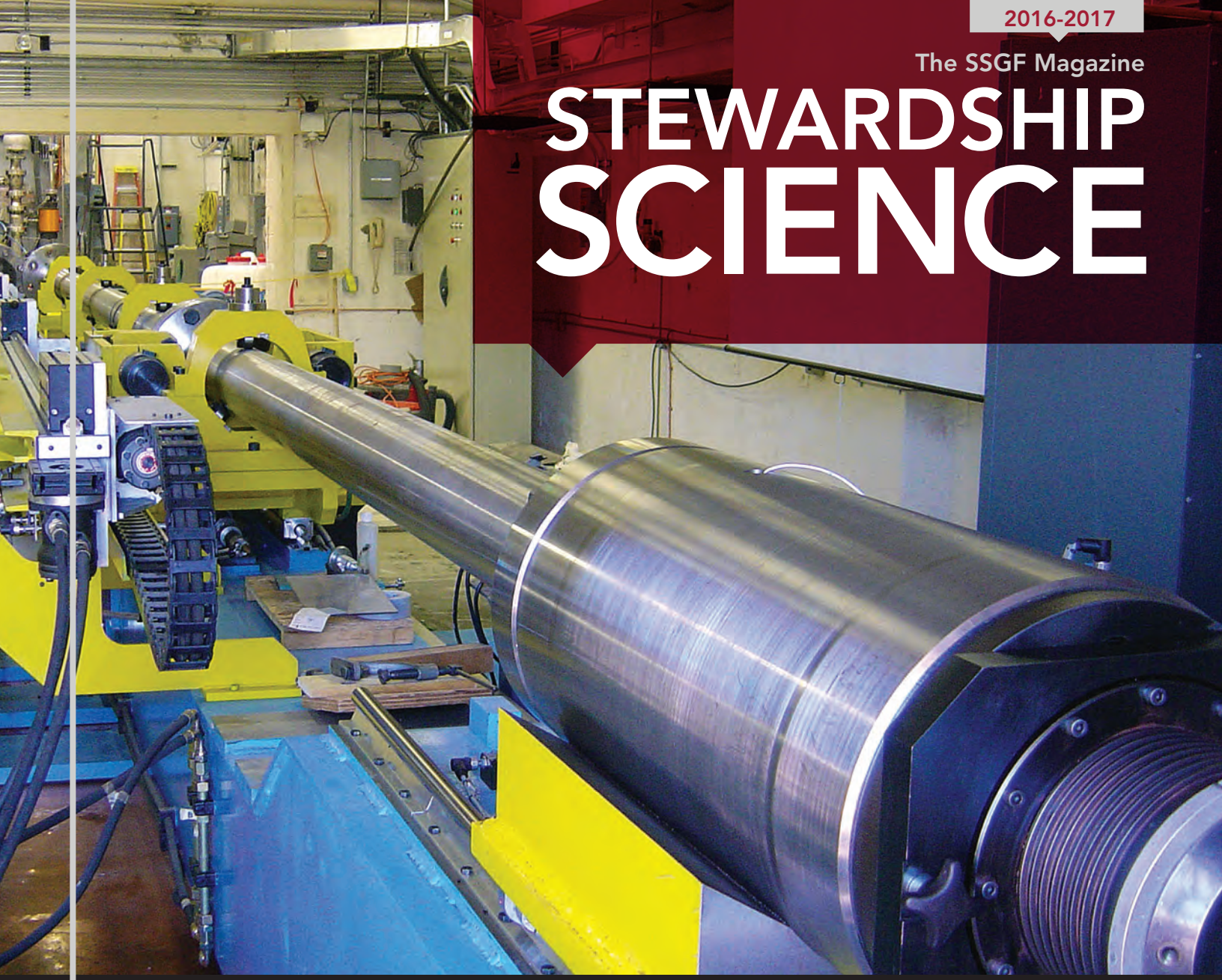
2016-2017
The SSGF Magazine

STEWARDSHIP SCIENCE



PINGING PLUTONIUM

Livermore in Nevada, firing up the big gas gun

Sandia: Swinging Thor's hammer

Los Alamos: Finding hidden explosives

Plus: Fellowship turns 10, an earlier Earth's core, metals' strength under pressure, fellows at the labs, a talk with the program's first alumnus, where one fellow was when the lights went out

Department of Energy National Nuclear Security Administration

STEWARDSHIP SCIENCE GRADUATE FELLOWSHIP

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

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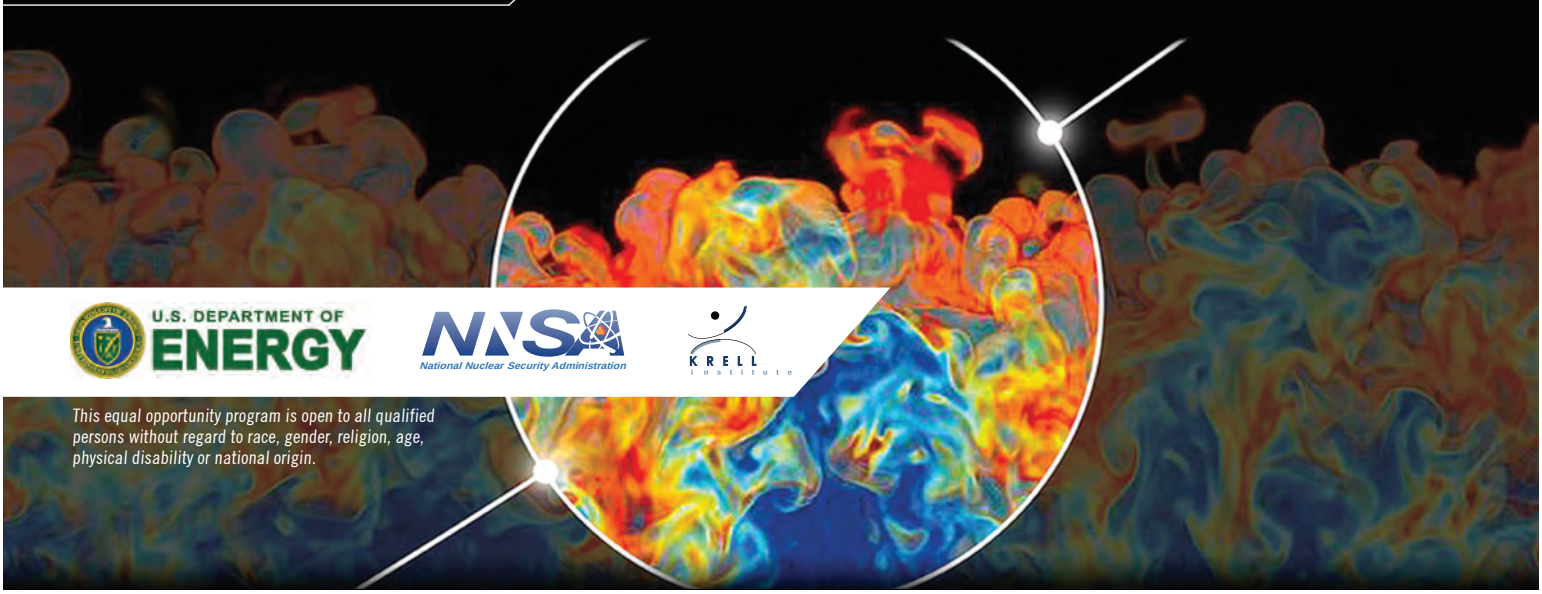

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Viva SSGF

THE NEVADA TEST SITE ORAL HISTORY PROJECT – a rich repository of voices from the Cold War, curated by the University of Nevada, Las Vegas – reports that from the 1950s until the final test in 1992, 1,021 nuclear devices were detonated at the 1,375-square-mile Nevada National Security Site (NNSS) northwest of Vegas. The moratorium has held for a quarter century. In that time, Congress created the National Nuclear Security Administration (NNSA) and the site's name changed to its current one, reflecting its new roles: stockpile stewardship and national security.

By 2011, Lawrence Livermore National Laboratory's Bruce T. Goodwin was telling *The Washington Post* that we have "a more fundamental understanding of how these weapons work today than we ever imagined when we were blowing them up." He was speaking specifically of supercomputer simulations, which are informed by the shock physics and hydrodynamics experiments of Livermore, Sandia and Los Alamos national laboratories, often in collaboration with NNSS site-operator National Security Technologies.

This issue of *Stewardship Science* features as its cover story research inside one of the workhorse facilities at NNSS: JASPER and its 30-meter-long, plutonium-compressing gas gun. Since 2003, data gleaned from experiments at JASPER have informed supercomputer calculations like those Goodwin noted. Also featured in this issue: Sandia's latest pulsed-power device, which goes by the whimsical name of Thor, and Los Alamos' ongoing research into new ways to detect hidden explosives.

Nevada and NNSS also played a large role in a milestone for the Department of Energy NNSA Stewardship Science Graduate Fellowship: the program's 10th anniversary. Commemorations included the 2016 program review in Las Vegas, featuring an NNSS tour and, as always, presentations from fellows finishing their final year in the program. Over the next few pages, you'll find stories about those fellows' national lab experiences – plus a talk with Lawrence Livermore National Laboratory's Miguel Morales, the fellowship program's first alumnus. Like him, most of the program's 30 graduates now work in areas important to the NNSA: high energy density physics, nuclear science and materials under extreme conditions and hydrodynamics.

Elvis may have left the building long ago, but the fellowship's mission of training the next generation of nuclear scientists and technologists has only just begun. Here's to the next decade.

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

2016 2017

STEWARDSHIP SCIENCE

DEPARTMENTS

FRONT LINES

SAMPLINGS

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COVER

SHOCK JOCK

A view of the JASPER gas gun looking from the breech to the pump tube, past the acceleration reservoir and the launch tube into the secondary confinement chamber. JASPER stands for Joint Actinide Shock Physics Experimental Research; the gun is housed in a facility at the National Nuclear Security Administration's Nevada National Security Site. When fired, the gun generates enough force to propel 15- to 30-gram projectiles down its 30-meter length and slam them into small plutonium targets at up to 18,000 miles per hour. JASPER shock physics results are crucial to nuclear stockpile stewardship efforts. Read more, starting on page 12.

Stewardship Science: The SSGF 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) program, which Krell manages for NNSA under cooperative agreement DE-NA0002135. Krell is a nonprofit organization serving the science, technology and education communities.

