STEWARDSHIP SCIENCE

2021-2022

THE SSGF/LRGF MAGAZINE

MAN OF NEW MEXICO

SSGF fellow Gabriel Shipley grows as he goes from Sandia to Los Alamos and back

Livermore: A program alumnus thrives under pressure

Sandia: A fellow squeezes insights from explosions

Plus: More science from shocked materials; diversity matters; other fellows, other locations; slipping into darkness under Italy

DOE NNSA FELLOWSHIP OPPORTUNITIES

BENEFITS

+ $38,000 yearly stipend
+ Payment of full tuition and required fees
+ Yearly program review participation
+ Annual professional development allowance
+ Renewable up to four years

The Department of Energy National Nuclear Security Administration Stewardship Science Graduate Fellowship **(DOE NNSA SSGF)** provides outstanding benefits and opportunities to students pursuing degrees in stewardship science areas, such as **properties of materials under extreme conditions and hydrodynamics, nuclear science, or high energy density physics.**

The fellowship includes a 12-week research practicum at Lawrence Livermore National Laboratory, Los Alamos National Laboratory or Sandia National Laboratories.

ELIGIBILITY: U.S. CITIZENS WHO ARE SENIOR UNDERGRADUATES OR STUDENTS IN THEIR FIRST OR SECOND YEAR OF GRADUATE STUDY.

www.krellinst.org/ssgf

The Department of Energy National Nuclear Security Administration Laboratory Residency Graduate Fellowship **(DOE NNSA LRGF)** gives students the opportunity to work at DOE NNSA facilities while pursuing degrees in fields relevant to nuclear stockpile stewardship: **engineering and applied sciences, physics, materials, or mathematics and computational science.**

Fellowships include at least two 12-week research residencies at Lawrence Livermore, Los Alamos or Sandia national laboratories, or the Nevada National Security Site.

ELIGIBILITY: U.S. CITIZENS WHO ARE ENTERING THEIR SECOND (OR LATER) YEAR OF GRADUATE STUDY.

www.krellinst.org/lrgf

These equal opportunity programs are open to all qualified persons without regard to race, gender, religion, age, physical disability or national origin.

A FINE 15 AND A FRESH DIRECTION

IT'S A SPECIAL YEAR for the Stewardship Science Graduate Fellowship. Fifteen years ago, the Department of Energy National Nuclear Security Administration (DOE NNSA) established the program to identify the country's most talented young scientists and introduce them to nuclear science and technology as practiced at U.S. national security laboratories. Since then, the program has graduated more than 60 researchers, many of whom now work at DOE labs.

This year also is a milestone for this magazine. Since our launch in 2010, we've covered developments in areas of importance to stockpile stewardship: high energy density physics, nuclear science, materials under extreme conditions and hydrodynamics. A couple of years ago, we incorporated the activities of a sister fellowship, the DOE NNSA Laboratory Residency Graduate Fellowship. This issue marks not so much a change in direction but a shift in emphasis. We will continue to feature outstanding science and technology at each of the labs – and in those fields – but our in-depth articles will profile current and past fellows.

Celebrating anniversaries and syncing content to evolving programs is all part of a larger goal of building a community of current and former fellows, laboratory staff and university scientists who advance science and technology in the national interest. We hope you enjoy this showcase of our extraordinary community's product.

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

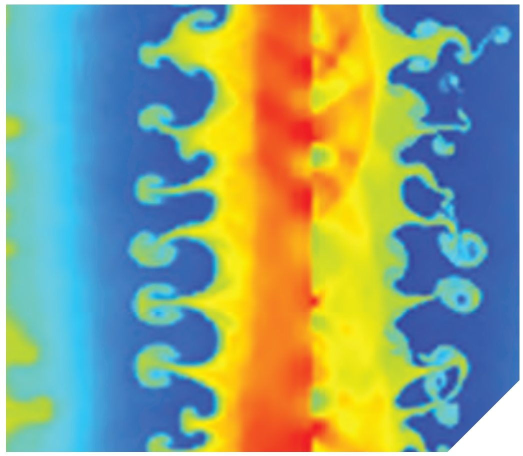
CELEBRATING SSGF 15 YEARS

STEWARDSHIP SCIENCE

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-NA0003960. 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

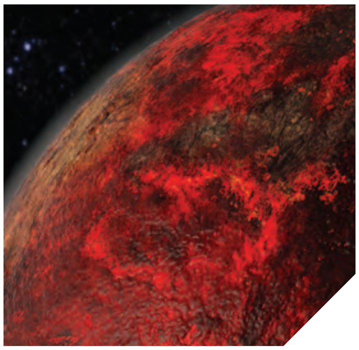
FEATURES

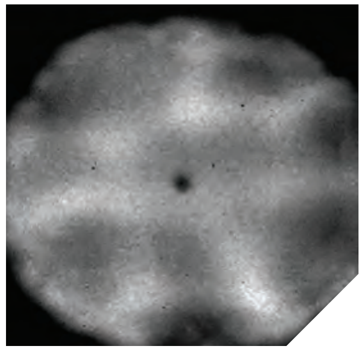


DEPARTMENTS

FRONT LINES

2021-2022 THE SSGF/LRGF MAGAZINE





CONVERSATION

ESSAY

FELLOWS ON LOCATION

ON THE COVER

Physicist and DOE NNSA SSGF recipient Gabriel Shipley on the campus of Sandia National Laboratories in Albuquerque, New Mexico, with public art fashioned from an early version of the Z machine. While a Ph.D. student at the University of New Mexico, Shipley simulated Z-machine experiments as part of his Los Alamos National Laboratory practicum. He also served as a principal investigator and principal designer for other Z experiments. *Sandia National Laboratories.*

PETN PR

KABOOM BOX

Scientists and engineers at Sandia National Laboratories in New Mexico routinely huddle around a boombox that is nothing like its 20th century portable-music namesake.

The toaster-sized device they designed and built was dubbed the Boombox for reasons less historical than literal: It allows them to safely detonate material in the lab and study how explosions start and grow.

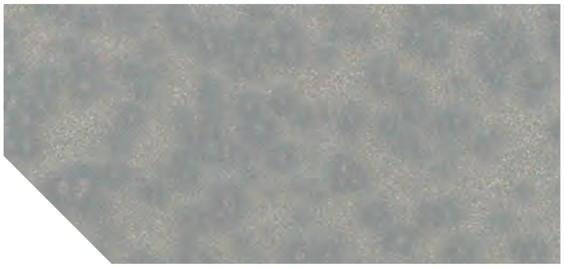
A key part of the effort was creating a thin film – as thick as just a few sheets of notebook paper – made of pentaerythritol tetranitrate, or PETN, a material often used by the military and in the mining, quarrying, and oil and gas industries that has roughly the explosive power of TNT. The researchers used a method called physical vapor deposition to grow PETN films on silicon substrates.

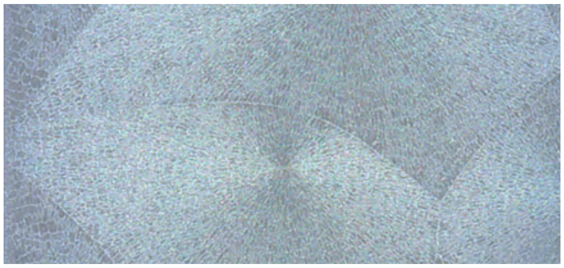
Sandia is the only lab in the nation that can make and study detonation-capable thin films on such a small scale.

The Sandia team began coating silicon surfaces with PETN more than six years ago, on a piece a quarter the size of a postage stamp. Some of the first films it grew were only about a tenth as thick as paper – too thin to detonate. The team gradually bulked up the PETN, vaporizing it in a vacuum, then depositing it on substrates.

More recently, the team found that depositing PETN on clean silicon surfaces cracked the explosive film in a pattern resembling dirt on a dry lakebed. Tests led by Eric Forrest, a Sandia principal R&D scientist, showed that even hair-thin surface cracks can stop a Boombox detonation in its tracks. Dirty surfaces, they discovered, alter the PETN crystals' dry-lakebed orientation. "We found that by applying different techniques, we could control the PETN film growth on an almost molecule-by-molecule basis," Forrest says.

PETN film microstructures, seen here a few millimeters across, differ based on the cleanliness of the underlying substrate. *Sandia National Laboratories.*





SHOWING ITS AGE

The technique is called image quantification. Lawrence Livermore National Laboratory researchers have teamed up with University of Utah computer scientists and used high-performance computing (HPC) to show that this special twist on X-ray computed tomography (CT) can systematically track subtle changes related to how materials were made and how they age.

What's more, the method can be applied generally to material systems to help ensure that aging doesn't impact reliability, says Richard Gee, group leader of Livermore's Reaction Dynamics Materials Science Division and the project's principal investigator. The technique enables long-term predictions of "material behavior much earlier, well before the material has changed to a point of manifesting as an issue," Gee says. "The approach represents new evaluation methods."

In a 2020 paper in *Computational Materials Science*, the authors note that, besides well-known uses in medicine and biology, X-ray CT is becoming an important non-destructive 3-D characterization tool in other fields, including geology, materials science and planetary sciences and in industry. The lab is interested in the method for, among other things, its potential to identify the effects of aging on stockpile-relevant materials. To make image quantification work, the authors say, the team had to devise a general-purpose algorithm and demonstrate its use in various realistic scenarios.

The Utah team members developed just such an algorithm for this study. It employs Morse complex construction, which Gee describes as a way to identify topological features that distinguish material domains within a microstructure.

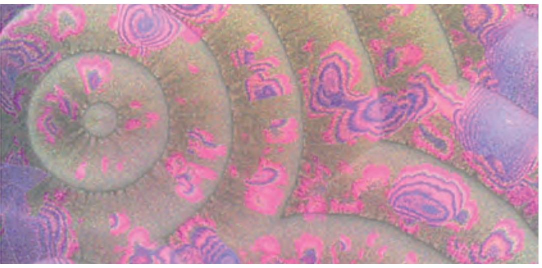
Meanwhile, participating Livermore materials scientists evaluated five differing lots of a study material, a plastic-bonded explosive formulated with pentaerythritol tetranitrate (PETN), selected because it is used in many commercially available applications and has been studied extensively, "therefore affording a rich data set to draw upon for future exploration." PETN is widely used for bombshells and missiles and in metallurgy, demolition and rock blasting and sculpting.

Fine, needle-like PETN crystals were slurry-coated and pressed into cylindrical pellets as they would have been if manufactured. Samples were heated for several weeks to mimic years of natural aging.

Had Livermore researchers been able to process enough samples – tens of thousands, Gee estimates – they could then have trained neural networks to uncover hidden aging patterns they'd sought through

To better understand explosions, the team used a technique known as schlieren imaging to visualize changes in air density and temperature as shock waves raced through the Boombox. Schlieren is German for "streaks." Other researchers have used the technique to study the role of air movement from human coughs, both with and without facemasks, in COVID-19 transmission.

To help document the thin-film research, the team attached to the Boombox a high-tech camera system capable of taking up to a billion images per second, Forrest says. Created using steel and polycarbonate – a tough, transparent plastic – the box was designed to contain detonation debris and prevent explosions while the device is open. "We can watch detonations and shock waves in the Boombox propagate in real time," Forrest says, "even when the material is moving at tens of thousands of miles per hour."



