STEWARDSHIP SCIENCE

The SSGF Magazine 2010-2011

PRESSURE PLANET

Livermore team recreates deep-Earth conditions

Los Alamos: Time projection gets small

Sandia: Diamond droplets and beyond

Plus: Nuclear forensics, DARHT toss, a conversation with NNSA's chief and SSGF fellows in first-person

STEWARDSHIP SCIENCE 2011 GRADUATE FELLOWSHIP

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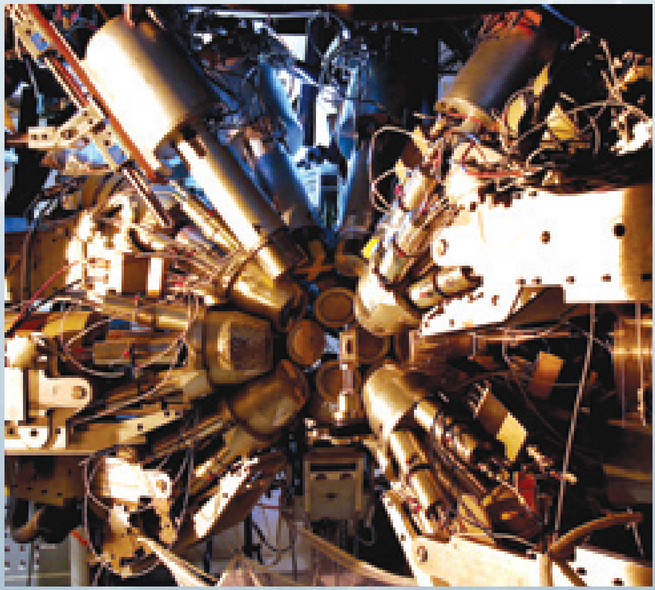
The Department of Energy National Nuclear Security Administration Stewardship Science Graduate Fellowship (DOE NNSA SSGF) program provides outstanding benefits and opportunities to students pursuing a Ph.D. in areas of interest to stewardship science – such as high energy density physics, nuclear science or properties of materials under extreme conditions and hydrodynamics. The program is open to senior undergraduates or students in their first or second year of graduate study. Fellows spend a 12-week research practicum at Lawrence Livermore National Laboratory, Los Alamos National Laboratory or Sandia National Laboratories.

Germanium Array for Neutron-Induced Excitations at Los Alamos Neutron Science Center - courtesy of Los Alamos National Laboratory



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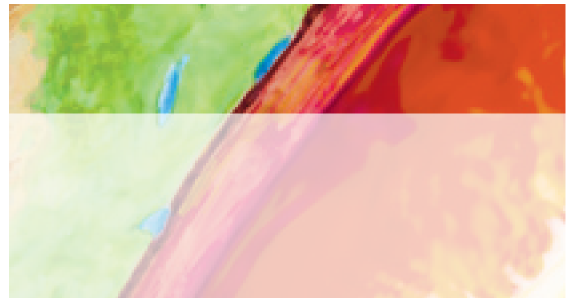
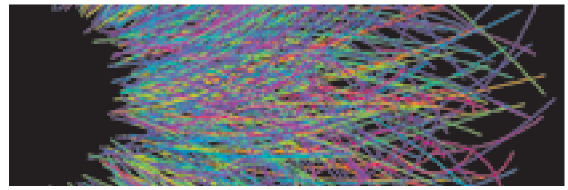
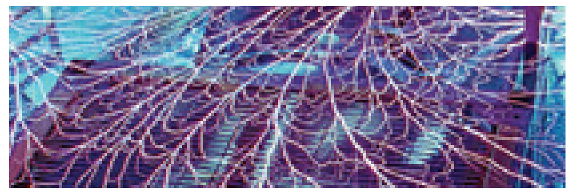
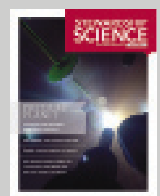






DEPARTMENTS

COVER



PICTURE BEFORE PULVERIZING

Materials that go through laser-driven ramp compression emerge "pulverized, scattered to the four winds," says Lawrence Livermore National Laboratory's Raymond Smith, whose work is featured starting on page 6 this issue in "Ramping Up the Pressure." "They're nice to look at and take a lot of effort to make, but you'd better take a lot of pictures before the shot because you never see them again." Even diamond, as shown in this time-integrated photograph (center, surrounded by diagnostic instruments) of an OMEGA laser experiment at the University of Rochester, eventually yields to tremendous pressures. The bright white light is ablated plasma and the radial yellow lines are tracks of late, hot target fragments. (Photo courtesy of Eugene Kowaluk, University of Rochester Laboratory for Laser Energetics.)

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Circular aluminum structures create magnetic fields in DARHT's accelerator, focusing and steering a stream of electrons.