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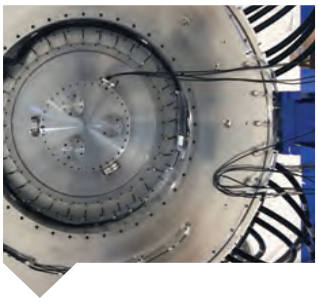
FEATURES



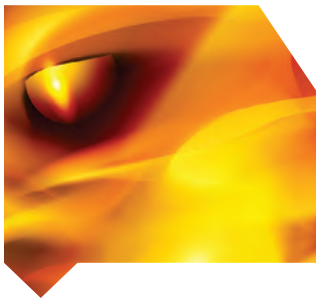


IMAGE CREDITS

Cover, Nevada National Security Site (NNSS); page 4, Lawrence Livermore National Laboratory (LLNL); page 7, Los Alamos National Laboratory (LANL); page 8, Sandia National Laboratories (SNL); pages 13 and 14, LLNL and NNSS; pages 15-19, David Reisman, SNL; pages 22 and 23, Purdue University/LANL.

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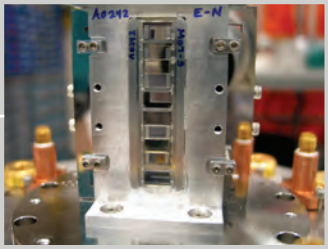
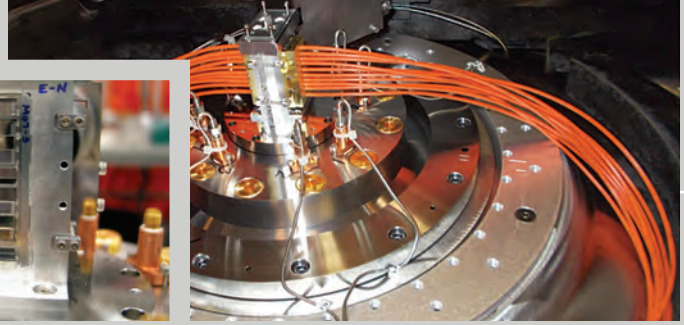




Iron Storm

Above: The 2-inch tall physics experiment package in the center of the Z machine chamber. Orange fiber optic cables transmit data from the package about the velocities of shockwaves and aluminum projectiles in the impact experiments. Inset: A close-up of one of the target panels in the experiment package, with 10 samples on each panel. Each experiment holds two panels, allowing the team to shoot 20 different targets on each experiment.

It may not have had the impact of a huge meteor striking the young Earth, but Richard Kraus' recent research still made a splash around the world. Kraus, a Lawrence Livermore National Laboratory research scientist, published experimental results that are challenging theories of how Earth formed. News outlets picked up the *Nature Geosciences* paper and *Discover* magazine named it one of 2015's top science stories. Far-flung friends and colleagues told Kraus they'd heard the paper's assertion that iron may have fallen like rain on the young planet.

Earth and other rocky planets formed through particle accretion and meteor and planetesimal impacts. As these planets grew, the collisions landed at ever-higher velocities, says Kraus, an alumnus of the Department of Energy National Nuclear Security Administration Stewardship Science Graduate Fellowship. Near the end of Earth's formation more than 4 billion years ago, giant, iron-rich rocks hit its mostly molten surface at 20,000 to 90,000 miles per hour.

Scientists believe the stony shower supplied most of Earth's iron, including the solid core and molten outer core responsible for Earth's protective magnetic field via the magneto-dynamo effect.

Under the impact of meteors and planetesimals, iron would have reached pressures two to three times that at Earth's center and temperatures in the tens of thousands of degrees, Kraus says. Yet "it's surprising that we don't know how it behaves" under those conditions. "What happens to it? Does it melt? Does it vaporize?" His experiments sought answers.

Using the Z machine, Sandia National Laboratories' massive pulsed-power facility, Kraus and his colleagues fired aluminum plates less than a centimeter square and about a millimeter thick into equally small iron samples at 30,000 to 37,000 miles per hour. At impact, the plates squeezed the iron samples to more than 630 gigapascals (GPa), about twice the pressure at Earth's center.

The shocks passed through the iron samples and into vacuum gaps. As the pressure released, the iron expanded across the gap, decompressing and accelerating into a quartz window, where instruments tracked the iron's velocity to determine its thermodynamic state.

The tests found iron vaporizes at lower impact speeds and shock pressures than previously thought, about 500 GPa instead 900 GPa. Or, as Kraus puts it, "for a given impact speed there's a lot more iron vaporized."

Iron in a meteorite striking the early Earth would have melted on impact. As the shock passed, the material would have decompressed, and the iron and rocky mantle around it would have vaporized, Kraus says. The vapor would have spread over the planet, condensing and raining as iron particles that mixed with the molten mantle.

The findings also help clarify how the core formed and materials spread through Earth's crust. Geochemists say elements should have mixed efficiently during crust formation, based on their distribution in the mantle. Geophysicists, however, say there's no mechanism for mixing. Standard theories say an incoming object would have splashed into the molten mantle, its iron core sinking deep into Earth. Kraus's findings support the geochemists.

The results suggest that the planet's core formed earlier than in some predictions: 30 million years after the solar system formed rather than 100 million.

Now Kraus is moving from inner Earth to outer space with more high-pressure iron experiments.

Astronomers have found dozens of exoplanets orbiting stars throughout our galaxy. They want to know whether these bodies, typically many times Earth's size, could sustain life. A protective magnetic field, like Earth's, is one necessary condition. Kraus's next experiments, at the National Ignition Facility (NIF) in Livermore, will look at how iron's state changes under the extreme pressures inside giant planets and the implications for a solid iron inner core and liquid outer core to produce the magneto-dynamo effect.

The NIF experiments will have two parts: First, lasers will vaporize a beryllium layer just a quarter of a millimeter thick, driving a shock of at least 300 GPa into an iron sample. Next, a laser pulse will ramp the pressure to 700 GPa and ultimately to around 2,000 GPa.

The test should emulate the circulation in a solid-liquid planetary core: Hot material at the base expands and rises to the outer layer, where temperatures and pressures are lower. Cooler material descends from the outer layer surface.

"We're trying to find the same thermodynamic path as the cool material at the outside of this liquid outer core," Kraus says, "and then asking will it solidify as we increase the pressure? And where does it solidify? At what point?"

What Kraus and his co-principal investigator, Russell Hemley of the Carnegie Institution for Science, learn could help astronomers identify which exoplanets are most likely to have magnetospheres.

–Thomas R. O'Donnell

Fellows on Location

The DOE National Nuclear Security Administration Stewardship Science Graduate Fellowship's outgoing class describes the national lab research experience.

FORCE OF NATURE

In his **Lawrence Livermore National Laboratory (LLNL)** practicum, **J. Scott Moreland** looked into a weakness in calculations of the strong nuclear force.

Quantum chromodynamics (QCD) theory portrays the strong force's effects and is a main research area for Ron Soltz, who supervised Moreland's work at LLNL in 2014. QCD calculations help researchers study matter's fundamental nature, especially in the microseconds after the Big Bang, when the quarks and gluons comprising matter briefly disassociated into a quark-gluon plasma (QGP).

Scientists recreate the QGP in particle colliders like Brookhaven National Laboratory's Relativistic Heavy Ion Collider (RHIC). In 2000, such experiments found the QGP behaves like a perfect fluid with minimal viscosity. Soltz is on one of two research teams that used lattice QCD simulations, which break QGP behavior into discrete pieces for computation, to calculate the QGP fluid's shear velocity and equation of state.

At Livermore, Moreland, a **Duke University** nuclear science doctoral student, compared the teams' data to analyze and quantify systematic and statistical errors in lattice equation of state calculations. As Moreland reported in his practicum evaluation, he found that systematic uncertainties contributed about 5 percent uncertainty in the production of anisotropic flow, an observable quantity used to constrain QGP shear velocity predictions. That suggested the teams' results were consistent with error in models of heavy-ion collisions. Moreland concluded that increasing computer power to refine the lattice equation of state and further constrain relevant QCD observables would have only marginal success.

Moreland, who does similar research at Duke under Steffen Bass, devised the heavy-ion collision simulations the analysis used and wrote code to handle results. The research was published in December at the ArXiv online repository.

J. Scott Moreland

Sarah Palaich

Mareena Robinson Snowden

WASTE NOT

Sarah Palaich's research at **Los Alamos National Laboratory (LANL)** focused on materials used to store nuclear waste.

Working in 2015 with supervisor Florie Caporuscio, a specialist in radioactive waste disposal, Palaich quantified the corrosion of copper exposed to high temperatures and pressures in hydrous media containing the clays found in engineered barrier systems. The systems are used in nuclear repositories and are important to the U.S. Used Fuel Disposition Campaign.

Palaich used reflected light and scanning electron microscopes to image the residual copper. From the images, she made about 800 measurements of pitting and copper byproduct growth to quantify the corrosion. Palaich, a doctoral student at the **University of California, Los Angeles**, is first author on a paper detailing her results.

Palaich did all the work with minimal supervision, Caporuscio wrote in his evaluation. He hoped to continue the collaboration. "She is a huge asset to the scientific community and would do extremely well in her desired field."

While at the lab, Palaich discussed her interest in science education with Claudia Mora, leader of the LANL Earth System Observations group and president-elect of the Geological Society of America. With Mora's help, Palaich plans to join the society's education committee.

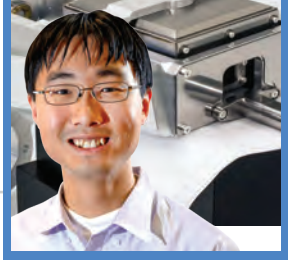
The LANL project stretched her knowledge and skills, Palaich noted. "I loved every second of it," especially doing a project different from her doctoral research, under Abby Kavner, which studies the structure and behavior of minerals in the deep earth. "I look forward to collaborating with the people I met at the lab."

FORBIDDEN FISSION

Sniffing out forbidden materials motivated **Mareena Robinson Snowden's** 2014 project at **Livermore**.

As in her thesis research at the **Massachusetts Institute of Technology**, she focused on finding ways to passively detect nuclear warheads to enforce weapons control agreements. Her goal: to use a warhead's natural radiation signatures to detect the high explosives within it.