The group's ability to finely control PETN deposition onto the silicon plates has enabled improvements in a Sandia computer model known as CTH, which companies, universities and the Department of Defense use to probe the physics of shock waves.

Sandia researcher Julio Peguero boosted the project by refining CTH to match data from experiments. Peguero previously worked on explosives research at the Energetic Materials Research and Testing Center, part of the New Mexico Institute of Mining and Technology in Socorro, his hometown and where he received his mechanical engineering master's degree in 2019.

In the Boombox project, Peguero and his colleagues plotted the velocity of shock waves during explosions. The team created various crack sizes on the PETN thin film, from slightly wider than a hair to one-third the width.

"We are trying to understand the effects of the small cracks we see and how they affect the success and failures of explosions," Peguero says. "Fundamental science like this can help increase the safety of explosions and also benefit our national security."

Forrest's team has worked with other Sandia thin-film-growth researchers on potential applications in renewable energy, including improving the performance of solar panels. *–Jim Scott*

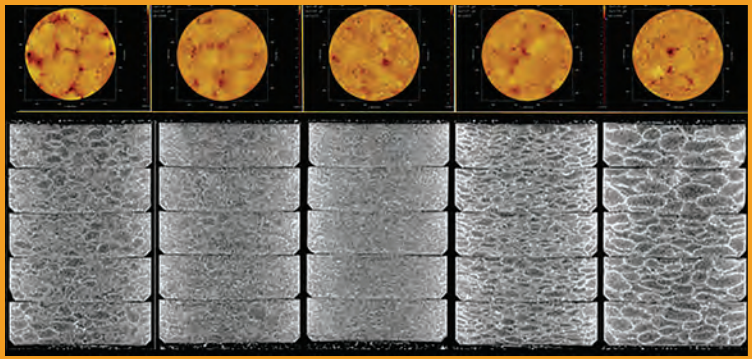
deep learning. That's a class of machine learning that searches the same raw data in repeated stages to uncover new information.

But time and costs limited their total samples to a few hundred. So Instead of deep learning, the researchers opted for statistical machine learning, which can identify small microstructure variations.

Gee says machines at both the University of Utah School of Computing and Livermore were used for the image processing, data reduction and statistical machine-learning evaluations. Meanwhile, a commercial instrument at Livermore's High Explosives Applications Facility supplied the X-ray CT analysis.

The researchers found that even small changes in how the materials were prepared showed up in the CT images. Variations in particle sizes and shapes, as well as changes in how the ingredients were distributed, could be identified by comparing five distinct sample lots. To reveal age-related changes from lot to lot, the team statistically analyzed the numbers of grains per sample, the total surface area of each grain and the persistence of documented features.

Next, he says, the researchers will improve their image processing and data analytics methods, then couple them to machine-learning approaches to extract features that further elucidate the physical and chemical processes that occur with age. *–Monte Basgall*



CT scans and X-rays provide the raw data for topological analysis of microstructure changes in aging materials. *Lawrence Livermore National Laboratory.*

SURFING SHOCK WAVES

When physicist Ralph Menikoff arrived at Los Alamos National Laboratory more than 45 years ago, running hydrodynamics simulations required preparing stacks of 6-by-3-inch punch cards and waiting for results. Computing and experimental diagnostics have changed dramatically since then, and Menikoff has not only embraced the advances but also pioneered approaches to the physics of extreme materials. His work modeling shock and detonation waves and reactive burn in chemical explosives led to his election as a Fellow of the American Physical Society in 2020.

Menikoff had studied particle physics at the University of Pennsylvania. To gain employment as a Los Alamos postdoctoral researcher, he had to switch to fluid dynamics. Disappointed at first that he couldn't find a job in his chosen field, he recalls, "it turns out I have much better intuition for fluid flow. I think it turned out well."

He started with Rayleigh-Taylor instabilities, which pop up when one fluid accelerates over a heavier one and perturbations arise at the interface. Menikoff investigated how fast such instabilities grow and how altering the fluids' surface tension, viscosity and other physical properties could mitigate those effects. He and his colleagues used novel mathematical approaches to simulate these physical problems.

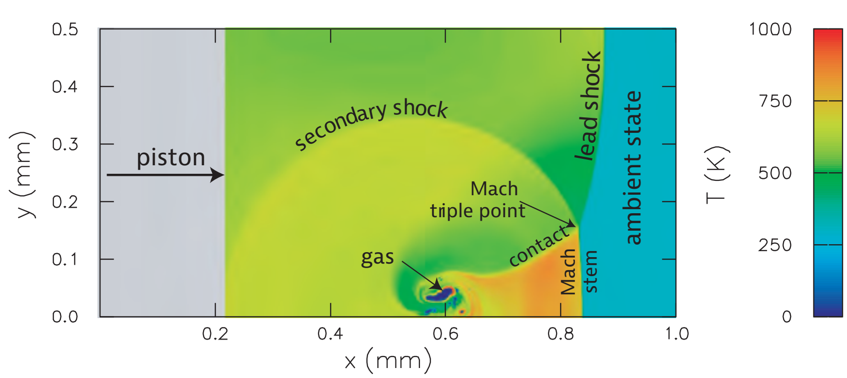
That work led him to examine compressible fluid flow and the three types of waves involved: compressive, shock and rarefaction. Compression waves increase fluid density and propagate shock and rarefaction waves. The waves' interactions are characterized by the Riemann problem, about which Menikoff wrote a key article in *Reviews of Modern Physics* with Bradley Plohr in 1989. It earned him the Los Alamos Fellows Prize the next year.

The Riemann problem's solution depends on a material's equation of state, which determines its pressure in terms of its density and temperature. Explosives-driven experiments at extreme pressures provided data for equation of state models, and Los Alamos published them in the volume *LASL Shock Hugoniot Data*. "You're talking about pressures of gigapascals to megabars, so it's 10,000 to a million times atmospheric pressure," Menikoff says. "You can't get that statically so easily. The dynamics from shock waves gives you data in that high-pressure region." Thermodynamics and the Riemann problem constrain equation-of-state models used in hydrodynamics simulations.

This past decade, Menikoff has focused on reactive burn models for detonation waves in high explosives. The problem is challenging and interesting because plastic-bonded explosives are heterogeneous materials comprising small explosive granules joined by a polymer-based binder. "What drives the reaction rate, when you send a shock through it," he explains, "is not the bulk temperature coming from behind the shock wave. Rather, it's then when you compress out the voids. You get local regions of high temperature, and they're called hotspots." Instead of examining the average over the whole material, scientists must understand how micron-sized hotspots are distributed. The idea that they dominate high explosives' behavior has been discussed since the 1960s, but Menikoff and his colleague Sam Shaw have developed a reactive burn model called SURF that better implements those concepts.

Scale variations are key challenges to modeling these explosives. Micron-sized spaces can be hard to resolve in a 15- to 30-centimeter charge, he notes. Menikoff has applied some of these models to study properties of explosives produced in new ways, such as additive manufacturing, also called 3-D printing. Typically, these explosives are molded and machined from material chunks. Printing them would expand manufacturing options but could alter densities or produce other variations in the explosives that would raise questions about quality control and predictability. Menikoff and his colleagues want to nail down those effects.

One of his former Los Alamos colleagues nominated him to be an APS fellow and attempted to keep the effort a secret, Menikoff says. But the colleague needed a copy of Menikoff's resume. "I gave them something really free-form, and he said, 'No, no, they need something more'" and told Menikoff why. "I didn't expect to be named a fellow, so that came as a surprise." *–Sarah Webb*



Shock waves can generate hot spots as pores (dark blue) collapse in plastic-bonded explosives. In this simulation, a piston (gray) drives the lead shock (green curve). The pore collapse leads to a high pore pressure that then expands, triggering a secondary shock (yellow curve). Reds and oranges show the hottest temperature regions and correspond to the hot spot. The high hot spot temperature is dominated by shock dissipation behind the Mach stem. *Ralph Menikoff/Los Alamos National Laboratory.*

Diversity and Inclusion in Technology and Policy

Mareena Robinson Snowden is a senior engineer in the Johns Hopkins University Applied Physics Lab's (APL's) National Security Analysis Department. She holds a Ph.D. in nuclear engineering from the Massachusetts Institute of Technology (2017), where she was a Department of Energy National Nuclear Security Administration Stewardship Science Graduate Fellowship (DOE NNSA SSGF) recipient (2012-16). She spoke with Stewardship Science's Sarah Webb. Her comments were edited for space.

What are you working on at the Johns Hopkins Applied Physics Lab?

I work half time on nuclear-related questions – for example, looking into the role of nuclear weapons in nuclear crises or supporting technical studies into future systems. The other half, I engage with questions outside my comfort zone. Most recently, I participated in a project looking at base resiliency to climate impacts, thinking about the risks to continental U.S. military bases in the 2030s and 2050s. It's been an exciting way to get my feet wet on climate work. APL is a great place where you can go a mile deep into a problem or carve a path with a broader focus.

Even before APL, as a Stanton Nuclear Security Fellow at the Carnegie Endowment for International Peace, you worked on technical problems that intersect with policy. What drew you to these complex issues?

I was never quite satisfied with just being in the lab. The nuclear security field is exciting because it's so interdisciplinary. To be an effective technologist, one has to have an appreciation for how the technology interacts with things that are much less quantitative. Understanding the culture and history in which technology will be deployed, or real-world constraints on development or implementation, increases the likelihood of successful adoption, in fields from radiation detection to education. Appreciating these subjective factors is essential for making the technological argument you put forward strong and effective.

What's the most rewarding part of your STEM advocacy work? What's the most challenging?

To me, science and engineering is a team sport. Broadening that community and feeling the support from and giving support to my colleagues and my peers – that is the most rewarding piece. Not only do you see the quality of the science improving, but also the people and the culture. The key is creating a space where people feel empowered to question conventional wisdom and the status quo. Respectful dialogue allows robust, innovative ideas to emerge.

One of the challenges is that diversity and inclusion work isn't a neutral conversation where there are no emotions; it is nearly certain that each person will be triggered at some point in some way. But that discomfort is not a reason to stop the conversation. Maybe we change our approach. Maybe we take a break. But inherently, the feelings themselves are not evidence that the work is going in the wrong direction.

What are the most pressing needs for fostering a diverse, inclusive scientific culture?

Much of diversity and inclusion work is grassroots. You need to honor the stories and experiences of the most marginalized groups to move the needle. At the same time, those grassroots efforts have to be met with a top-down commitment to remove obstacles. Some leaders are not content experts on diversity, equity and inclusion issues and may feel uncomfortable about interventions and solutions proposed by their staff. So that requires an added level of consciousness to really reflect on where any discomfort might arise and its true cause. Today we have a direct test case for diversity in leadership: The current presidential administration now has the most diverse cabinet in history. This didn't happen by accident. It was signaled from the top down.

It's also important to ask what work this representation should be doing. Is this diversity the ends or is it the means? And the means to what? When we're thinking about topics, like deterrence or arms control or safeguards, is this cultural and gender diversity supporting the status quo, which isn't always promising? Or is that diversity trying to challenge systems, reinvent and innovate? Once we've achieved diversity, what work is it doing? The jury is still out about how diversity will shape policy and technical questions. But that's the next step in this work.

