simple products such as small carbon particles (graphite or diamond), ammonia and water.

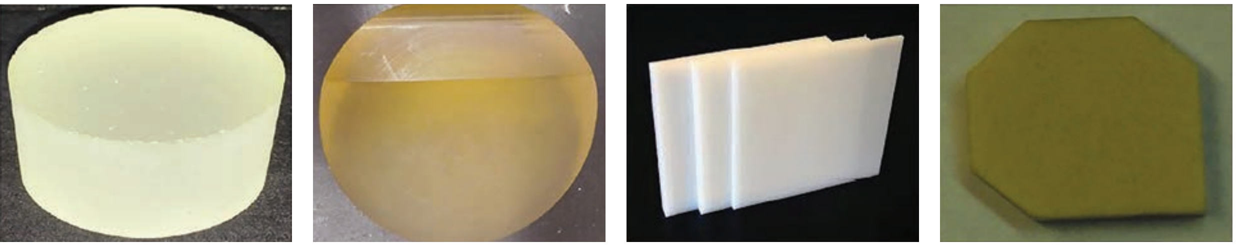
MANY PATHS CONVERGE AT SHOCK PHYSICS

The field offers engineers, physicists and chemists a range of opportunities.

Mechanical engineer Eric Brown joined Los Alamos as a postdoctoral researcher working on high-energy shock responses in polymers. He found the job rewarding because it combined fundamental and applied research. Brown has published numerous journal articles and received academic recognition for contributing to basic science. And the work has a range of real-world applications for stockpile stewardship, weapons development, new body armor and more.

Chemist Dana Dattelbaum moved into shock physics at Los Alamos in 2004. She first came to Los Alamos as a graduate student, making time-resolved measurements of excited states. She later worked on high-pressure spectroscopy as a postdoctoral researcher and staff member in the lab’s Polymer and Coatings Group. These areas integrate similar challenges and goals – understanding material behavior under extreme conditions. Shifting research areas while on staff can be challenging, she says, but she had patient advisors who helped her. “It was an environment where I was really mentored well,” she says, by people who unselfishly supported her and shared their knowledge. One of those mentors was Stephen Sheffield, a now-retired engineer who had worked alongside experts such as Sandia’s Robert Graham and Los Alamos’s Ray Engelke.

The combination of supporting classic techniques and embracing new *in situ* methods makes it an exciting time to work on these problems, Brown says. “For someone who is interested in doing something a little bit different than they did in graduate school, this is an opportunity to jump into a new and exciting field.”



Soft materials important in stockpile stewardship include (left to right) epoxy, polysulfone, polyethylene and polyurethane.

As they incorporate polymer behavior into hydrodynamic simulations, the scientists often must use two separate equations of state for the polymer components – one to represent the polymer before it decomposes and another to represent the products after they fall apart. As they reconstruct more of those mechanistic details, they'd like to develop a reactive burn model that incorporates the energetic details of that chemical transformation.

Understanding the shock behavior of solid polymers is challenging enough, but Dattelbaum's team is working on an even more complicated problem: shock behavior in polymer foams. These materials support structures and cushion impacts. They have the same chemical composition as their solid counterparts but are manufactured with air pockets to create materials with defined, but lower, densities and specific structural properties.

Adding pores introduces different compression behavior. "Once you introduce even a moderate amount of porosity, you never compact a foam to the point where it behaves like the solid polymer," Dattelbaum says. Instead, the foams get so hot that they expand, a feature known as anomalous compression.

In that way, polymer foams behave even more like explosives than their solid counterparts. Even with just 25 percent porosity, shock heating dominates, she says. "That was completely new and pretty surprising" and has important implications for modeling in a range of situations because foams cushion shocks in many systems, including in inertial confinement fusion experiments. The anomalous behavior – limiting compression – could be helpful for mitigating shocks, Dattelbaum adds. "It's almost like pushing back and expanding relative to compression."