Using MCNP, a neutron transport code developed at LANL, Robinson Snowden modeled the radiation interactions of spontaneous fission neutrons in a crude warhead design. With the model, she was able to make preliminary estimates that identified the presence of a weapon's high explosive from


Hong Sio


Sabrina Strauss


Christopher Young

gamma rays generated during thermal neutron capture and from inelastic scatter inside the material.

She next used californium-252, a strong neutron source, and a simulated high explosive to experimentally investigate the emission strength of these higher-energy gamma rays.

It was Robinson Snowden's second LLNL practicum. Both connected directly to her research, under Richard Lanza, to develop radiation-detection systems to verify bilateral nuclear disarmament treaties. She expects to use the warhead model she developed as a basis for future detector designs.

WARM RECEPTION

Hong Sio waded into warm dense matter (WDM) at **LLNL**.

Working with Gilbert Collins and Yan Ping in 2014, Sio designed and conducted experiments to measure thermal conductivity in WDM, a phase of matter found deep inside giant planets and created in inertial confinement fusion (ICF) experiments like those at LLNL's National Ignition Facility.

The measurements, Sio wrote in his evaluation, will be used to test heat conduction models in strongly coupled plasma phase space. They're important to understanding aspects of ICF experiments, in which powerful lasers generate radiation to implode tiny capsules containing hydrogen isotopes. If all goes well, the hydrogen nuclei fuse, releasing energy.

Sio used the radiation-hydrodynamic code HYADES to simulate how the warm dense matter target evolves during and after proton heating. He chose a final design for the experimental target based on data from multiple simulation runs, each with varying target thickness and material parameters.

Sio later helped with the experiments at LLNL's Jupiter Laser Facility. He also worked to analyze the results, some of which were published in 2015 in the journal *Physics of Plasma*. Sio's designs will be used in future experiments and the data he produced will become part of how researchers predict and analyze high energy density (HED) experiments.

Sio, who studies aspects of ICF implosions under Richard Petrasso at **MIT**, said he's long been attracted to the national laboratories' HED research facilities. His experience at Livermore reinforced that appeal.

SUPERHEAVY STUDIES

Sabrina Strauss spent several weeks at **LLNL** studying one of the newest entries on the periodic table.

Working with Nicholas Scielzo in 2014, Strauss analyzed the structural properties of superheavy elements. She focused on flerovium, element 114, created in 1998 when Russia's Flerov Laboratory of Nuclear Reactions bombarded plutonium 244 atoms with calcium-48 atoms.

Flerovium is a short-lived element, and scientists have observed fewer than 100 atoms. They have gathered data about lighter flerovium isotopes, produced through a calcium-48 reaction with plutonium-239, to study both the structure of superheavy elements and the limits on their stability.

Strauss' job was to make sense of data the Flerov lab gathered on these lighter isotopes. Because the reactions produced few statistics, the analysis also had to calculate background radiation's contribution.

In his review of Strauss' research, Scielzo said she helped determine nuclear decay properties and production cross-sections for the calcium-48 reaction with plutonium-239 and compared them to results from experiments using heavier plutonium 242 and 244 targets.

To analyze the background potential, Strauss wrote a code incorporating a Monte Carlo random probability technique to interpret the results and determine their statistical significance.

Strauss researches nuclear structure and astrophysics in her doctoral research under the **University of Notre Dame's** Ani Aprahamian. The LLNL project was in the same field, but "it was a far different region of study than the experiments I normally do," she reported. "I was given an opportunity to expand my views of what nuclear physics covers."

Scielzo, meanwhile, planned to continue the collaboration: "I hope this is the beginning of a strong partnership between LLNL and Notre Dame."

PLOTTING PLASMAS

Particle-in-cell, the standard technique in plasma physics simulation, lacks dynamic range and is subject to statistical noise. Other methods become too computationally demanding as the problem size and complexity increases.

Despite having little background in computational physics, **Stanford University** doctoral student **Christopher Young** worked with chunks of code **LLNL** practicum supervisor David Larson had gathered over the years – and added his own work – to implement a new approach, the Shape Function Kinetics (SFK) method. SFK converts the plasma constituents into finite mass packets that move and stretch in time under the influence of external and internal forces. In the remap step, new shape functions are periodically fit to a particular state of the data. Young produced the first results with a Gaussian mixture model remapping, combined with the expectation-maximization algorithm.

By the end of the 2012 practicum, Young had modeled a quiescent plasma – a simple electron distribution with fixed ions – showing the SFK approach is viable. He identified a bottleneck in the algorithm's remap step, paving the way for later improvements.

Young learned the Fortran 90 programming language to do the work. Though he had some experience with programming and plasma simulation, he noted afterward he faced "a steep learning curve, as the SFK method is pretty unique."

His doctoral research into plasma diagnostics under Mark Cappelli is largely experimental, but with some work the SFK method could help validate and predict tests. He and Larson published their findings, including additional test cases, in the March 2015 issue of the *Journal of Computational Physics*.

Jet-setting Cerium

Impacts, explosions and other fast, powerful phenomena generate shock waves that distort, deform and destroy the materials in their paths. With what they learn from these shocks, scientists could better understand meteorite strikes and engineers could design stronger armor for soldiers and new materials for cars and airplanes.

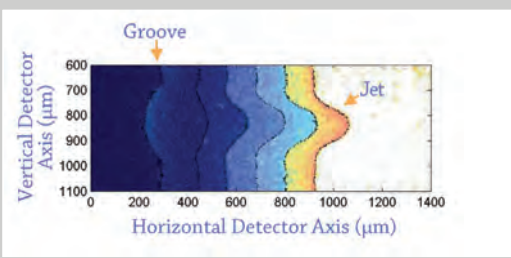
"Shock waves provide a well-defined, well-controlled way to reach the high pressures required to begin studying strength," Los Alamos National Laboratory's Brian Jensen says. Over the past decade he and his colleagues have explored the fundamental physics of materials under extreme conditions, simulated by shock waves, with an initial emphasis on iron and cerium.

Cerium, a rare-earth metal, "has numerous phases more easily accessible than other materials," Jensen says. It displays a variety of structures in its solid and liquid states over a relatively moderate range of temperatures and pressures. That's led Jensen and his colleagues to use gun systems and explosive loading on cerium samples to simulate extreme events such as a meterorite impact or explosion. The researchers then observe changes in the metal's structure.

To build a foundation for its work, the team described how cerium behaves at the macro scale. Jensen and his colleagues have learned how it compresses and flows and the critical temperatures and pressures where the metal transforms between various liquid and solid states.

But what happens at the micro – or even atomic – scale is critical for watching these events in real time and understanding how extreme conditions affect material properties, including strength. So the researchers have pursued X-ray techniques that could allow them to zoom in and observe materials in new ways.

Jensen and colleagues at Los Alamos and Argonne national laboratories and National Security Technologies LLC developed the IMPact system for ULtrafast Synchrotron Experiments (IMPULSE). It's based at Argonne's Advanced Photon Source (APS), a synchrotron radiation source that generates bright X-ray pulses. In what the researchers call a "dynamic compression framework," IMPULSE employs a gun system that generates shock waves, allowing the scientists to study matter under extreme conditions.



Multiple images of a cerium jet captured by a detector after X-rays from Argonne National Laboratory's Advanced Photon Source have been converted to visible light. A team led by Los Alamos National Laboratory generated the image by firing copper projectiles at a cerium sample etched with shallow grooves, one of which is visible at left.

One of the system's first experiments observed jets that formed in cerium when shocked.

The team fired copper projectiles at a cerium sample etched with shallow grooves on its back. The impact created an instantaneous pressure, generating a shock wave that traveled through the sample and interacted with the grooves. That caused the cerium to flow and squirt out ahead of the rest of the sample in a jet, Jensen says.

As the jet forms, the metal's strength reins it in, preventing the material within the jet from escaping. The researchers used a technique called X-ray phase contrast imaging to capture snapshots of multiple cerium jets as they evolved over time.

Obtaining these data required precisely timing the impact with the X-ray pulses and the detectors. To study shock waves, researchers

continued on page 8

must observe the material in the infinitesimal fraction of a second after impact. "With a synchrotron, you can get an X-ray pulse every 150 millionths of a second that can be used to study the material deformation. That X-ray pulse is typically vary narrow in width, less than one nanosecond" or billionth of a second, Jensen says. The team had to time experiments to that single X-ray pulse, capture what the material was doing, and be able to detect it.

Synchrotron systems like Argonne's APS can produce those pulses, but such experiments typically average the results over many pulses – sometimes occurring over seconds and minutes. Jensen and his colleagues had to design a new detection system that could obtain an image from a single X-ray pulse and get the timing exactly right. The new system couples commercially available detectors with a custom-designed optics system. And because it can capture multiple images from a series of individual pulses, the team obtained the first shock-movies using the APS X-ray beam.

– Sarah Webb

Forecasting Failure

Welders have known for centuries that when they connect two pieces of cast metal, the joint is susceptible to splitting, cracking, buckling and, even worse, failing. When the consequences of weld failure could be catastrophic – mid-flight, say – minimizing that risk is paramount. But predicting failure in various real-world scenarios remains based on experience and conjecture.

"When a manufacturer says, 'we made some welds and got N-number of pores in there, is that OK?' the answer to that question currently is, 'I don't know,'" Sandia National Laboratories' Brad Boyce says. Boyce is co-principal investigator of the Predicting Performance Margins (PPM) program, a lab initiative to bring science-based predictive capabilities to questions of material strength and reliability.

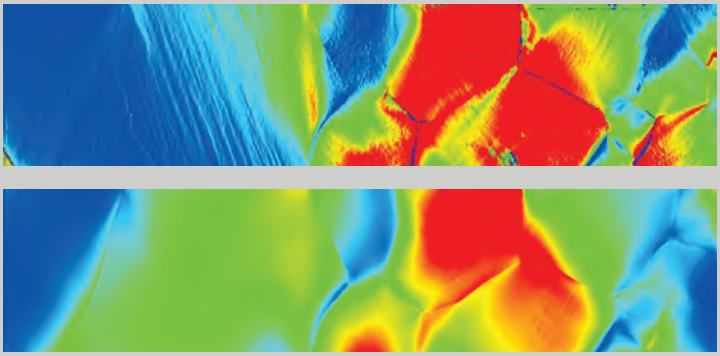
Now in its fifth year, PPM is closing the gap between atomic-scale modeling and bulk materials behavior by exploring physics at the micrometer scale. This intermediate, or mesoscale, science is the least understood aspect of material properties. Engineers expect mesoscale advances will help them move beyond validation of material performance and toward accurate prediction and control in the design process. It offers clues as to how impurities affect crystal formation and how crystal structure deformations lead to the resulting bulk-scale material's behavior under working conditions.