Who are your inspirations?

Many people inspire me, including my girlfriends from the different chapters in my journey. I don't think we have space to name them. Of people you may know, Dr. Shirley Jackson. She was the first Black woman to get a Ph.D. at MIT and went on to chair the Nuclear Regulatory Commission and become president of Rensselaer Polytechnic Institute. I remember looking at the large plaque about her work in the Infinite Corridor at MIT, reminding me that if she could do it back then, in the 1960s and '70s, there was little excuse for me. For so many women, and particularly Black women, she's the epitome of excellence in science. Also, Ambassador Bonnie Jenkins. In the last few years she founded an organization, Women of Color Advancing Peace, Security, and Conflict Transformation, and it's really become such a vibrant space for women of color to form security policy ideas, amplify our proposals, and advocate for each other's success.

The author is beginning her second year in the DOE NNSA SSGF at Rice University. This was the winning entry in the 2021 Essay Slam.

Into the Darkness

By Sophia Farrell

Where there is darkness, there is light. We hear this proverb echoed in epic stories like *The Lord of the Rings* and *The Odyssey*, in prayers and throughout generations of old tales. But for me – and 180 fellow scientists around the world – the timeless struggle between darkness and light is literal.

Miles below the Earth's surface, near a centuries-old mountain town in Italy, lies the world's cleanest, darkest and largest vat of liquid xenon: We call it the XENONnT experiment. Housing almost 9,000 kilograms – or about 10 tons – of ultrapure xenon, our beautiful experiment's many superlatives are all the product of a mission to detect dark matter. Dark matter makes up five times more of the universe than all the other matter that we know and love, like stars and planets. Normal matter interacts with light; it's why we see stars in the sky, or why you can read the words on this page. However, dark matter interacts with normal matter so rarely that we cannot see it from Earth or space. Instead, we go underground, hoping that there the world is so dark that dark matter might just shine brighter.

Our subterranean lab is quiet, cold and damp. It's also free from nearly all the atmosphere's radiation, thanks to the halting force of the mountains that shield our xenon. Here, we set up an ingenious detector to observe what particles interact with xenon far underground. There are the usual-suspect interactions, like background radiation from the detector materials or errant ultra-energetic particles from the atmosphere. But occasionally something unexpected happens.

The work of a physicist under this mountain is anything but glamorous. After you don a hardhat, steel-toed boots and, if you are working on the detector itself, a hazmat suit, you enter a delicate ecosystem of intricate electronics, cryogenic pumps, purification systems and, of course, the xenon detector itself. Yet except for the fortunate few (myself included) who helped build the detector, most XENONnT scientists may never see their own detector. We shield the detector from the radiation in the mountain and in our own bodies by sealing the device inside a three-story-tall water tank. Our detector rests contentedly while we buzz about, monitoring its many systems. The pumps, labyrinthian in their complexity, hum in unison; their rhythmic melody to us means, "We aren't broken!" We work in similar fashion, flowing along, intertwined throughout the lab. There is always an expert and a student, though each of us is a student in many respects. Working together on site keeps us informed and constantly learning. The more we can learn about the detector's every aspect, the better we can look for dark matter.

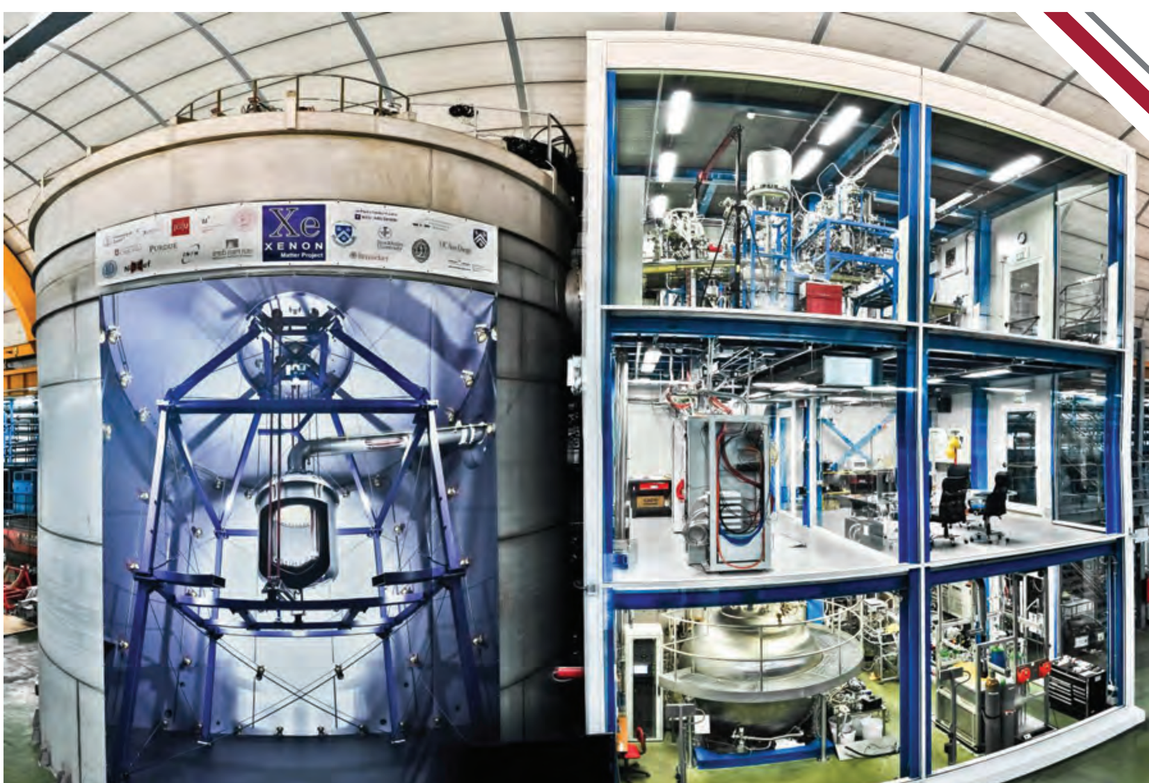
We see signals from our detector with cameras that record specks of light. We have to infer for every interaction the likelihood that it came from dark matter interacting with xenon. This is where I enter the scene. We can't see into our detector lest we contaminate it. Instead, we must observe its behavior with non-invasive sensors. Each signal is unique, imparting to the sensors hints of its origin via a digital fingerprint. I translate these signals into physics.

We reconstruct each fingerprint to determine whether a dark-matter particle left it behind or if it's from a blithe neutron or some other particle. So far, only known particles have come out to play in our xenon, but observing what we know is not always a bad thing. It offers glimpses of particles behaving in new ways, and that has led to discoveries like the rarest nuclear decay ever recorded, that of xenon-124.

Our gentle giant, XENONnT, provides us hints at not only what dark matter is and is not but also how our known universe and its constituents behave. This helps us reconstruct the universe's past and infer our Earth's state today. Our detector tells us acutely about its surroundings. Particles that pass through us invisibly are blinding beams to the xenon atoms, allowing us to put our dark matter detector to practical use in many particle physics applications.

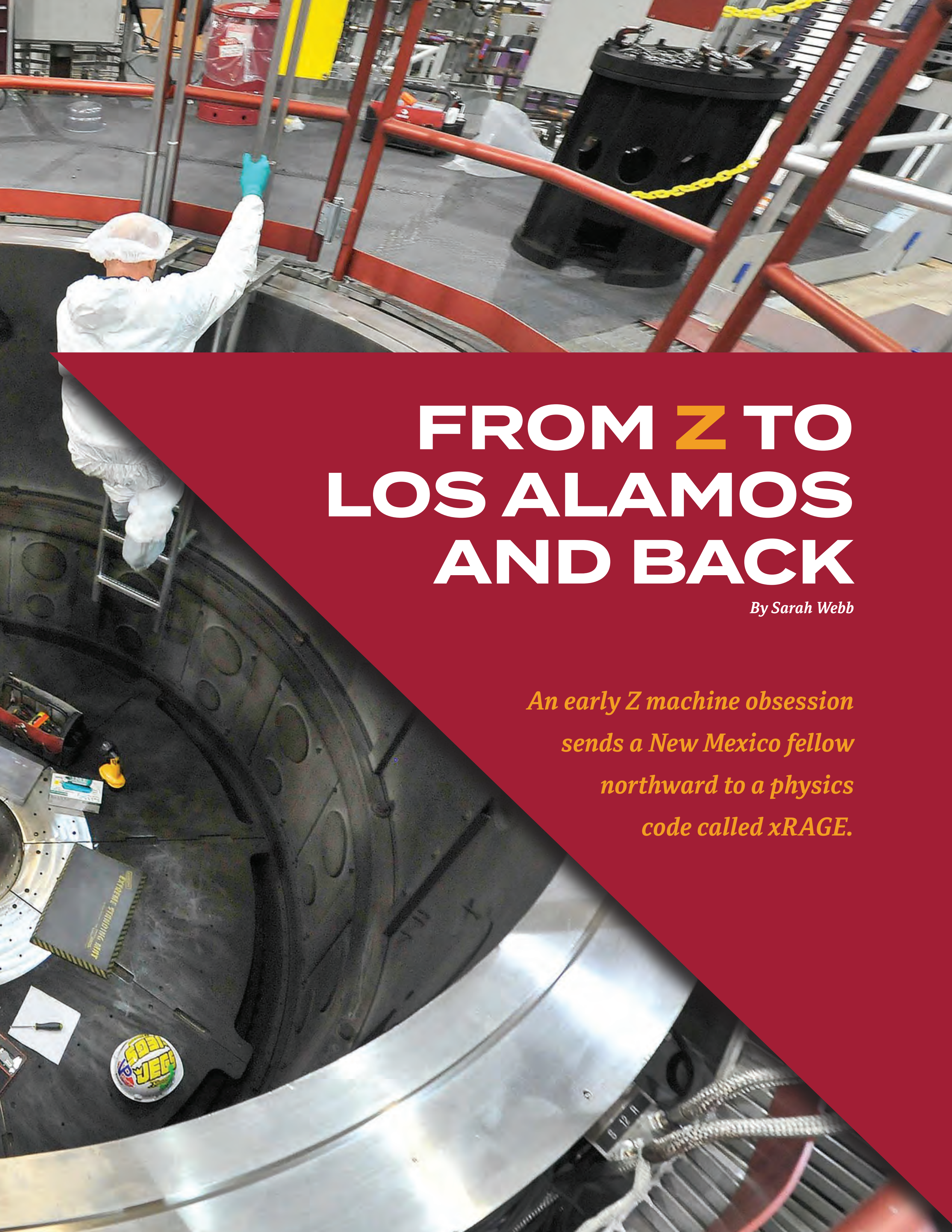
But the story is not all dark and light. There are gray areas as well. Recently, we saw a curious fingerprint, a slight excess of signal, that led to more questions than answers. It was unlike anything we had predicted. Perhaps nature is playing games with us. Or maybe it is humanity's first glimpse of dark matter. Only time, and the 180 passionate scientists devoted to this project, will tell.