Understanding this behavior in foams could lead to new materials. If researchers can exploit shock wave coupling to porous structures, they could take advantage of this feature to control the wave's dynamics. Dattelbaum has a laboratory-directed research and development grant to explore this idea in more detail.

Because shocking foams produces more heat, foam polymers also decompose at far lower shock magnitudes. Their Hugoniots show transitions at pressures closer to a few GPa instead of 20 GPa. Because these reactions burn hotter sooner, they also produce a more complex mix of products. For example, with a solid polymer, assuming that the carbon product is solid graphite or diamond is reasonable. But at these even higher temperatures, at least some of that carbon could be liquid, Coe says. The researchers will need better models for liquid and other carbon phases and ways to characterize size effects in carbon. "Carbon is the hard part from an EOS perspective," he adds.

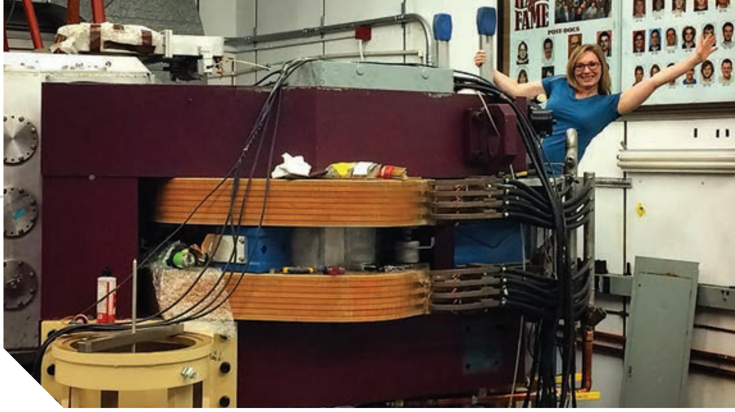
Meanwhile, new tools for studying material behavior under extreme conditions have come on line. At the Dynamic Compression Sector at Argonne National Laboratory's Advanced Photon Source and at the SLAC National Accelerator Laboratory's Linac Coherent Light Source, X-rays can offer a new look at compression and phase changes in carbon and polymers under extreme shocks and more information about the products formed. Higher energies and more X-ray brilliance could enable simultaneous small- and wide-angle X-ray diffraction experiments.

Those instruments would allow the researchers to monitor structural modifications during shock experiments such as changes in molecule structure and bonding, Brown says. "It's something that we were never able to do before."

Eventually Dattelbaum hopes to incorporate X-ray-based spectroscopy techniques to uncover the full chemical details of how polymers and explosives decompose. The complexity of the materials, the difficulty in penetrating them and the incredibly short reaction times all make this process challenging.

Brown notes that polymers were historically viewed as a simple commodity, but they're an important part of DOE NNSA weapon life-extension programs. "There are a lot of really important things within the details of how those materials behave in extreme environments," he says. "We want to make sure that we understand the materials that we're putting into the stockpile going forward."

When Physics Becomes Art



Louisiana State University's Erin Good with the split-pole spectrometer she uses in her experiments, located at Florida State University in Tallahassee. The fourth-year fellow is the winner of the 2019 SSGF Essay Slam, an annual writing contest open to current and former fellows.

Nuclear physics captured my imagination as a child. Living within the 10-mile evacuation radius of a nuclear power plant that is famous for a meltdown will do that to you. But I didn't think I'd be a grad student studying the subject and creating experimental works of art in epoxy and metal.

To explain: I build detectors. Some are mundane metal boxes, filled with hundreds of wires, that I've pumped full of gas thousands of times. Some are gorgeous, sparkling cone-shaped constructions of silicon wafers that stand proudly at attention in starkly empty chambers.

They never work properly the first time. Hours and hours are spent troubleshooting. Is it the detector? Is it the electronics? Is that a faulty wire? Is there a leak or – on a rough day – did I forget to turn it on? It may take a while, but I always figure it out eventually.