At the micrometer scale, the PPM team combines high-performance computing with novel experiments to explore the pores, divots, gaps and other imperfections that weaken a weld joint or polymer seal.

In a 2015 proof-of-concept study in the *International Journal of Mechanical Science*, the PPM team used some of the highest-resolution metallic-grain-deformation data published to date to demonstrate that its experimental results and computational models align quantitatively. Researchers developed a heat treatment to form tantalum oligocrystals with large, 1-millimeter grains that spanned the entire width of the sample, creating a monolayer that made surface measurements possible. They also created a customized loading stage coupled with a high-resolution digital image correlation method that let them collect detailed data from the entire sample.

On the computational side, postdoctoral scientist Hojun Lim worked with co-principal investigator Corbett Battaile to perform simulations that closely matched the experimental conditions. They built a crystal plasticity model that described the evolution and propagation of dislocations using continuum state variables and coupled that model with Sandia's Sierra Solid Mechanics multi-physics code, which was developed as part of the Advanced Simulation and Computing (ASC) program.

To compare measured and simulated results, the researchers mapped experimental data to the model's finite element mesh. Model predictions of both surface strains and grain rotations at a range of applied strains matched experimental results well enough to validate the computational model.



Top: A high-resolution digital image correlation, a technique that measures strain that shows on the surface of a specimen, in this case tantalum oligocrystal. The colors correspond with the magnitude of the strain, with blue lowest and red highest. Bottom: The predicted strain for the same sample as simulated via crystal plasticity finite element modeling. The prediction agrees well with the measured strain.

The team can begin to answer this question: Will it hold? And nowhere is that quandary more pertinent than in 3-D printing or, as it's known in industry, "additive manufacturing." Sandia engineers have been among the pioneers in the field, developing Laser Engineered Net Shaping (LENS), a process to print complex metal parts from powders poured into molds and fixed by laser energy. Manufacturers are excited about the potential of this process, but many questions remain about its performance under the stringent standards required for an airplane or, say, as a replacement part destined for the nuclear stockpile.

–Karyn Hede

Conversation

An Alumnus 'Obsessed' with Enigmas

'After the practicum, it was extremely clear what my career path would be.'

Miguel Morales is a research scientist at Lawrence Livermore National Laboratory's Condensed Matter Physics and Materials Division. He was a DOE NNSA SSGF recipient from 2006 to 2009.

You create and run first-principles models of materials under extreme pressures and temperatures. Why is it important to understand these things?

There are technological and fundamental reasons. On the technological side, for example, there's the National Ignition Facility, which studies materials under the extreme physics found in nuclear detonations. You have to compress materials to extremely high temperatures and densities. You reach scales that are completely unknown and do things that we have never been able to do in a lab. The physics at these scales is not only new but unexpected, in some cases, so we need tools that allow us to understand the properties of these materials and some of the physical processes occurring in the experiment. Then we can use that information to design the experiment.

From a fundamental point of view, hydrogen, for example, is the most abundant element in the universe. Most of the giant planets are mostly made of hydrogen and helium. The pressures inside the cores of these planets are extremely high and materials behave differently there. We need to understand and predict that behavior in order to understand things about planets and galaxies.

What advantages does working at a national laboratory provide you?

I do computational work, and the national labs have some of the best computational resources on the planet. Also, because it's such a multidisciplinary environment, there are great chances for collaboration. And anytime I need to find an expert in any topic it's very likely I'll find someone around here who knows about it.

In 2014 you received a Presidential Early Career Award for Science and Engineering. What has that meant for your research?

It's been a very positive experience. It's allowed my career to grow at a pace that I don't think would have been possible otherwise – funding opportunities, collaboration opportunities. It also allowed me to be placed in leadership positions I probably wouldn't have been in otherwise.

You were the first graduate of the DOE NNSA SSGF. In general, how is the program viewed, 10 years after it was founded?

We have many alumni in the labs, particularly here at Livermore, so as a recruiting tool it has been extremely successful. It also fills a void, funding-wise and opportunity-wise, for people working with materials in extreme conditions and other areas the fellowship funds. And it brings an incredible opportunity for people in the labs to access these fantastic students during practicums and for the students to learn what actually happens inside the labs. The program should be seen, I hope, extremely positively for both the universities involved and for people from the national labs.

How did your time as an SSGF recipient influence your career?

It influenced it completely. After doing my practicum at Livermore, it was clear this is the place where I wanted to end up. I'm not sure I had a clear long-term career path before I had the fellowship. But especially after the practicum it was extremely clear what my career path would be, or at least what I wanted it to be.

You've been honored as a role model for Hispanic youth. What can we do to engage underrepresented groups in STEM (science, technology, engineering and math)?

We have to pay attention to them. There's a real need to provide the necessary opportunities to our youth and to present science and STEM fields to them as attractive possibilities. In most underrepresented communities, there's little understanding about STEM or the idea that you can have a fulfilling life doing science, technology, engineering and math, so we need to bring in successful scientists and people within STEM fields and present them to kids as role models and people to aspire to and be inspired by. This needs to be done on a regular basis and in a widespread way.

What element of your work excites you the most?

I love solving problems. Every time I stumble on a problem that I cannot quite figure out, I get obsessed.

COVER STORY

FIRING UP THE BIG G

TECHNOLOGY THAT WAS GOOD FOR GENERAL MOTORS AND NASA INSPIRES LAWRENCE LIVERMORE NATIONAL LABORATORY PLUTONIUM SHOCK PHYSICS RESEARCH.

UN

BY MONTE BASGALL

A WARNING SIREN SOUNDS as the control room staff at the Nevada National Security Site (NNSS) tenses in concentration. With a rumble, the latest JASPER shot ignites. In far less than a heartbeat, energy from up to three and a half kilograms of ignited gunpowder generates enough force to hyper-accelerate 15- to 30-gram projectiles. They fly down a 30-meter-long two-stage light gas gun and slam into similarly small plutonium targets at up to 18,000 miles per hour, nearly three-quarters the escape velocity from Earth. The resulting shock wave assaults the plutonium with up to 6 million times atmospheric pressure (600 gigapascals), greater than the load at Earth's center.

Such cosmic smashups at JASPER, an acronym for Joint Actinide Shock Physics Experimental Research Facility, are revealing otherwise unobtainable details about plutonium. The experiments are an alternative to the underground nuclear tests that ended decades ago and provide information that's key to maintaining the reliability of the nation's nuclear stockpile.

"Aside from being radioactive, plutonium is one of the most complicated metals there is because of its different potential structures," says Neil Holmes, the program's originator and a physicist who leads Lawrence Livermore National Laboratory's gas gun dynamic-shock research.

"Plutonium is complicated because of the complicated physics involved to understand it. It has so many protons (94) that even relativity is important to the theory." Because it's one of the most difficult metals to calculate, it's also "a great challenge for theorists."

JASPER's stockpile-informing findings are classified because plutonium is used in nuclear weapons. From its first shot in July 2003, its data have consistently been deemed so close to perfect, Holmes says, that theorists and modelers use it to underpin supercomputer calculations that the nation's Stockpile Stewardship Program relies on. JASPER is one of the main experimental facilities of the National Nuclear Security Administration's Science Campaign.

"No one has ever done what we have," Holmes says. "Plutonium had been studied for decades, but the data were never quite good enough. I had a new idea about how to do it." Holmes drew inspiration from three similar gas guns General Motors originally built for NASA to evaluate nose-cone re-entry.

GM later sold those, one each, to his and two other national labs, Los Alamos and Sandia. Holmes recalls proposing, "Why don't we build another gun like the one here (at Livermore) but in a place that can be safe to do experiments with plutonium?" The new gun was assembled at NNSS Building 5100 for about $20 million and costs about that much to operate each year.

There are no explosions or radiation inside JASPER's long barrel, Holmes emphasizes. Working with it is thus far less messy and far more economical and surgical than a nuclear test would be.

His technology burns conventional propellants that pressurize common gases (see sidebar, below) to launch flat-faced impactors at up to 8 kilometers per second but

INSIDE THE BIG GUN

The two-stage light gas gun used at the Joint Actinide Shock Physics Experimental Research (JASPER) Facility fires special scientific bullets called impactors, specially constructed so they can be accelerated to half a million times Earth's gravity without suffering damage from such intense forces.

"It's gentle enough; that's why we do it," says Neil Holmes, the Lawrence Livermore National Laboratory physicist who came up with JASPER. "The impactor arrives at the target intact, unheated, unchanged."

They also use a low-molecular-weight gas, typically hydrogen, which increases the projectile's allowable speed. "Roughly speaking, we can get 10 times the shock pressure with a two-stage gun," Holmes notes.

Workers load three different kinds of gunpowder in the gun's breech to provide initial energy. The burning powder pushes a deformable piston made of plastic, copper and wax along a pump tube at up to 2,200 mph.

The piston serves to trap and squeeze a reservoir of hydrogen where the tube tapers down into the beginning of a narrower barrel. A rupture valve there opens when pressures reach about 5,000 atmospheres (75,000 psi), launching a 28-millimeter-diameter impactor placed beyond the valve towards its plutonium target.

On the way, a series of sensors activate an explosive ultrafast closure system by crunching an aluminum tube into a seal just after the projectile passes, blocking the escape of radioactive plutonium fragments. A shock wave occurs when the impactor hits the target and diagnostics measure the response.

After the experiment is completed, the primary target chamber where the plutonium was mounted is sent to the Department of Energy Waste Isolation Pilot Plant in New Mexico for disposal.

Meanwhile, the now-deformed piston has sealed off the gun barrel's other end, leaving only gas from burned gunpowder on the other side. After that is vented, the gun is disassembled and cleaned. JASPER can now be prepared for its next experiment.

lasting only as long as 1.5 millionths of a second. Striking plutonium targets with such a massive momentum sends hyper-intense shock waves through them before they self-destruct.

JASPER's main experimental focus is to understand the basic physics of plutonium, Holmes says. By adjusting variables like the force of propellants or the mass and makeup of impactors, his team can study how plutonium responds at high temperatures, densities and pressures.