We must always remind ourselves of our purpose, especially in times of darkness. Why go to these lengths? Why push xenon, physics and even ourselves past where we haven't gone before? For me, the reward of discovery is worth the struggle, the light brighter and more precious when it is seen in darkness. If we can see the dark matter, we know the story of our universe, and our place in it, that much more clearly. In pushing the bounds of dark matter to their limits, we push ourselves, too. Perhaps that pursuit is equally worthwhile.



The three-story-tall XENONnT dark matter experiment, cocooned inside a mountain in Italy. *XENON Collaboration.*

Inside the Sandia's Z machine between experiments. *Randy Montoya/Sandia National Laboratories.*



FROM Z TO LOS ALAMOS AND BACK

By Sarah Webb

An early Z machine obsession sends a New Mexico fellow northward to a physics code called xRAGE.

Gabriel Shipley

Future physicist Gabriel Shipley was an Albuquerque high school student when a friend's father told him about pulsed-power nuclear fusion and the Z machine, a few miles down the road at Sandia National Laboratories. Shipley was blown away that the world's most powerful X-ray facility was in his backyard and that these sophisticated instruments could theoretically supply limitless power of the kind that fueled stars. "The fire got lit," he says.

The flame drove Shipley to take multiple science and math courses and to read books on high energy density physics, fusion energy and other topics. "This is the hardest problem we've ever tried to solve," he remembers thinking. "Man, I want to work on that."

After a few years of ingesting engineering and science, Shipley knocked on Sandia's doors. He started his Ph.D. program at the University of New Mexico on a Department of Energy National Nuclear Security Administration Stewardship Science Graduate Fellowship (DOE NNSA SSGF) and then, in 2018, headed north to Los Alamos National Laboratory to learn programming. "My goal in going into the practicum was I'd like to do something that I've never done before that will be difficult," Shipley says. "I hadn't run one of the big lab codes before and heard they were very difficult."

He teamed with Forrest Doss, a Los Alamos scientist and fellowship alumnus. Doss was using computational tools to simulate experiments at large-scale laser installations such as OMEGA at the University of Rochester and the National Ignition Facility at Lawrence Livermore National Laboratory. He wanted to extend the work to the Z machine and designed a protocol that linked xRage, a Los Alamos-developed code, with Sandia's version of the GORGON simulation tool

'I got to be a principal investigator for experiments on Z, which was a dream come true.'

These codes allow researchers to simulate hot, flowing plasmas under the extreme conditions – intense magnetic fields and radiation – that occur when the Z machine compresses and heats fuels toward thermonuclear conditions. The Sandia code supplies the critical magnetic physics to calculate the initial implosion. The Los Alamos code lacks those features but is adept at simulating small-scale instabilities without making the simulations too computationally expensive.

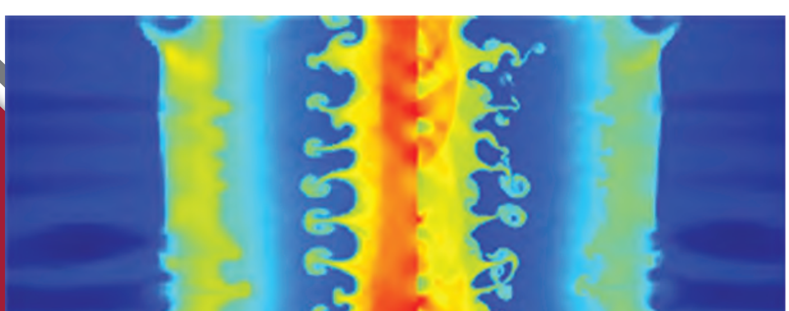
"My task was to learn how to run xRAGE and learn how to go in and break things in the GORGON-xRAGE linking tool," Shipley says, so the team could test and improve it. He and Doss then used the link, called RageRunner, to simulate implosion instabilities observed in experiments from an ongoing Z campaign. RageRunner let them directly compare their detailed predictions with experimental results.

"It was a 'wow.' This is a powerful tool," Shipley says. Doss adds that "we could use the combination of tools that we made to model new things about the experiments that neither lab really could alone." The team published its work last year in the journal *Physics of Plasmas*, including Shipley and Doss's computational results.

Back at Sandia the next year, practical issues nudged Shipley toward computation. Increasingly, he needed three-dimensional codes to answer important research questions. With experience from his practicum, he decided he'd learn to run the codes himself so that he could probe more of the questions he wanted to address. "I've definitely been on more of a simulation bent ever since," he says.

The ambitious choice has paid off. Recently Shipley took on the rare dual role as both principal designer and co-principal investigator on several Z experiments while also completing his doctorate. He will remain at Sandia for the next three years as one of the lab's 2022 Truman Fellowship recipients.

Besides pursuing science, Shipley is a serious saxophonist. He was a high school drum major and performed with New Mexico's All-State Band. He briefly considered a musical career and even auditioned at Boston's Berklee College of Music before choosing science instead. He continues to play, sometimes with a small jazz combo and has also taken up ukulele, guitar and drums. He also loves alpine skiing and reading philosophers such as Albert Camus, Arthur Schopenhauer and Aristotle.



Density maps of simulated hydrodynamic instabilities under Z machine test conditions. Left of center shows the simulation at two levels of adaptive mesh refinement, a numerical method for improving a model's spatial accuracy; right of center, the simulation at four levels of refinement. The images were produced with RageRunner, a Los Alamos-developed code. *Gabriel Shipley.*

With his sights set on Z, Shipley started an undergraduate major in nuclear engineering before pivoting to physics. In 2012, he sent a couple dozen applications for Sandia internships and received a single call from Dave Cole about working in his group, which focused on explosives – both arming and firing systems and ways to defeat improvised explosive devices. "It was a fantastic job and was so fun," Shipley says, "and I learned a lot."

Shipley spent a year working in UNM's Pulsed Power, Beams and Microwaves Laboratory on pulsed-power accelerators and high-power microwave sources, then in 2013 moved into a Sandia nuclear engineering group that focused on nuclear reactor design. Shipley enjoyed that work too but continued to seek opportunities to work on Z.

Shipley was taking a beam physics course when he met Derek Lamppa, a Sandia staff engineer who was working on his Ph.D. Lamppa's team had recently shifted its laboratory to electrical engineering to support the Z machine, particularly its magnetized liner inertial fusion (MagLIF) experiments. Lamppa recalls that the course professor mentioned he might hear from Shipley, whom the professor described as a "kid who is really gung-ho about trying to get involved with Z."

Shipley never pestered him about his Sandia duties, Lamppa says. Instead, as the two became acquainted through the course, Lamppa mentioned his work and offered to bring Shipley into his group and introduce him to scientists within the Z community, where he might find a Ph.D. project niche. Shipley picked up electrical engineering skills during that phase, Lamppa says, and then "very quickly transcended them by diving into the physics of the experiments, which are much more challenging plasma physics." Lamppa also taught him to use Ansys Maxwell, commercial software for designing electromagnets and studying the dynamics of electromagnetic fields.

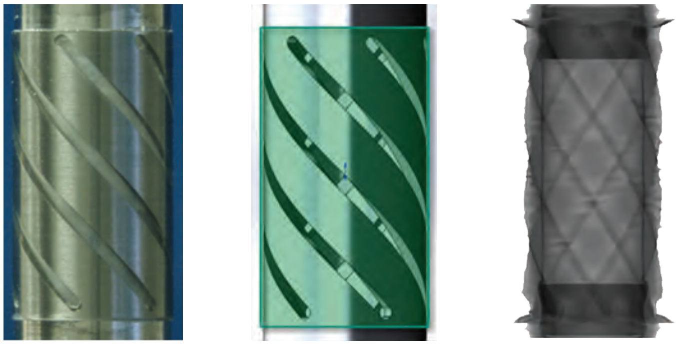
As Shipley sought Ph.D. projects, he knew that lab scientists usually have a long list of research questions they didn't have time to pursue. "There are always these things that are on the edge of someone's desk," he adds. Shipley asked staff scientists about those lingering projects and whether he could start working on them.

One of those researchers was Sandia physicist Thomas Awe, who immediately mentioned a project on auto-magnetizing liners, shortened to AutoMag, a novel way to produce powerful magnetic fields inside Z targets. Scientists had proposed the theory but hadn't tested it with experiments.

MagLIF trials use cylindrical targets filled with fusion fuel. External coils magnetize the target assembly. A laser then heats the fuel and intense pulsed electrical current from the Z machine compresses it, imploding the fuel to thermonuclear conditions, a process called inertial confinement fusion (ICF). The implosion lasts about a hundred nanoseconds; instabilities can develop that prevent effective compression and heating. But premagnetizing the fuel helps to thermally insulate it, letting researchers reduce heat losses and achieve significant thermonuclear reactions.

Traditionally, researchers have produced these magnetic fields with copper coils wrapped a few centimeters from the targets, but at the necessary intensity – often 30 to 50 Tesla – they are difficult to work with. "They can blow up," Shipley notes. "It's a hard problem." The large coils needed to generate the magnetic field also can impede diagnostic instruments that observe the implosion.

AutoMag removes the coils and magnetizes the fuel via the cylindrical liner itself. Instead of using a solid liner, the researchers designed a new one that included conductive helices – to direct current and produce a strong internal magnetic field aligned with the liner's axis – and gaps between them.



An auto-magnetizing (AutoMag) liner (left) is made of discrete conductive helices that replace the copper coils in MagLIF targets. Center: a model of the liner. Right: An opacity map from a simulated AutoMag implosion. *Gabriel Shipley.*

Awe had done some initial research on the project and had even talked with other students about working on it. "Gabe had lots of enthusiasm and free energy, and more than that he had (computer-aided design) skills," Awe says.

A few months later, Shipley had drawn up the target and devised an elegant way to make it. Awe was impressed, and the pair applied for a lab-funded grant for six months to build the targets and do initial experiments on Sandia's Mykonos accelerator, a pulsed-power facility a twentieth Z's size.

After a couple years of rigorous Mykonos tests, careful analysis and a published paper, the duo applied for and received three Z machine shots. "I got to be a principal investigator for experiments on Z, which was a dream come true," Shipley says. Part of his Ph.D. work described how AutoMag targets depend on a magnetic field's size. They showed that with AutoMag they could reliably produce fields of up to 100 Tesla. On Z, they observed symmetrical, cylindrical implosions, even with the liners' helical nonuniformity.

"Gabe became the poster boy for how LDRDs (laboratory-directed research and development grants) succeed," Awe says. "He did great work on a small facility, vetting the concept, and then it turned into a part of Sandia's ICF program and saw significant time on Z."

Shipley had also been working on the dynamic screw pinch concept, a novel strategy for stabilizing implosions. Unlike the AutoMag approach, this strategy maintains the solid cylindrical liner but uses exterior metal posts wrapped helically to generate a continually rotating magnetic drive field that partially stabilizes the system. Sandia physicist Paul Schmit produced a paper in 2016 outlining the idea's theoretical physics but hadn't described a detailed testing scheme or received experimental time to test it.

Schmit knew about Shipley's AutoMag success and in 2017 approached him about working on the dynamic screw pinch. Shipley explored helical coil designs to create the stabilizing magnetic field and incorporated window-like spaces so that X-ray diagnostics could measure the implosion within.