They're delicate in some ways – a fingerprint on the mirrored surface of a silicon wafer or the bursting of a shiny foil window are tragedies – but sturdy in others. They operate under gas pressures that would suffocate humans and measure radiation doses that would kill us, yet carry on contentedly.

The detectors measure qualities of the charged particles that contact them – protons, deuterons, tritons, alphas and more. What they quantify depends on the detector and on the reaction.

They're all different, but in one way they're the same: I built them. You can't work with something for months on end without making it personal. When you're the expert on a detector's every little setting and quirk, it becomes special to you. Of course, they'll be sent around or installed at another lab permanently, but I'll always think of them as my creations.

My detectors work with a phoenix reborn: an old, well-loved split-pole spectrograph, a gigantic, exquisitely designed magnet we acquired when a small university accelerator lab closed.

The old behemoth got a makeover after its long truck ride down I-95 – new lab, new concrete pedestal to sit on. It was polished and painted to within an inch of its life and now sits proudly in the middle of the facility.

The spectrograph is a marvel – a 34-ton monstrosity in steel with a power supply the size of a walk-in closet. It bends the paths of charged particles to sift them by their speed and charge, creating finely sorted groups as they exit the magnet, but on its own it's silent. To be heard it needs my detectors.

My detectors work in tandem with the magnet to tell us things. A beam of particles comes into a chamber ahead of the magnet and hits a target of our choosing, creating the nuclei we want to study. They remain in the chamber while lighter, leftover nuclei continue surging into the magnet.

My focal plane detector sits at the magnet's exit and tells us where the leftover particles land and how much energy they have. This is the instrument that's filled with gas and wires, enclosed by fragile mylar foil windows. When it's placed just so, it precisely resolves the particle groups, focusing them into the narrowest points possible.

My silicon array sits in the target chamber just ahead of the magnet. It's the shiny array that looks like a space-age lampshade and surrounds the beam before it hits the target. The array tells us what nuclei we created that were left behind in the chamber and what particles they shoot out as they calm down.

If all goes well, my detectors and this colossal magnet will be together for years. Other nuclear physicists will use them to study how nuclei are excited, how they decay, and how they behave differently at different angles. With that information, they'll figure out how the protons and neutrons are arranged in various nuclei, gleaning information about intrinsic characteristics such as spin and how often they react with other particles at different energies.

I'll use the magnet with my detectors to see how many times a specific neon nucleus decays after its formation. That will help me figure out how many times a different oxygen nucleus captures an alpha particle in a stellar explosion called an X-ray burst. With that snippet of information, we'll try to better understand which elements are created where in the universe and why astronomers see what they see when stars explode.

Hopefully, I'll work on figuring out where the elements are made for a long time and use other detectors that work in totally different ways from the ones I've built. I look forward to meeting other detector designers and hearing about how their frustration and dedication came together to create a vital tool for research.

Maybe I'll build more detectors in the years to come, or maybe I'll never touch another soldering iron. Either way, I've left a legacy in detectors at a lab that will use them for years.

DOE NNSA SSGF/LRGF FELLOWS ROSTER

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KEY
(academic advisor); national laboratory practicum location:
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LLNL = Lawrence Livermore
SNL = Sandia National Laboratories
TBD = to be determined

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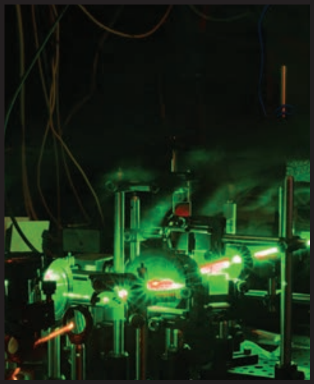

HEAT LAMP

At the Massachusetts Institute of Technology, outgoing fellow Cody Dennett and his colleagues use the lasers pictured here to thermally excite metal surfaces and generate acoustic waves for probing material defects. To learn more about his research and ongoing collaboration with Sandia's Ion Beam Laboratory, see page 4.

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