This temperature-density-pressure relationship is formally known as the equation of state. "When many solids are pressurized or heated, the atoms rearrange themselves into new stable solid crystalline patterns called phases," Holmes says. "Those phases can act like very different metals. They might conduct heat or electricity differently. They might even look very different. Plutonium is noteworthy because of the many and complicated crystal phases it can form."

Doing shock wave experiments on plutonium is no easy task. Plutonium doesn't exist in nature but instead is made in a nuclear reactor. It is highly reactive chemically and can occur in many isotopic forms (with differing numbers of neutrons). It's hard, brittle and extremely radioactive.

"So it is no wonder that experiments to measure the shock properties of pure plutonium at high pressures have been going on for a long time," Holmes says. "It's simply hard to do." That form wasn't completely characterized until his group did it in 2015, capping a 50-year effort. "That's what JASPER has done."

JASPER operates with a team of more than 70 people, about 40 from Livermore and 35 to 40 from National Security Technologies, the NNSS management and operating contractor, on-site project manager Trenton Otteson says. The team includes engineers, scientists and technicians. Some have such striking mechanical abilities that Holmes labels them artists.

When Holmes was interviewed in early 2016 for this article, the big gun was awaiting Shot 139. Each experiment is an extended logistical challenge that can take a year or more to prepare. Because JASPER aims to do one shot a month, Otteson adds, "there's a lot of work, and it's very hard a lot of times."

To complement those so-called hot shots, the team also has conducted 40 or 50 surrogate shots. These are used to test various components or new technology without using real plutonium targets. Surrogate targets are typically made of

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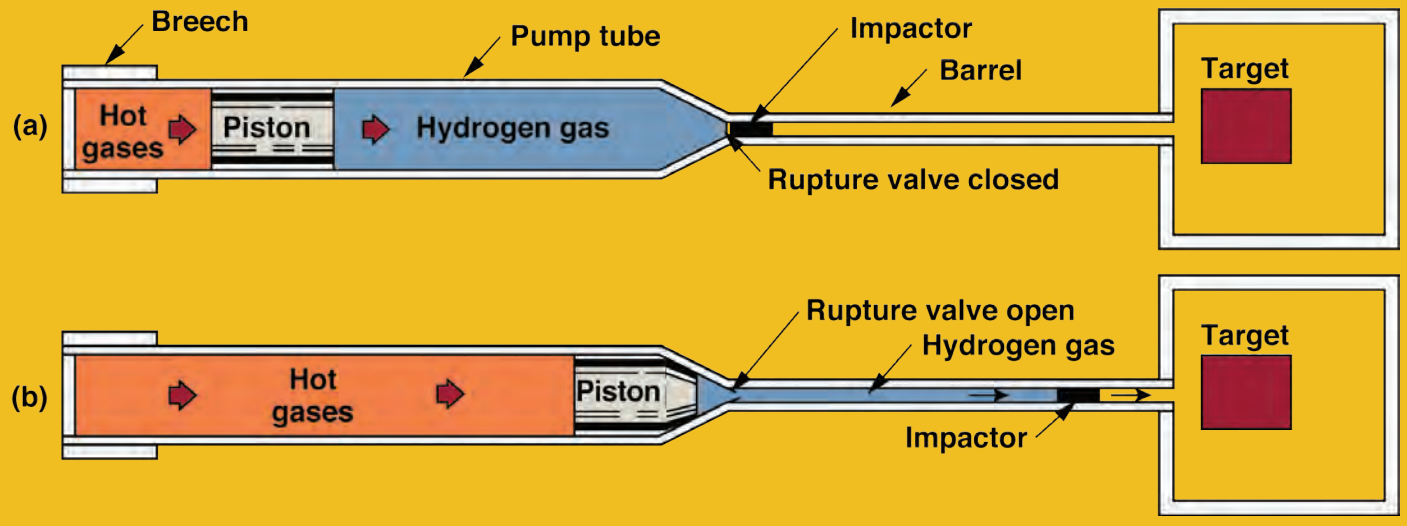


simple metals like aluminum or tantalum – tantalum being close to plutonium, Holmes says.

"If we go through major maintenance, we'll do another surrogate shot to make sure everything still works as we expect. Every time we have a new target design, or a new diagnostic, we'll do a surrogate test."

The researchers also use diagnostic instruments to measure gun performance and how plutonium responds during the shock generated at impact. There are electrical pins, for example, that short out to log passing shock waves and two flash X-ray units that measure projectile velocities. There's also a velocity interferometer system for any reflector, or VISAR, and photonic Doppler velocimetry, two more techniques for measuring speed by evaluating light-interference patterns.

Although temperatures are hard to measure precisely under these conditions, they can be inferred by radiometry, which uses photomultiplier tubes to measure light that shock wave-heated targets emit. Researchers also measure how metals conduct electrical current – used to help interpret radiometry. The team is adding another detection method, X-ray diffraction, to determine the crystal structures of shocked plutonium samples.

X-ray diffraction evaluations are already underway at Livermore's High Explosives Application Facility (HEAF), home of one of the GM-built guns JASPER is modeled on. That HEAF gun also is the test bed location for many of JASPER's surrogate shots.

JASPER's dime- and nickel-sized targets – too small to go "critical," Holmes says – are made at Livermore's Superblock, one of the nation's two defense-related research and development sites for plutonium. Working there, inside a radiation-stopping glove box with the added protection of 1/8-inch-thick gloves, deft technicians hand-lap the metal surfaces to a flatness within 2 microns or better of perfection. That tolerance is "about one-thirtieth to one-fiftieth the thickness of a human hair," Holmes marvels. From the Superblock, carefully packaged plutonium samples are shipped to the Device Assembly Facility at NNSS for final assembly into gun targets.

Meanwhile, other Livermore craftsmen expertly assemble the two kinds of impactors that strike those targets.

The first are solid metal impactors, designed to produce single steady waves that provide simple shocks, Holmes says. With precise velocity measurements during the experiment, "we can determine the final pressure, density and internal energy of the sample using relations that express conservation of mass, momentum and energy."

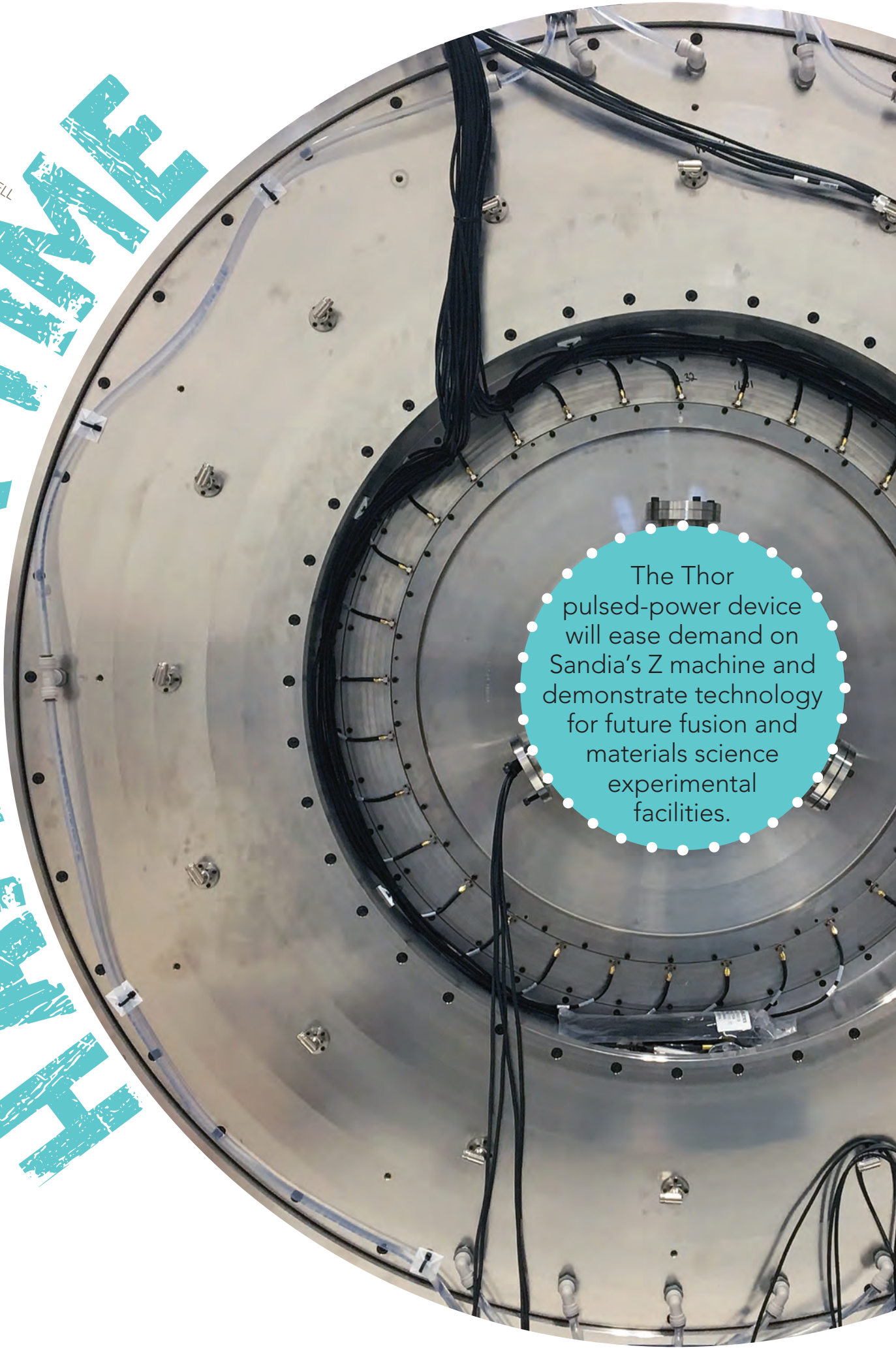
The others, called graded density impactors, or GDIs, are made of up to 100 layers of different densities and materials and "gets us to places we can't with simple experiments," Holmes says. Building a GDI requires embedding powdered metals, typically magnesium, aluminum, copper and tantalum, in a plastic matrix which is then cut like cookies, stacked, heat pressed and finally reheated to cook out the binder. "Eventually you get something you can machine," Holmes says. "It gives you unparalleled access to the kinds of thermodynamic states you couldn't reach otherwise."

How long will the JASPER program continue? "I'm guessing more than 10 additional years at least," Holmes says. "The next five years are mapped out. I think it might go on indefinitely because, as we learn more, there are more questions. We need to make basic measurements that we are still learning to do." SS

A view inside the gas gun's secondary confinement chamber, looking at the primary target chamber that was designed by Lawrence Livermore National Laboratory and built by National Security Technologies.