But after another colleague did larger dynamic, 3-D simulations, the team realized that the initial design had flaws. When Shipley decided to spend a year learning a Sandia 3-D multiphysics simulation code to run the more sophisticated calculations himself and troubleshoot the potential vulnerabilities, Schmit was floored. "Full disclosure: I've designed 65 experiments on Z to date," Schmit says. "I don't even know how to run a 3-D calculation. As a trained experimentalist, it's almost unheard of for someone like Gabe to pick up this immensely useful and complementary skill."

Afterward, Shipley and Schmit wrote another proposal for a Z shot to test their ideas and were awarded four experiment slots. Says Schmit, "I know for a fact that it was only because of Gabe's contributions that we got shot time on Z."

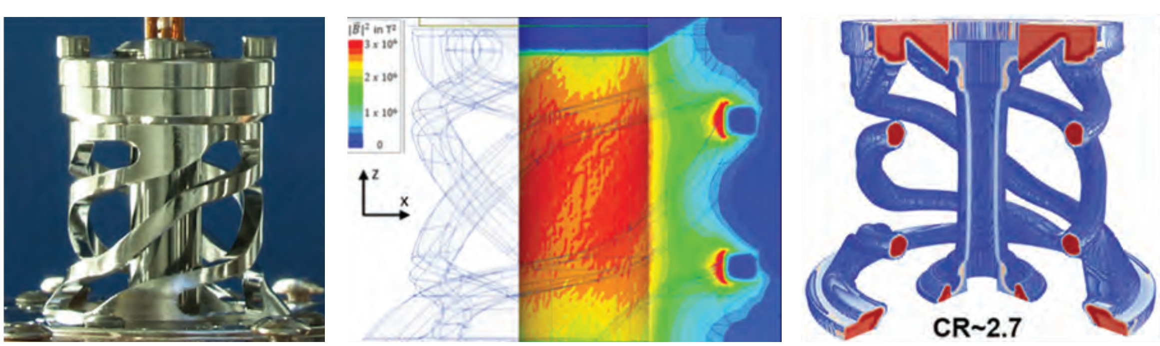
Shipley filled key leading roles on these experiments, which were completed in March 2020 and February 2021, as both principal designer and co-principal investigator. It's unusual for a graduate student to take on either of these roles, his Sandia colleagues noted. It's also incredibly rare for a single person, even staff members with years of experience, to fill both jobs. Although the team just finished the experiments, their new designs appear to have improved on earlier approaches and could support a larger research campaign, Schmit says.

As a Truman Fellow, Shipley can continue with established projects on Z and refine the 3-D simulations that have fueled his recent work. "It is an ideal opportunity," he says. "The rigor has been ratcheted up along with the freedom to explore topics beyond those I've dedicated my Ph.D. research to."

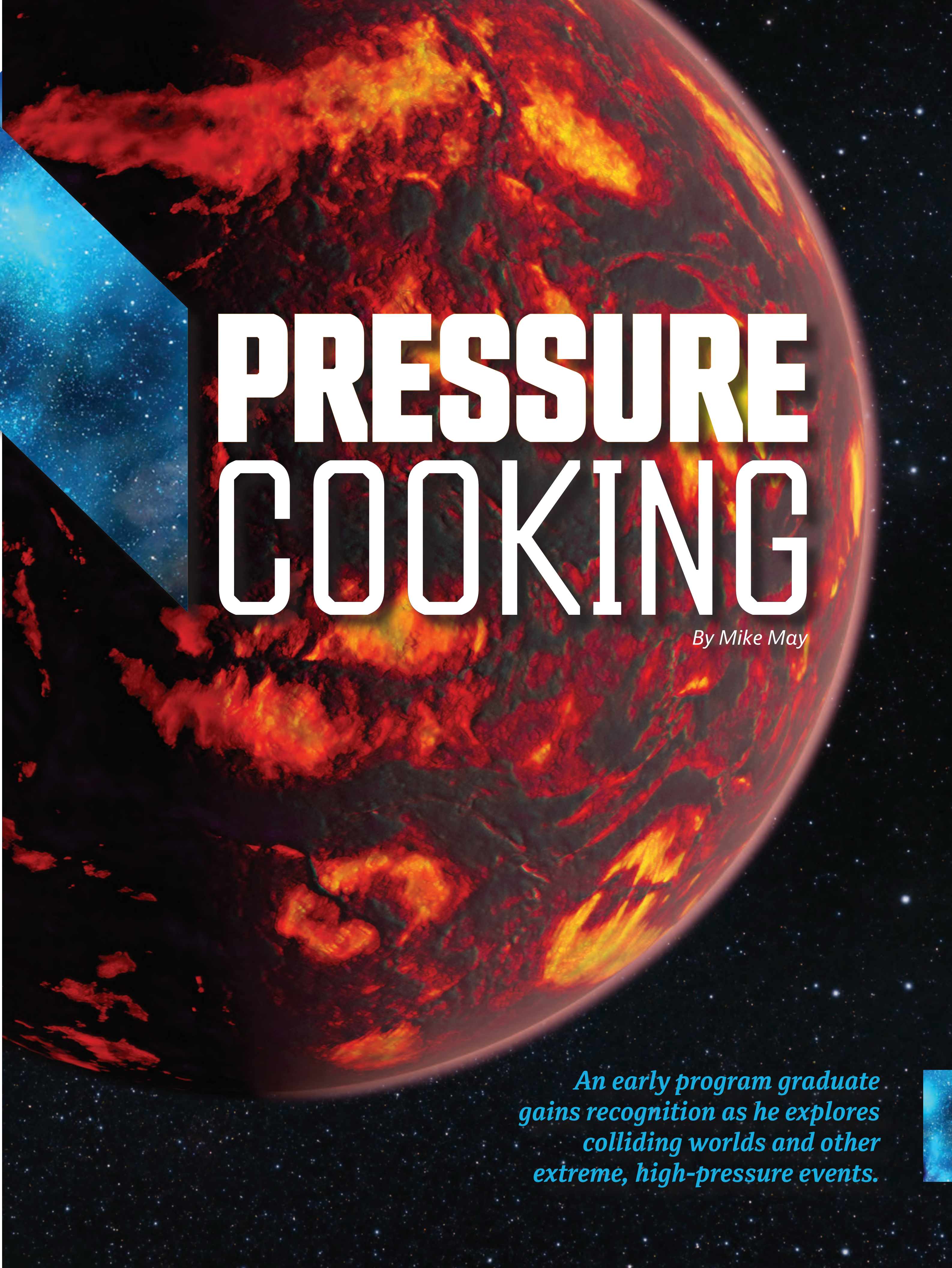
In his new work, Shipley will use 3-D simulation to model initial small-scale instabilities, starting at just a few microns, that form in magnetically accelerating materials on Z and better understand how they grow into larger ones, greater than 100 microns. Such work could improve target-design simulations, reducing the number of numerical approximations needed. What's more, these tools could help researchers understand the instabilities that might occur in larger, higher-energy experiments, thus aiding in the design of future accelerators. Schmit says the problem is universal and will be relevant to other NNSA facilities that also grapple with modeling instabilities under extreme conditions.

Shipley's colleagues attribute much of his success to his team-building talent. "He's effective at making collaborations win-win," Awe says. "He knows when to ask for help, and when he does, he makes it a synergistic relationship. It's not just 'can you help me learn this?' but helping others move their projects forward, too." Shipley also is tenacious, Doss says, in tracking down problems and building the needed skills to pursue important experiments.

Perhaps most impressive, Schmit adds, is Shipley's humility. "He takes nobody for granted." Shipley's personal connections with technicians, engineers, computational designers and the experimental community give him a wide network. "He's a kind of glue that can really hold a collaboration together. He doesn't inject a lot of ego into it. He's driven really by this fascination and curiosity with achieving something difficult."



The solid liner dynamic screw pinch hardware (left) tested on the Z machine. Center: The simulated magnetic pressure mapped within the dynamic screw pinch target geometry. Right: A density map from a 3-D implosion simulation. *Gabriel Shipley.*



PRESSURE COOKING

By Mike May

An early program graduate gains recognition as he explores colliding worlds and other extreme, high-pressure events.

Rick Kraus

As a Harvard University doctoral student, Rick Kraus studied shock physics, in particular the enormous pressures created when planets collide at 30,000 kilometers per hour. Today, as a Lawrence Livermore National Laboratory (LLNL) research scientist, he applies his knowledge of high-pressure physics to stewardship of the country's nuclear stockpile.

Since completing a Department of Energy National Nuclear Security Administration Stewardship Science Graduate Fellowship (DOE NNSA SSGF) in 2012 and joining the lab, Kraus's career has been on a steady ascent. He's published landmark papers and has accreted lab leadership positions and accolades, not least a 2019 Presidential Early Career Award for Science and Engineering (PECASE), recognized as the U.S. government's highest honor for a young researcher.

PECASE noted that Kraus has advanced "the field of materials science, planetary science and material issues that are critical to the nuclear security mission, through elegant and innovative design, analysis and understanding of dynamic compression experiments using gas-gun, magnetic compression and laser sources."

When he discusses the honor, Kraus downplays his personal achievement and emphasizes the value of collaboration. "I had many incredible mentors along the way that have made this achievement possible," starting with his high school math and physics teachers and then as an undergraduate at the University of Nevada, Reno, where he met physics professor Aaron Covington.

Kraus thought he might be able to make extra money grading papers. Covington had no such financing, but he did run an NNSA-sponsored research lab. Kraus says he "started working in the lab, kind of getting my hands dirty but also connecting that experimental research with what I was learning in class. Those connections were really amazing." Kraus immediately found the experiments challenging and rewarding. He was hooked on physics, but it wasn't clear what kind of career he might pursue until he spent two summers working with Damian Swift at Los Alamos National Laboratory. "That's really what cemented it," he says. "Even as an undergrad I thought there's this exciting experimental science that you can do, but in a way that is also beneficial to our national security."

Previous page: An artist's rendering of 55 Cancri e, a carbon-rich exoplanet. Rick Kraus was part of a large team at the National Ignition Facility that achieved the extreme pressures like those in carbon exoplanet interiors. *ESA/Hubble/M. Kornmesser.*

‘It is very likely that previous studies have underestimated the amount of vapor produced during planetary impact events.’

At Harvard, Kraus worked with advisor Sarah Stewart, who is now at the University of California, Davis. Kraus wanted to know how materials behave when they’re subjected to very high pressures and temperatures. He and Stewart were particularly interested in improving the field’s understanding of how the Earth formed.

Grasping planet formation requires lots of work on the fundamental physics of collisions. “Planets grow by a series of impacts, and so understanding how a planet grows and evolves into its current state – say, a habitable environment like Earth – depends a lot on how it got there,” Kraus explains. “My thesis work involved performing experimental research at facilities like (the Janus laser) at LLNL and the Z machine at SNL (Sandia National Laboratories), some theoretical development, and computational modeling describing the detailed processes of growing a planet.”

In 2014, for example, Kraus and his colleagues reported in the *Journal of Geophysical Research* that when planets collide at speeds starting at around 10 kilometers per second, “the internal energy increase is sufficient to melt and vaporize a large fraction of the colliding bodies.”