HAMMER TIME

BY THOMAS R. O'DONNELL



The Thor pulsed-power device will ease demand on Sandia's Z machine and demonstrate technology for future fusion and materials science experimental facilities.

THE Z MACHINE, Sandia National Laboratories' famed pulsed power facility, has a new little brother – and it's bringing down the hammer.

Thor, which began making test shots in 2016, is a condensed, less-powerful version of Z. But it's agile, making it especially useful for discovery in materials science and geophysics, and has advanced technology that could find its way into an upgraded Z.

Z, perhaps the most famous device at Sandia National Laboratories' New Mexico location, takes its name from the Z-pinch: using powerful currents that run in the same direction as the z axis on three-dimensional graphs to contain plasma, a hot mix of ions and electrons. Massive banks of capacitors in the 10,000 square-foot facility deliver a thousand times the energy in a lightning bolt but in a time span 20,000 times shorter. The brawny charge produces tremendous, finely focused magnetic fields that crush tiny targets and squeeze plasmas as a step toward possible nuclear fusion.

Z has proven itself in experiments exploring the forces and radiation found in nuclear weapons detonations, the secrets of fusion energy and the properties of materials under extreme conditions, but it's tricky to use. Its devastating power heavily damages shot hardware, and it's difficult to calibrate the length and strength of its pulses. Z can fire only about once a day.

Enter Thor. It covers just 2,000 square feet and, when it reaches its full capacity, will deliver 100 kilojoules of energy (a speeding bullet has about 1 kilojoule of kinetic energy) compared to Z's 20 megajoules. Thor will produce pressures of about a million times that of Earth's atmosphere – equal to pressure at our planet's core. Z shots can produce pressures of up to five million atmospheres.

But Thor is more than just Z light. Its size and technology means it can do two or more experiments per day, generating more understanding of how materials behave under high pressures, what happens in planetary interiors and more.

David Reisman, a Thor designer and its lead theoretical physicist, says he once asked a researcher studying a material's strength how many experiments he gets to run on the Z machine. "Well, I get maybe four a year," the scientist replied.

"Thor could do four shots in two days," Reisman says. "It allows people to do many more experiments, and they don't necessarily need the super-high pressure" that Z produces. Researchers may want to know how a material's phase changes

The Medusa-like central power flow structure in Thor, Sandia National Laboratories' latest pulsed-power device. The black cables supply pulses from racks of capacitor bricks. Intermediate support towers – spools of supply cables – are to the left and right.

A view inside the central power flow structure. The isentropic compression experiment panel is at center, in copper. Thor's magnetic fields shocklessly ramp up tremendous pressures on materials held here.

at lower pressures, for example, or they may want to test new diagnostic instruments that gather experiment data. Testing such tools "may be more difficult, more risky on a big machine, where you know there's a lot of expense per shot and limited shots."

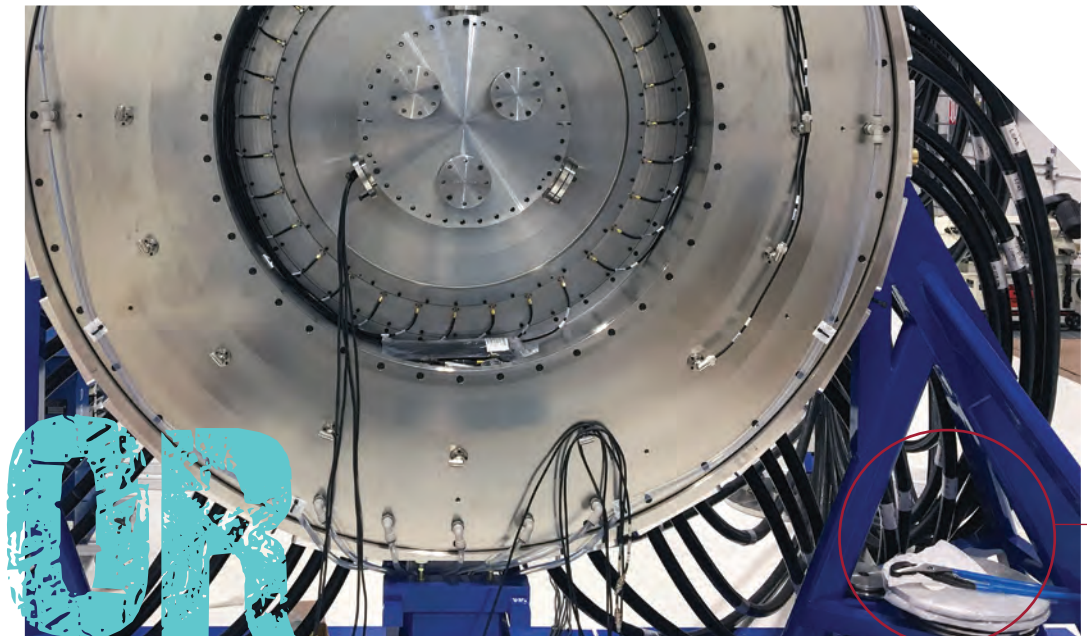
Firing the Z machine is an attention-getting exercise, with alarms and countdowns and technicians sitting behind banks of computer screens. Occupants of nearby buildings can feel the shock of the pulse and spectacular lightning-like arcs cross the pool of oil and deionized water that insulates the transmission lines.

Firing Thor is a calmer event. "It's run from a laptop computer," Reisman says. For what it lacks in flashiness, Thor makes up for in flexibility, allowing "physicists to come in, try new ideas, have more experiments, more data, more throughput, and consequently produce more work, more papers and more understanding."

Z's power comes from 36 Marx generators, capacitor banks that are 8 feet square and 12 feet tall, with tree-trunk-thick transmission lines. Like a camera's strobe light, the banks gradually build electric charge, then release it in one huge, incredibly rapid burst that's funneled into a thimble-sized target.

But the pulse isn't short enough for some experiments. Z technicians must hand-tune transmission line switches to cut the pulse length from microseconds (millionths of a second) to nanoseconds (billionths of a second) and increase impact on the target. The switching cuts Z's energy efficiency and the lifespan of some components.

Instead of monumental Marx banks, Thor uses a series of small advanced capacitors, grouped by twos into cubic-foot bricks. The more bricks – 144 in Thor's final design – the more powerful the pulse will be. During discharge, output ramps up over periods as



Thor's central power flow structure has a target chamber at the center where massive electrical pulses create powerful magnetic fields, crushing materials specimens. The clear and translucent tubes carry deionized water to insulate transmission lines. Note the wrench at lower right for scale.

short as 100 nanoseconds. Energy travels from each brick, through individual cables, into a ring-shaped central power flow structure about two meters in diameter and onto centimeter-sized targets lined up on a thin strip. (The structure's relatively small size means Thor should easily fit into other facilities, allowing access to unique diagnostic instruments.)

"Because we have many of these bricks, we're able to fire them individually or in small clusters" and at precisely spaced intervals to control the speed and strength of the current and resulting magnetic force. Materials scientists want to squeeze their test samples gradually – a process called shockless loading or isentropic compression – rather than with a sudden jolt that could instantly liquefy the substances. "Every material has an ideal pulse shape that it needs in order to maintain shockless loading, and you need to have the ability to tailor a pulse in order to avoid shocks." Firing capacitors in just the right number of bricks lets researchers mold the pulse for each material.

Thor's decoupled structure, with separately cabled capacitor bricks, also means "the pulse is simply a linear combination of all these small pulses." Designing an optimal pulse takes just seconds using simple optimization software.

Figuring out how to shape a pulse on Z, however, requires a huge computer code, Reisman says, comprised of around 50,000 circuit elements. Technicians spend days calculating the ideal pulse shape and sometimes must use precious test shots.

That's partly because Z wasn't designed for isentropic compression experiments. Around 2000, Reisman and colleagues from Sandia and Lawrence Livermore National Laboratory (where he worked at the time) recognized the machine could shocklessly compress materials.

"From that point onward, we started developing the Z machine as, in addition to the fusion mission, a materials science platform" via complex pulse-shaping steps.

Eight-foot-tall racks of capacitor bricks supply powerful pulses via heavy cables to Thor. Eventually the machine will have 144 bricks generating magnetic pulses capable of pressures as high as a million Earth atmospheres.

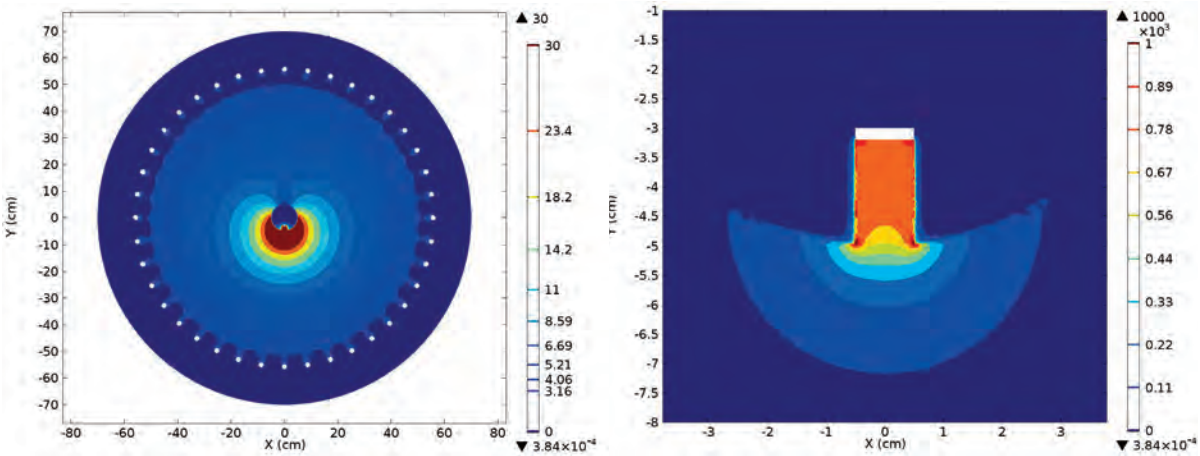
Reisman was still at Livermore when he first heard about the Thor concept. Bill Stygar, manager of Sandia's Advanced Accelerator Physics department, approached him about building the machine. "I started working on it and I realized, boy, this is a really good idea," Reisman say. "This is a very efficient machine and it can accomplish a lot of things in a small space." He moved to New Mexico and joined Stygar's department in 2014.

Thor incorporates advanced capacitors based on the linear transformer driver (LTD), a device Sandia researchers pioneered in collaboration with a team in Russia. The bricks charge and discharge faster than Z's Marx generators, making for a simpler, more compact design that also eliminates much of the complex insulating material and transformers Z uses.

The devices and their efficient switches will make Thor, once it grows to 144 capacitor bricks, 40 times more efficient than Z in producing magnetically generated pressure.

Pulsed-power researchers are watching Thor's technology and considering adopting it in an upgraded Z or entirely new machine. In a 2015 *Physical Review Special Topics – Accelerators and Beams* paper, Stygar, Reisman and several colleagues described plans for Neptune (so named because deionized water would be the chief transmission line insulator), a device that would yoke 600 capacitor bricks and produce pressures as high as 10 million atmospheres.

"The architecture can be expanded to different types of designs, but it's all built around the concept of adding currents and isolating each of the bricks from each other so you can



Simulations of the magnetic field strength contour plots for Thor's central power flow structure (left) and experiment strip line (right). Colors indicate field strength, ranging from weakest (blue) to the strongest (orange and red), about 800 Tesla. An 800-Tesla field corresponds to a magnetic pressure of 250 million pascals.

create these linear combinations of current," Reisman says.

Eventually, Stygar – whose group designs and builds LTDs – foresees pulsed-power machines that might produce magnetic pressure powerful enough to achieve ignition, in which a fusion target releases more energy than was put into it. That goal is years – and hundreds of experiments – away, however.

Meanwhile, Thor will provide a testbed for diagnostics and a place to refine experiments before they run on Z. For example, researchers could test a material's strength with a series of lower-pressure Thor shots before going to Z's high pressures.

But Thor will produce plenty of science on its own. For instance, researchers have built theoretical models of how the elements cerium and lithium behave at high pressures, including the points at which they change phases. "But really, there isn't a lot of experimental data in those regions," Reisman says. Tests next year will gather information scientists can check the models against.

"The goal is to compare between theory and experiment in the regions of very high pressure, to validate computer models" of material strength and phase transition (from solid to liquid to gas) and "to understand the complex material properties as things undergo high-pressure conditions."

Reisman wants to use Thor in combination with X-ray diffraction diagnostics that can capture a material's properties *in situ* – while actually under pressure. Most previous experiments have relied on velocimetry, which measures the response of a material surface to compression. Researchers then use math to reconstruct phase transitions, a process that can be imprecise. With diffraction, "we can actually look at the atomic structure dynamically and we can identify the different phases." He's "really excited about doing those types of experiments," starting with elements like zirconium, cerium and lithium.

Research groups from Sandia and from outside universities are showing similar enthusiasm, with several already seeking time on Thor.

Some experiments will have to wait until Thor reaches its full size, with 144 capacitor bricks. Reisman and his colleagues are scaling up the device, gradually adding bricks and making shots on simple copper targets to test electrical systems. The team had tested Thor-16 in summer 2016 and planned to add eight bricks this fall to bring the configuration to Thor-24. In the coming fiscal year, the researchers will begin live experiments as the machine grows to Thor-48 and Thor-72. Eventually it will again double in size to reach its full configuration. SS

Senior Science Editor Thomas R. O'Donnell has written extensively about research at the DOE national laboratories.

A LOS ALAMOS TEAM TEASES OUT DIFFERENCES BETWEEN HIDDEN EXPLOSIVES AND HARMLESS MATERIALS.

'TICKLING

THE DRAGON'

BY ANDY BOYLES

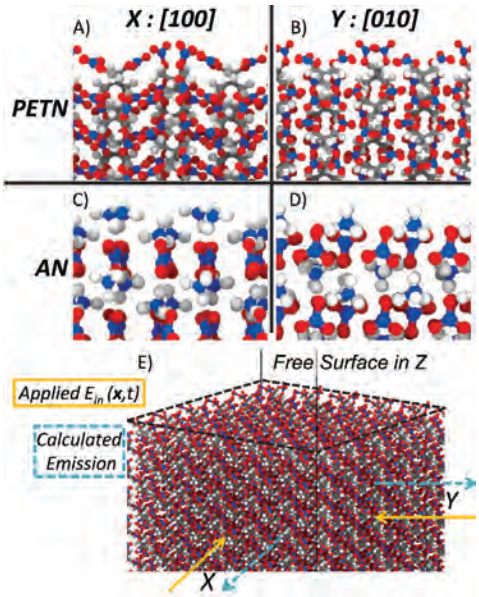
ABOUT SEVEN YEARS AGO, David Moore, a research scientist at Los Alamos National Laboratory (LANL), thought of a way to detect hidden explosives. As a physical chemist with LANL's Explosive Science and Shock Physics Division, Moore knew that as helpful as bomb-detection strategies are, none could see into packages and determine with reasonable certainty whether a concealed substance is explosive. Two technologies – X-ray and infrared – can identify devices that might be bombs, but they also flag innocuous objects that must be ruled out as threats. For people who screen suspect items, those nuisance alarms halt inspections and ratchet up psychological stress.

Moore was working on a project unrelated to explosives detection when he envisioned another application. The radiation he was studying was at a frequency in a narrow gap in the electromagnetic spectrum between the infrared and microwave ranges. He knew that energy in that frequency range, from gigahertz to terahertz, can penetrate fabric and paper packaging and stimulate materials inside. Unlike X-rays, it does so without harmful ionizing radiation.

Those properties resonated with Moore, who is also team lead for Shock and Detonation Physics in the 57-member Los Alamos Collaboration for Explosives Detection (LACED). "I had the idea that we could use the denial system on explosive materials, and we might see new signals," he says. "I suspected you would get heating under terahertz illumination, and that would give off vapors or reaction products."

Heating an explosive material slightly, well below its detonation point, is known in the field as "tickling the dragon." A future technology might use terahertz energy to penetrate packaging and heat suspected explosives, causing the bulk material to emit distinctive spectra. At higher intensities, the energy would stimulate chemical reactions in the material, which might yield additional spectra. Those spectra could be measured in light returning from inside the package to a detector, then serve as fingerprints in the field, not only to confirm that a suspicious object is an explosive device but also to identify which material it contains.

In short, an explosives detection technology based on gigahertz to terahertz light has the potential to reach new levels of both certainty and safety. For the past six years, Moore and his colleagues have been working toward such a technology.



Representative views for electromagnetic pulse propagation and emission in simulated molecular dynamics (MD) for two explosive materials, PETN and ammonium nitrate (AN). Panels (B) and (D) show the [010] direction – a vertical edge of the cube of modeled material – in either material. The crystals shown are unusual because the molecules are arranged differently from how they're configured along another, presumably equivalent, cube edge. (E): Perspective view of the simulation domain showing how the free surface is created in MD; the propagation direction of both applied and emitted fields is perpendicular to this free surface. This simulation setup enables realistic molecular dynamic absorption and emission polarizations. Atom colors correspond to carbon (gray), hydrogen (white), oxygen (red), and nitrogen (blue).

Two studies led by LANL theoretical physicist Diego Dalvit and published in the same 2016 issue of *Physical Review Applied* have advanced that work. In the first, a group of scientists created microscale images and simulations of the interiors of explosive materials as gigahertz waves irradiate them. In the second, a smaller group created simulations that identified potential signature spectra explosive materials might emit.

In principle, scientists and security personnel could use a database of signature spectra to screen suspect objects and packages, Dalvit says. "The problem is typically the spectra in the terahertz region are very congested, so it is very hard to really do a one-to-one match between the spectra you measure and those in the database." Further complicating matters, the spectrum of a given material can vary with temperature and in the presence of other materials. The new studies addressed these challenges.

The first study, Dalvit notes, may be the first full 3-D simulation of a heterogeneous explosive interacting with light. The results delivered tools needed to predict how explosives will respond to electromagnetic stimulation.

To begin, the group chose two common forms of the explosive and propellant HMX. Like forms of the material used in practical applications, the two samples were heterogeneous materials made by bonding HMX crystals, each in a different type of polymer. As a result, the samples offered all the complications and confounding factors of real-world explosives, including energy-concentrating air pockets scattered through the polymer.

Brian Patterson and Nikolaus Cordes in LANL's Materials Science and Technology Division created high-resolution, three-dimensional computed tomographic (CT) images of each sample. Dalvit's team then simulated the sample interacting with electromagnetic millimeter waves, causing local heating from 295 to 460 Kelvin (from room temperature to that of a baker's oven). For this stage of the research, the team chose not to heat the samples enough to cause phase transitions or trigger chemical reactions. Instead, the researchers wanted to pinpoint hot spots, places on the HMX crystals where electric fields concentrate, temperature rises and, they hope, useful emissions will originate.

The high-resolution CT images enabled an accurate simulation of hot-spot formation in the sample. "Doing CT scans at this high resolution to understand these details is not routine," says LANL experimentalist Amanda Duque, who participated in the study. "Intuitively, all of the important properties of explosives in general happen at the mesoscale – a regime of a couple hundred nanometers to microns – and that's been an area that unfortunately is not well understood. We know hot-spot formation happens at this scale. It's got to be somewhere at this regime that the explosive material is going to begin to differ in behavior from something inert, like sugar."

Before the team could hope to predict and interpret the results of future experiments, it would have to develop a computer simulation of the HMX samples, a problem solved by Wilton Kort-Kamp, a postdoctoral research associate in the LANL Theoretical Division with Dalvit as his mentor. "The main obstacle was to incorporate the CT data into electromagnetic numerical solvers, and Wilton really excelled in this," Dalvit says. "We were stuck on the simulations for more than a year. He came to Los Alamos, and in just two months, he moved forward."

Kort-Kamp began with finite element methods (FEM), breaking the modeled HMX volume into tetrahedra, hexahedra and other three-dimensional shapes that fit together into a mesh of small parts. "Finding a suitable mesh that provides an accurate solution in a reasonable time can be challenging, depending on the geometry we want to simulate," Kort-Kamp says. Prior explosive materials models were two-dimensional, simple structures. "In our case — a 3-D geometry with realistic structural data from CT images — meshing was one of the main difficulties, since the energetic material had HMX crystals and void volumes with many different sizes and shapes."