To predict the likely amount of melting and vaporizing caused by impacts, Kraus and his colleagues used the Janus laser to put samples of quartz under enough heat and pressure to set off the vaporization of silica. Then they measured the sample’s temperature over time after being shocked, which showed that less shock than expected was required to trigger vaporization. “Given our improved understanding of the physics of shock-induced vaporization of silicates,” Kraus and his co-authors concluded, “it is very likely that previous studies have underestimated the amount of vapor produced during planetary impact events.”

Kraus did part of his doctoral research, including the practicum project described above, at Livermore, putting him in contact with what he describes as “a community of folks who were both really engaged in their scientific pursuits but were broadly capable.” He learned the many benefits of collaborations connecting people with diverse interests and capabilities; in fact, he saw how a broad scope of expertise is needed to solve most large problems.

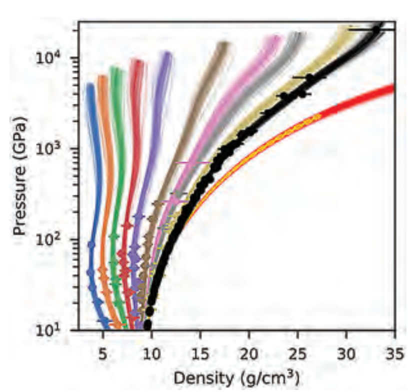
During his fellowship, Kraus also grew interested in labs composed of “really big teams solving really big problems,” he recalls. “That was one of the first times I really engaged in that thought.”

As a graduate student, he explains, “the goal was for you to become the world expert in this little bit of science – you really push the envelope.” Now “it’s about being able to put things together and grow a team and engage a team such that you solve the problems of the NNSA or, more broadly, the U.S. government.”

The doctoral research he performed at the national labs helped Kraus land a Lawrence Fellowship at LLNL. He continued to explore fundamental geophysics questions, but Kraus started to think ahead – to consider what kind of physics career he really desired. One such challenge that intrigued him, even as a student, was ensuring that the U.S. maintains a reliable nuclear deterrent.

“The country supports these really amazing scientific resources,” he remembers thinking at the time, “but they also build these large capable teams where everyone has a really critical role working for a purpose.” He soon knew that he wanted to be part of that, and landed his LLNL staff position.

Maybe that’s not pushing the academic envelope, but it certainly takes science to the edge of what’s possible, especially in maintaining the weapons stockpile without a nuclear detonation since 1992. Instead of testing devices experimentally – actually setting one off to see how it works – Kraus and his colleagues must run trials that stay below nuclear criticality (the point at which an atomic chain reaction begins) and simulate the rest.



An ensemble of equation-of-state models for copper that statistically represents the uncertainty in the underlying experimental data. *Reproduced from* Journal of Applied Physics ***128****, 185902 (2020) with the permission of AIP Publishing.*

One person – world expert or not – cannot run such exercises and simulations and provide accurate data on how devices would perform. It's a big challenge; a team project. And it's up to the NNSA laboratories, including Kraus and his many colleagues, to continually determine the stockpile's status.

Despite the transition to big teamwork, Kraus says his work continues to focus on understanding processes. "How do materials behave at really extreme conditions?" Now he pursues the answers in diverse applications, mostly related to national defense, in three large efforts.

The first involves the U1a Complex, an underground laboratory at NNSA's Nevada National Security Site used in the Stockpile Stewardship Program. Started as an unused borehole for a 1960s underground nuclear test, today's U1a Complex provides a place to run subcritical trials. In the next few years, Kraus will lead a large team of scientists and technicians on experiments there that, he says, will measure important high-pressure materials properties that cannot be measured anywhere else.

Kraus also is working with Los Alamos and Sandia scientists to develop NNSA-backed projects at a couple of powerful DOE Office of Science light-source facilities: the Advanced Photon Source at Argonne National Laboratory and the Linac Coherent Light Source (LCLS) at the SLAC National Accelerator Laboratory. "We came together over the past two years and re-evaluated our mission need for understanding the fundamental mechanisms controlling material performance at extremes," Kraus says. The team concluded there was a coming gap in scientific capabilities, with a demand for instruments that penetrate mid-scale materials to observe mechanisms that control their dynamics. These light sources will be used to improve understanding of high explosives, plasma physics and material science, supporting stewardship of the nuclear stockpile.

Not least, he serves as a project lead in LLNL's Global Security Directorate for, he says, "the material modeling work we do to understand and assess the nuclear threats we might one day face." His team works on "detailed calculations that sometimes requires material models we don't currently have."

If there's a common thread running through Kraus's research portfolio, it might be how to account for uncertainty. If experimental data gets collected and then used in detailed calculations without considering the fundamental uncertainty it holds, that's a problem.

"We have been thinking a lot about how scientists communicate their confidence in what they're doing," he explains. "One of the things I'm most proud of is that we've developed this methodology and a process to perform this transfer of information.

"So that starts to give our scientists who are making assessments – people who are running calculations – the ability to say, 'I know that this calculation is correct to this level of accuracy because I can tie my calculations back to the uncertainties in the original data that constrained it.'"

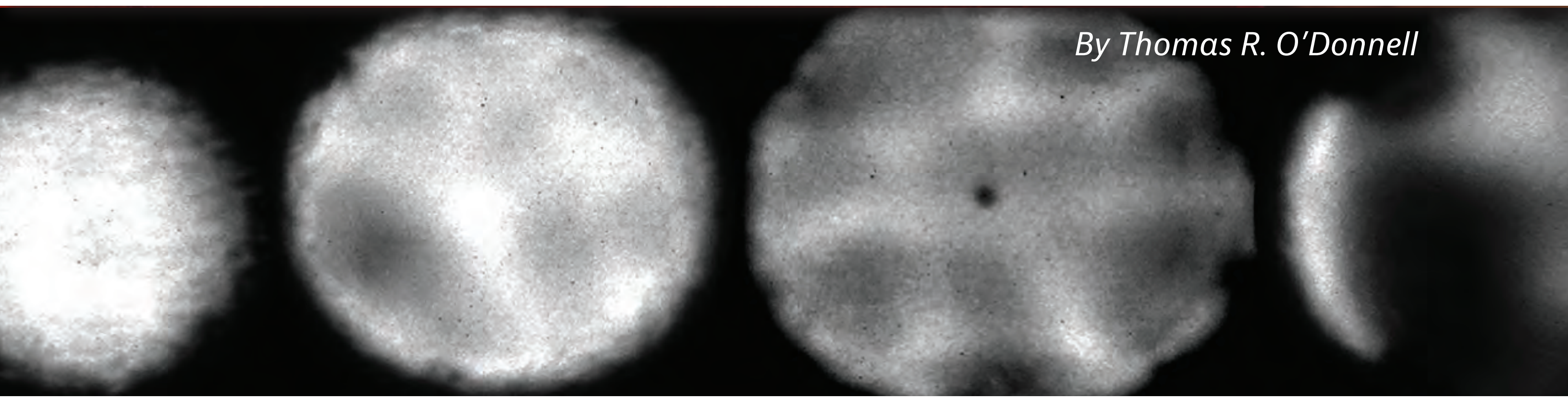
With such challenging work, Kraus has little uncertainty in a career that explores the fundamental physics behind stewarding the nuclear stockpile. SS

The undulator hall at the Linac Coherent Light Source. *SLAC National Accelerator Laboratory.*

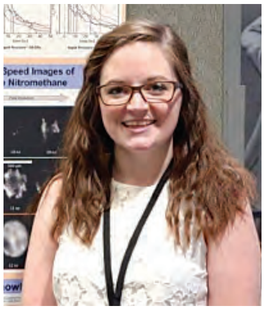
Destination:

DETONATION

By Thomas R. O'Donnell



Diverted from water, a fellow turns to blasts that offer a glimpse into explosions' early moments.



Erin Nissen

An undergraduate astrophysics class at Colorado Mesa University led to Erin Nissen's fascination with how strangely compounds behave under the pressures and temperatures found inside planets. "I got a taste of the more bizarre things that can happen in the universe," she says, and liked that there is much yet to learn about materials under extreme conditions.

Even seemingly familiar stuff like water that "we think we know so much about at ambient conditions," she says, will do radically different things at high pressures and temperatures. "We don't know some of the very basic things that are going on."

So when Nissen, who recently finished her Department of Energy National Nuclear Security Administration Stewardship Science Graduate Fellowship, joined chemist Dana Dlott's group at the University of Illinois at Urbana-Champaign for doctoral studies, she intended to focus on how water behaves when squeezed to astronomical pressures. After two years of refining an experiment, however, a key diagnostic necessary to track the results broke. Repairs – in Japan – took 18 long months.

With the water project dried up, Dlott asked Nissen to collaborate with Mithun Bhowmick, then a postdoctoral researcher who was studying how nitromethane, a liquid explosive, reacts – especially how it detonates – under sudden pressure.

Nitromethane, Dlott says, "is an age-old model system for explosives." It's transparent, so reactions are easier to track, and has a simple, homogeneous chemistry absent in most solid explosives.

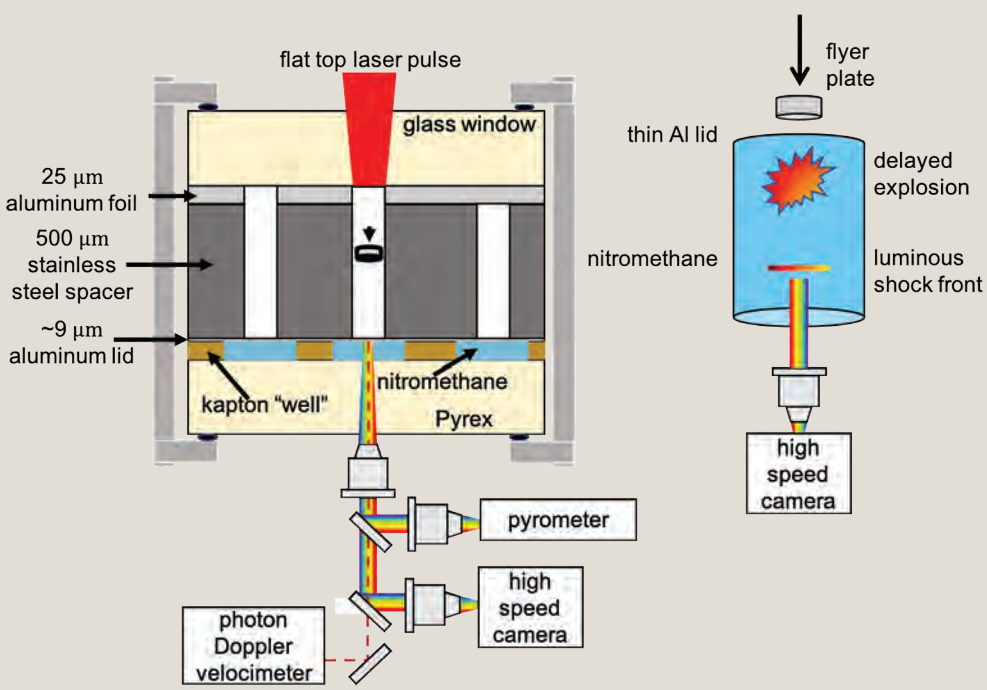
Plus, Nissen says, "if we don't understand (nitromethane) then we're going to have a much harder time" modeling more complex reactive compounds. "And so really understanding the fundamental nature of something so simple really helps with predictive modeling" crucial for maintaining the nation's nuclear stockpile.