The team chose to model a 1.5 mm cube from each sample. But even with

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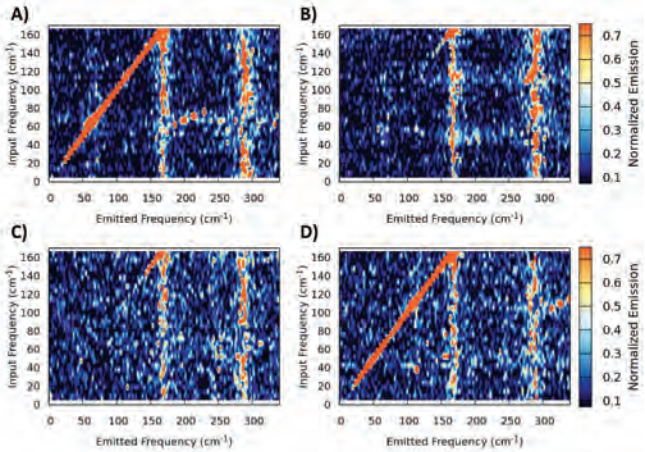


Simulated emission signals from one of the explosives, PETN, along the [100] (*x*) direction for electric field pulses applied in the (A) [100] and (B) [010] directions, with complementary emission signals with pulses along the [010] (*y*) direction for the (C) [100] and (D) [010] applied field directions. Where the emission signals are aligned with the pulse polarization, Rayleigh scattering dominates the observed emission. Perpendicular directions reveal emissions at unique frequencies different from the applied pulse, confirming the frequency conversion is from signals scattering from the material's interior.

this small volume, the algorithms couldn't perform all the necessary calculations on all the elements at once. Kort-Kamp's simulation-enabling solution: Split the CT image into several images and perform the mesh in each crystal and void individually and then merge all of them into a single file.

The simulation was a multiphysics combination of equations for electromagnetic fields and heat diffusion. Here, Kort-Kamp's experience in simulating novel solar-cell metamaterials was an advantage. Those simulations also demanded a marriage of electromagnetic and heat energy calculations, but in a two-dimensional framework. "To give you an idea of how complicated it was to perform the HMX simulations, I should mention that we dealt with over 2 million degrees of freedom," he says, referring to the multiple variables in multiple equations that had to be populated with data before the simulation could run. "Typical metamaterial simulations that I work with have less than 10,000 degrees of freedom."

Kort-Kamp started the simulation on his desktop computer, and two days later it was done, offering a glimpse of a hot explosive, represented in unprecedented detail. The research team has begun the next phase of its research: incorporating phase transitions and chemistry in the HMX crystals and vapors emanating from them. At that point, they will be simulating a true tickling of the dragon.

"Then if we crank up the field intensity, we could also have the possibility of finding nonlinear effects," Dalvit says. "Typically, in optics, any material will reflect light at the same frequency. But in a stronger field the material starts to also emit at different frequencies from the incoming one. So there are frequency conversions. And we have been making studies of these frequency conversion characteristics for explosives, as compared to inert" material.

These nonlinear phenomena, such as Raman effects – inelastic scattering that shifts a photon's frequency – may bear the fingerprints of explosive materials. The second study explored this possibility by simulating the effect of terahertz light on two widely used explosives, PETN and ammonium nitrate.

Sandia National Laboratories postdoctoral researcher Mitchell Wood performed the simulation portion of that study while a graduate student at Purdue University. "Mitch was the key person for the success of this part of our project, thanks to his extensive expertise in molecular dynamics simulations of energetic materials," Dalvit says.

To begin, the group had to choose which explosive materials to simulate. "The main challenge was with the appropriate use of the simulation tools," Wood says. "Molecular dynamics strictly describes materials using classical mechanics, which was in contrast to the quantum nature of absorption and emission of light. In all, it probably took us a few weeks to design the numerical experiment after we had agreed on which materials and which frequency range was most important."

Wood then created molecular models of bulk pieces representing the two explosive materials and bombarded them with simulated pulses of enough terahertz energy to evoke nonlinear effects. To the team's satisfaction, emission signals from PETN bore two bright lines – marks of Raman scattering and a potential signature for the explosive. Results from the parallel study of ammonium nitrate are "not as definitive," Moore says, but still point to areas in the terahertz spectrum to look for potential fingerprints.

Perhaps the most significant finding was that the two materials reflected spectra that are markedly different from each other, offering hope that many explosives also will have unique terahertz emissions. "This work is just a first step," Dalvit says. He wants to extend analyses to various other energetic materials.

Moore, Dalvit, and their colleagues are aware that adversaries have found creative ways to elude detection, and they may develop more in time. At any given moment, Moore says, a gap remains between what adversaries have at their disposal and what technologies can detect. "We're constantly thinking of ways that we can close that gap." SS

Dark Room, Bright Ideas

BY MAREENA ROBINSON SNOWDEN

Scientific presentations are tools – objects scientists use to build and advance their fields. At the rawest level, presentations must tell a story, complete with a foundational question, pivots that serve as plot twists and a resolution, all working to convey the research's significance.

In 2014, that was my intent: give a presentation revealing the source of my enthusiasm for disarmament. But then the power went out.

As a third-year Ph.D. student in the Nuclear Science and Engineering (NSE) Department at the Massachusetts Institute of Technology, I was chosen to give a featured presentation for our Graduate Research Expo. As I stood before the audience, with my title slide looming behind me, I was excited. It was time to perform, and I had an interesting story to tell.

My graduate work focuses on approaches to verify compliance with nuclear arms reduction agreements. This field has a significant history, and it was important that I provide this context for my research. Building on decades of arms control collaboration, the United States and Russia in the 1980s added on-site radiation detection as a verification option, ushering in a new era. Significantly, this shift toward on-site inspection using radiation detection allowed scientists and engineers, like me, to develop systems that provide more detailed evidence of compliance than previous methods.

Thirty-five years later, I stood before my department presenting what I saw as the next challenge: how best to verify the dismantling of nuclear warheads. This differs from previous arms control verification because it specifically examines the warheads themselves, not the missiles or bombers that deliver them. In the context of verification, scientists and engineers must give treaty negotiators a list of technologies to confirm warheads are dismantled so they can choose the most politically feasible option.

I confidently walked spectators in the packed auditorium through this, using my slides to orient them in a sea of dates, numbers and concepts. Then, as I finished explaining my research motivation, everything went black. Only a dim glow from my laptop screen was visible.

My thoughts dashed to my remaining slides. I had yet to provide what academics value most from a Ph.D. candidate: my novel approach to a solution. One of the most compelling portions of any scientific presentation is the data – the preliminary or well-established proof addressing the promise of one's idea. My mind raced as I considered how to best depict the graphs and images I intended to show – the visuals that captured the essence of my argument.

Once the seminar chair verified that we didn't need to evacuate, I decided to continue, with only my words and passion for my research as tools.

Consulting my laptop, I painted a picture of my idea to develop a passive approach to verify a warhead's presence. I explained the need to balance assuring compliance with avoiding intrusion into a country's national secrets. I walked listeners through the basic open-source knowledge of nuclear weapon designs. Then I explained my idea: leveraging the natural radiation interactions between the warhead's neutron-emitting plutonium and the high explosive surrounding it to tell us about the object to be dismantled. I paced in front of my audience, trying to read faces for looks of puzzlement or affirmation, gauging the effectiveness of my communication.

As hands shot up during the question and answer period, I realized that continuing was the right decision. Just as an audience shows its appreciation for a performance by applauding, scientists and engineers know that questions following a research talk are signs of interest and affirmation of a job well done.

As idealistic as it may sound, I believe all things work for the good. In science, as in life, an experience's impact is as much a function of how one responds to it as it is what actually happens. On that day, in that 30-minute free-style talk, a new aspect of my identity, as a strong scientific communicator, was cemented in my mind and the minds of my peers.

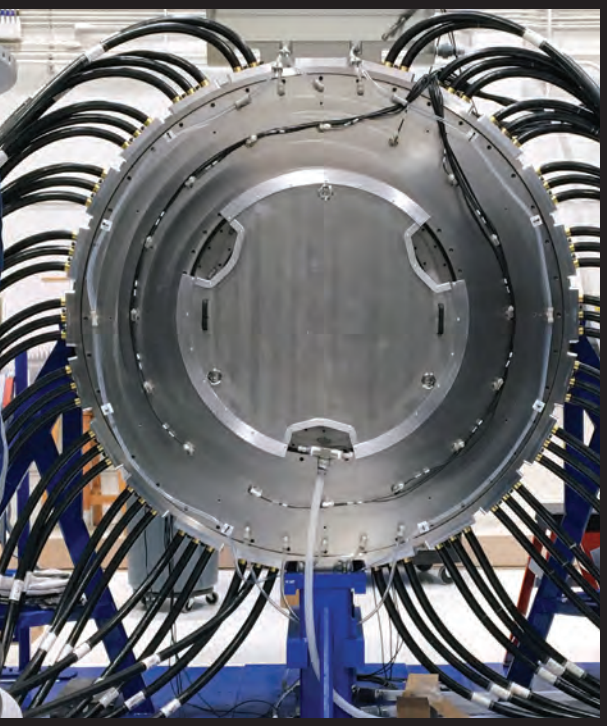
This gained significance when I was approached about becoming a coach in the new NSE Communication Lab, an initiative aimed at empowering scientists and engineers to become more confident and effective communicators. Nuclear engineering graduate students, trained in effective communication, work with members of the NSE community on how best to convey their scientific ideas. By focusing on tailored messaging and emphasizing the work's impact, I help my peers cultivate skills needed to engage their communities, thereby increasing the exchange of ideas in nuclear engineering.

I could not have imagined myself in this role. The abilities I exhibited during that Graduate Research Expo presented it to me. A non-ideal situation let me demonstrate key qualities of a successful researcher: confidence, resilience and grit. These aspects of my identity have allowed me to persist in the interdisciplinary field of nuclear arms control and turned what could have been my worst scientific presentation into one of my proudest moments.

This is the winning entry in the 2016 SSGF Essay Slam contest.

A complete listing of current fellows and alumni can be found on the DOE NNSA SSGF website:
https://www.krellinst.org/ssgf/

PULSE-POUNDER



Cables snake from the central power flow structure in Thor, Sandia National Laboratories' latest pulsed-power device. The black cables supply pulses from racks of capacitor bricks (not shown). Thor harnesses magnetic fields that apply extreme pressures to materials. Read more about Thor, starting on page 15.

KRELL institute

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