Nissen's experiments produced tiny explosions on a glass plate. A laser pulse disintegrated an aluminum foil 25 microns thick – the width of a thin hair. This sudden ablation produced a powerful discharge that launched an aluminum plate, just half a millimeter across and 25 microns thick, as fast as 4.5 kilometers per second.

The flyer plate crashed into an aluminum-film-capped well of nitromethane just 2 millimeters across. Instruments, including high-speed cameras and others that measure velocity and temperature, gathered information about the resulting detonations.

With this experimental framework, Nissen has probed how nitromethane reacts with additives that could accelerate or slow the reaction. She's also studied how physical or chemical modifications to the surface that initiates the shock propagate in the nitromethane reactions.

In a 2020 *Combustion and Flame* paper, Nissen, Dlott and Bhowmick, now at Miami University of Ohio, used the experiment to track the kinetics of detonating nitromethane. They verified that the explosion



Schematic, not to scale, of an experiment in which a laser-launched flyer plate strikes a nitromethane cuvette array made from Kapton polymer tape sealed with a 9-micron (μm) thick aluminum foil lid. Photon Doppler velocimetry measures the velocity of the lid's interior to determine the input flow velocity, or the velocity of the Pyrex window when the shock breaks out. Nitromethane explodes with a time delay, producing shocks that collide with the leading luminous shock front to generate characteristic cellular structures in the thermal emission. *Erin Nissen.*

took place in two stages, starting just nanoseconds after a short, powerful shockwave hit the liquid. The initial shock would decay, the paper says, except for the chemical explosion behind it, which launched shocks that merged with the leading shock front. The more powerful merged shock was strong enough to sustain the detonation. The second shock eventually combined with the leading shock well downstream of the initial reaction.

What's more, high-speed imaging found that as shocklets – tiny explosive shocks – collided with the leading luminous shock front, they boosted density, temperature and heat emissions and produced a distinctive grid pattern.

Other scientists had doubted the experiments would find these structures. "Some people were saying they wouldn't be there at all," Dlott says, whereas others "were saying it may be there, but you couldn't see it because (the patterns) would be too small." With microscopic instruments, however, the grid stood out and "told us where the reactions were happening in time and space. So she answered a longstanding question about whether they exist and used them to unearth more (information) about the mechanism."

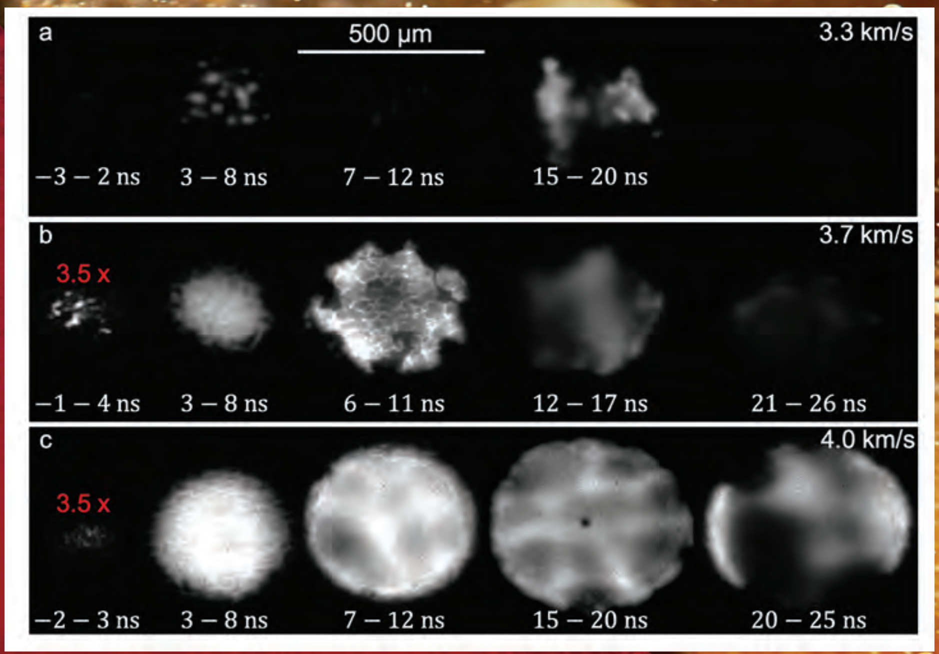
Nissen believes no one had ever imaged the patterns in liquid nitromethane. "That was something we were really excited to see, that it was making these structures," she says. Moreover, their size was tunable, meaning the researchers could change them by varying the experiment's conditions.

The idea that detonation is "creating these beautiful cells over and over and again at the exact same point in the reaction" shows they're fundamental to detonation, Nissen says. "Understanding why that's happening, why nature is continuously creating these cells, I thought that was very interesting on its own."

The experiment was possible only because Nissen overcame a significant obstacle: how to produce the tiny pockets, or cuvettes, that the equally minuscule flyer plates strike. She spent much of her first year of graduate school seeking a workable method. "Creativity hour, I would call it, but the hour was actually months." In the end, "we went with the most simplistic route, which is nice for me when I do experiments."

Nissen settled on a simple piece of polymer tape, varying in thickness from 25 to 90 microns, applied to a quarter-inch-thick Pyrex glass plate. (The tape thickness determines the cuvettes' capacities.) A laser milled a series of 2-millimeter-diameter holes in the tape. "Then we have these little baby cuvettes, and I can pipette the liquid (nitromethane) on top of the surface," filling each of them. Next, Nissen applied the aluminum film with a roller, squeezing out the excess liquid and sealing each cuvette. The process produced around 50 targets each time, enough for a day's worth of experiments.

"The nice thing about our tabletop setup is I can look in the microscope and see every single cuvette. I always know what I'm firing at. I know if it's empty, I know if there are bubbles inside, I know if the lid is wrinkled or weird," potentially skewing the results.



Nanosecond-scale time lapse images, left to right, of thermal emission produced as a flyer plate struck nitromethane. In image series a, at top, the plate traveled at 3.3 kilometers per second; in b, middle, at 3.7 kilometers per second; and c, bottom, at 4 kilometers per second. Hot spots coalesced into a uniform shock front that evolved into a structured front with cells, most noticeable in c, that are measured in millionths of a meter. *Erin Nissen.*

The arrangement's simplicity surprised Dlott, who had imagined something more complex. "I had all this stuff that was going to take NASA and Intel to make it happen, and she did it with chewing gum and Scotch tape," he jokes. "It was one of the examples when I told her it would never work and she went ahead and made it work. She's good at not listening to me when it matters." The experimental technique is widely applicable to other liquids – and perhaps even gases – and has become a standard tool in Dlott's lab.

Once the data were in, Nissen says, she and Dlott had to convince the explosives research community that their apparatus worked and produced valid results. Most experiments like these take place at much larger scales, from gas guns to the massive Z pulsed power machine at Sandia National Laboratories. "People didn't think we were going to be capable of producing a detonation on our tabletop system," Nissen says. "That took quite a while to prove to people that no, we are doing this. We are creating a detonation." Now researchers occasionally visit the Dlott lab to study the equipment and perhaps duplicate it.

Nissen got her chance to study water on her 2018 practicum at Sandia's New Mexico campus. She worked with Daniel Dolan to study the formation of ice VII, a phase of water found only under high temperatures and pressures. The extreme pressure forces the water molecules into a repeating, cubic lattice. Once the pressure releases, ice VII returns to normal liquid water.

'She's good at not listening to me when it matters.'

The research explores fundamental properties of phase transformations, says Dolan, who first studied water under extreme conditions for his doctoral thesis. Astronomers also think ice VII could be found on bodies where high pressures exist, such as the moons of Jupiter and Saturn and on giant exoplanets circling other stars.

"We know a lot about ice VII already," Nissen says, including whether it freezes in varying ways or homogeneously and at what pressures it transitions. But, Dolan notes, most of those measurements are under static compression: "You squeeze your liquid sample, and it appears to turn to ice instantly."

In their experiments, Nissen and Dolan focused on the effects of two factors: the initial temperature and pressure that ramps up gradually – albeit over an incredibly short time. The key questions: If the water's temperature varies when compression starts, what's the effect on when it will freeze to ice VII? And if you change how fast or slow you ramp up the pressure, will that also affect when the water transitions?

With ramp compression, Nissen says, "you're mitigating the temperature, so you have a much, much lower temperature at, say, the same pressure that you might reach with shock compression," which boosts pressure suddenly. "You might be at the same pressure, but the temperatures are way hotter in shock compression."

The experiments ran on Thor, a Sandia machine whose brief, powerful electric pulses generate magnetic fields and tremendous pressures. Thor let Nissen ramp up pressure so quickly, Dolan says, that "there's a point where the water *wants* to be ice VII, but that doesn't mean it can just instantly *become* ice VII because the molecules all have to arrange themselves in just the right configuration for that to happen."

Researchers have long wanted to quantify the lag between when water crosses the phase boundary and should be solid and when it actually freezes. To the human eye, it appears instantaneous but actually can span millionths of a second.

In multiple shots on Thor, Nissen and Dolan compressed tiny water samples at varying ramp rates over millionths of a second. The tests reached maximum pressures of from around 7 to 9 gigapascals – 70,000 to 90,000 times Earth's atmosphere. That's high but at the low end of extreme-pressure experiments.

Diagnostic instruments tracking the water's phase found that a higher initial temperature produced a water-to-ice VII transition at a higher pressure, around 9 gigapascals. Decreasing the ramp rate to compress the water more slowly caused ice formation at lower pressures. That effect was less significant, however, than the one produced by changing the initial temperature.

In a 2019 paper in the *Journal of Applied Physics,* Nissen and Dolan say the research provides additional benchmarks for phase-transition simulations. It was the first paper based on results from experiments on Thor, Dolan says.

Although Nissen had no experience working with magnetic-drive compression, Dolan says she needed little supervision after learning the fundamentals. "Erin is just intense and very independent," he says, and quickly "knocked out a whole bunch of work."

The practicum, Nissen says, had a huge impact on her research and career plans, introducing her to different kinds of science and to work at the national laboratories. It also whetted her appetite for research into water and other materials under extreme conditions.

"I'd like to move away from explosives and move more into planetary science and the interiors of planets," possibly with a focus on water, Nissen says. She hopes to pursue those studies on a return to Sandia, where she began work as a postdoctoral researcher after graduating this spring.

Dlott says Nissen won't stay in one position for long. "She likes science, she likes the research," but she wants a job "that will give her the best career opportunity, as opposed to 'I've got to study x or y.'" When possible employers ask about Nissen's future, Dlott tells them, "Oh, she's going to be your boss."

Outgoing fellows describe their research experiences. (Abbreviation key: SSGF/LRGF = DOE NNSA Stewardship Science Graduate Fellowship/ Laboratory Residency Graduate Fellowship.)

THEORY IN PRACTICE

Yale University's Paul Fanto embraced physics relatively late, switching from political science his junior year at Princeton University. He was inspired by how physicists defined specific, addressable problems, checked their answers and built on their results.

Paul Fanto

His first semester-long research experience at Princeton: a theoretical project to simulate operation of the Large Hadron Collider's proton accelerator beam. Researchers assumed that the protons acted independently of each other, but Fanto examined whether correlated behavior among the particles could introduce error and how that might change experimental results. A senior year working with Princeton physicist David Huse inspired him to pursue graduate school in theoretical physics.

At Yale, Fanto worked with advisor and nuclear-reaction code expert Yoram Alhassid on a new way to calculate nuclear-state densities that help determine the number of stable configurations the nucleus can access as a reaction gives off energy. These values help researchers understand reactions because nuclear processes are more likely to occur if more energy levels are available for decay.

Fanto and Alhassid's simulations are based on Hauser-Feshbach theory, a long-standing framework that lets researchers use nuclear reaction experimental data to extrapolate to nuclei that haven't been tested. During his 2018 practicum at Los Alamos National Laboratory, Fanto worked with Toshihiko Kawano, who employs Hauser-Feshbach theory to produce nuclear data libraries used to model key stockpile stewardship-related reactions.

A cover of the Yale science webzine Paul Fanto cofounded.

Working at Los Alamos fueled Fanto's budding interest in national security and defense research. After completing his Ph.D. in 2021, he started a research position at the Institute for Defense Analyses (IDA), a think tank in Alexandria, Virginia. Fanto learned about the institute from a Los Alamos postdoctoral researcher and later met another IDA researcher, SSGF alumnus Angelo Signoracci, at the fellowship's 2019 program review. Those connections led him to his new job.

Beyond his graduate work, Fanto sang with a Yale a cappella group and cofounded the online science magazine *Yale Distilled.*

PHASE DECIPHERER

LRGF recipient Dane Sterbentz was drawn to the University of California, Davis, and advisor Jean-Pierre Delplanque through a shared fascination with the mysterious behavior of compressed water. Delplanque also had research connections with Lawrence Livermore National Laboratory (LLNL), which led Sterbentz to residencies there with Philip Myint and Jonathan Belof in 2019 and 2020.

Sterbentz studies phase transitions that happen when water is steadily squeezed or rapidly shocked. His test case is ice VII, a phase found on oceanic exoplanets and in other astronomical settings but also in compression experiments that force molecules into a repeating, cubic lattice.

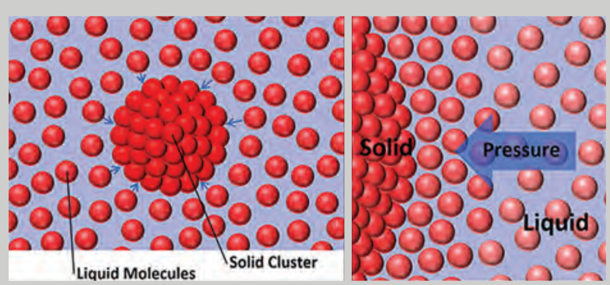
Phase transition kinetics dictate the magnitude of an energy barrier water molecules must overcome to form a stable cluster of solid molecules, a process called nucleation. These solid clusters can then grow to complete the transition. With Myint and Belof, Sterbentz modeled ice VII nucleation and found that interfacial free energy – involved in disrupting molecular bonds – may have had more influence in phase transitions than transient kinetics. They described the work in an October 2019 *Journal of Chemical Physics* paper.

In another project, Sterbentz modeled experiments – conducted by Erin Nissen, an SSGF recipient (feature this issue, page 19), during her Sandia National Laboratories (SNL) practicum – that used powerful magnetic fields to ramp up pressure on a water sample to make ice VII. Sterbentz also has modeled laser-driven results from the University of Rochester's OMEGA, an NNSA-supported laboratory.

Sterbentz used Ares, an LLNL hydrodynamics code, to simulate Nissen's experiment and paired it with an optimization algorithm that seeks the problem's best solution from myriad options. The algorithm varied drive pressure values through multiple simulations until it found ones that produced output pressures matching real-world results. Because the approach doesn't explicitly simulate the pressure-producing drive mechanism, it's widely applicable to other compression experiments. The project led to a 2020 *Journal of Applied Physics* paper.

Sterbentz finished his dissertation in December 2020 and soon after started an LLNL postdoctoral research appointment. He hopes to land a staff job there or at another national laboratory.

Dane Sterbentz



In dynamic-compression experiments (right), pressures tens of thousands times Earth's atmosphere push liquid molecules toward solid, nucleated clusters, leading to rapid growth and a phase transition that can occur within a microsecond. *Dane Sterbentz.*

IMPACT FACTOR

Gil Shohet

A lot happens in the nanoseconds after micrometeoroids smaller than sand grains collide with objects moving faster than a bullet. “There’s so much physics going on,” says Gil Shohet, a Stanford University doctoral student and SSGF recipient.

Material, mostly from the impacted surface, melts, vaporizes and ionizes, spewing into the vacuum as a charged-gas cloud of warm dense plasma before soon expanding into a low-pressure plasma.

There’s evidence that the dusty plasma’s oscillating and interacting electrons produce radio-frequency radiation and electromagnetic pulses, like tiny lightning strikes or nuclear explosions. Scientists don’t completely grasp the mechanisms of these bursts but fear they could interfere with or damage a spacecraft’s electronics.

A satellite or spaceship could suffer catastrophic harm when a large particle strikes, Shohet says, but “you have these much more frequent, smaller impacts that have the potential to cause electrical damage and they’re harder to characterize and detect.”

Such crashes can be informative, however, when they’re on asteroids, comets or planets. The resulting plasmas could provide clues to an astronomical body’s origin and mineral composition without having to land a spacecraft on it. For now, scientists are restricted to computational simulations and Earth-bound experiments, both of which occupy Shohet’s research with advisor Sigrid Close. “You have these many, many orders of magnitude in density,” Shohet says. “You need many models” to emulate the phenomena.

Shohet delved into particle-interaction calculations during his 2018 practicum at SNL. With Michael Desjarlais and Josh Townsend, he learned density functional theory, a method that includes the strange effects of quantum physics when computing molecules’ electronic structures.

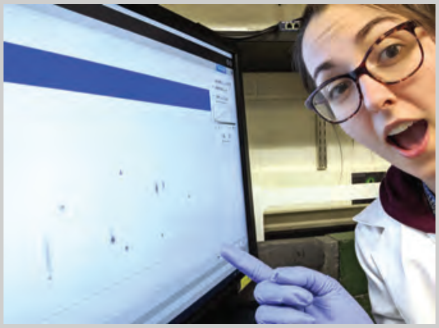
Shohet focused on forsterite, a magnesium-oxygen-silica compound found throughout our solar system. He ran multiple calculations of forsterite’s critical point – the phase in which its vapor and liquid states are indistinguishable – and pressure under extreme densities and temperatures, leading to a publication in *Geophysical Research Letters.*

After graduating in 2021, Shohet expects to continue doing fundamental research, location to be determined.

FRAGMENT COLLECTOR

At Michigan State University, Paige Abel produced radioactive nuclei in new ways that take advantage of the school’s National Superconducting Cyclotron Laboratory and its other nuclear research facilities.

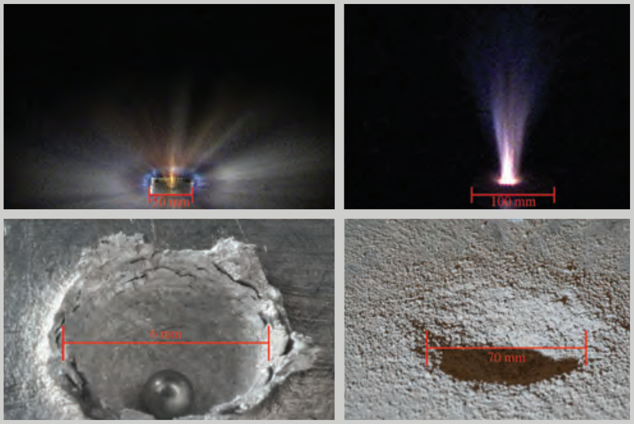
The machine beams heavy oxygen and uranium nuclei – and everything in between – at half the speed of light and smashes them into targets, producing exotic fragments for study. Abel and her colleagues devised a way to send the beam to a flowing water target to collect interesting isotopes, particularly calcium-47, from one of the more commonly used beams, calcium-48. Calcium-47 decays to scandium-47, a difficult-to-produce nucleus that may have use as a diagnostic tracer molecule and in cancer therapy.



Paige Abel

During her 2019 LLNL practicum, Abel worked with Ken Moody and Narek Gharibyan on a nuclear forensics project designing a method for producing tungsten-188 nuclei, which are rare and can be made when a nuclear weapon detonates. The material can be used for experiments on complex nuclear reactions and to interpret data from past nuclear tests. It was an ambitious project to carry out in just a few months, Abel notes. But she completed training, worked on separation methods, participated in the beam experiment and separated the resulting radioactive samples. “I don’t think I could have asked for a better practicum experience,” she says. “I got to experience a wider range of what radiochemistry has to offer.”

Abel completed her degree in December 2020 and now works as a radiochemist for Niowave, a Lansing, Michigan, company that produces radiopharmaceuticals. Besides the practicum experience, she says the SSGF offered opportunities to learn about other disciplines and to share her own research. “It pushed me out of my comfort zone and helped me have intelligent conversations with other scientists about their work.”



Impact flash and craters from gas-gun impacts on aluminum (near right) and regolith simulant, material with the composition and texture of space dust (far right). *Gil Shohet.*

MEET THE NEW DOE NNSA GRADUATE FELLOWS

STEWARDSHIP SCIENCE GRADUATE FELLOWSHIP

John Copley
Princeton University
Materials Under Extreme Conditions

Garrett King
Washington University in St. Louis
Nuclear Science

River Leversee
University of Colorado Boulder
Materials Under Extreme Conditions

Benjamin Reichelt
Massachusetts Institute of Technology
High Energy Density Physics

Yoni Xiong
Vanderbilt University
Nuclear Science

LABORATORY RESIDENCY GRADUATE FELLOWSHIP

Alexander Kavner
University of Michigan
Physics
Lawrence Livermore National Laboratory

Brianna MacNider
University of California, San Diego
Materials
Los Alamos National Laboratory

Brian Rodgers
Colorado School of Mines
Materials
Lawrence Livermore National Laboratory

Brendan Sporer
University of Michigan
Physics/Pulsed Power
Sandia National Laboratories, New Mexico

For the complete listings of current fellows and alumni, please visit the fellowship websites.

https://www.krellinst.org/ssgf/
https://www.krellinst.org/lrgf/

For more information, contact program coordinator Kris Moran, kmoran@krellinst.org, (515) 956-3696.

EXPLOSIVE EXPRESSIONISM

A Sandia National Laboratories team has mastered the fine art of depositing thin explosive films on silicon to study how small surface cracks, caused by substrate contaminants, affect the explosive's performance. This is a closeup of one of those surfaces. For more, see page 4.

The Krell Institute
1609 Golden Aspen Drive, Suite 101
Ames, IA 50010
(515) 956-3696
www.krellinst.org/ssgf