In Latest Tests, DARHT Pulses Hit Bull's-Eyes

Movie theaters aren't the only places where three-dimensional technology is hot. At Los Alamos National Laboratory, scientists are obtaining 3-D information about nuclear weapons in the early stages of detonation.

That's the mission of the Dual Axis Radiographic Hydrodynamic Test (DARHT) facility. Its two powerful accelerators – placed perpendicular to each other – fire short, intense X-ray pulses at mocked-up nuclear weapons (with surrogates like depleted uranium replacing fissile material) as they undergo primary detonation in a confinement vessel, providing 3-D information about the device's performance.

DARHT data can contribute to verification and validation of computer simulations, helping assure that the nation's nuclear arsenal is viable without live tests. The first accelerator, Axis I, went into operation in 1999.

The second beam line, upgraded to capture a series of images, gathered its first radiographic data in November 2009, when LANL researchers completed their first dual-axis shot. As explosives launched a metal flyer plate, the Axis I accelerator fired a single 60-nanosecond X-ray pulse. The Axis II accelerator fired four pulses of 20, 45, 65 and 65 ns.

The Axis II series captured the initial shock wave traveling through the flyer plate. Its third shot coincided with the Axis I shot so that scientists could compare them to generate a 3-D image of the shocked material.

In December researchers performed the first double-viewpoint hydrodynamic test of a nuclear weapon component mockup. They plan four shots in support of the facility's national security mission this year, then will turn to R&D efforts associated with low-current radiography.

~ Thomas R. O'Donnell

TRACE ELEMENTS

BIG SHOCK

The new full function test (FFT) device at Lawrence Livermore National Laboratory has set a new magnetic energy and power record for U.S. experiments, researchers report. The device, based on high-explosive pulsed power technology, delivered 66 megajoules of energy with a peak power of 10 terawatts. The FFT is designed to investigate the properties of materials under extreme pressures. Published in *Review of Scientific Instruments* 81, 036109 (2010); doi:10.1063/1.3359998.

PLANAR PINCH

Brent Jones and Sandia National Laboratories colleagues in New Mexico have tested an indirect-drive Z-pinch implosion configuration using planar compact wire arrays, which allow less primary hohlraum surface area compared to cylindrical loads. Implosions at up to 15 terawatts of X-ray power on the lab's Saturn accelerator produced radiated yields exceeding the calculated kinetic energy, suggesting other heating paths. Published in *Physical Review Letters* 2010 Mar 26;104(12):125001. Epub 2010 Mar 22.

APPLYING STUD TO PLASMA

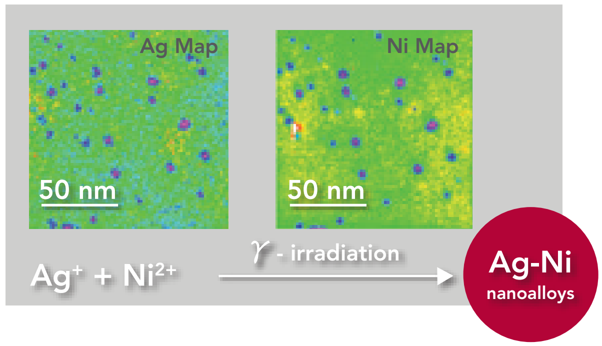
STUD (spike trains of uneven duration or delay) pulses on Los Alamos National Laboratory's Trident laser controlled plasma instabilities, says Bedros Afeyan of Polymath Research Inc., member of an international research team. That could be an important step toward higher-yielding fusion energy reactions. Presented at an Applied Plasma Physics and Fusion Energy Seminar, University of California, San Diego. Research sponsors: LANL, NNSA Office of Fusion Energy Sciences Joint HEDLP program, Feb. 3, 2010.

NOT-SO-FAST IGNITION

The initial burst a laser can apply for fast-ignition (FI) inertial confinement fusion is limited, LLNL's Andrew MacPhee and an international team of researchers say. The lab's Titan laser fired a pre-pulse and main pulse into a hollow copper cone. After a 7.5-milli-joule pre-pulse, the main pulse generated a filament of energetic electrons that bored through the pre-plasma to the cone's tip. But after a 100-mJ pre-pulse, most of the energetic electrons were diverted, showing that limiting the pre-pulse is critical for full-scale FI, the team says. Published in *Physical Review Letters* 2010 Feb 5;104(5):055002. Epub 2010 Feb 4.

Sandia Proves Its Metal

Metal alloys have fueled human technology for millennia. The eureka-moment that accompanied the smelting of bronze from copper and tin rated its own age-suffix in human civilization. So it's no understatement to say a new metal alloy can revolutionize technology, and scientists at Sandia National Laboratories have just created one.



Colorized energy filtered transmission electron microscopy (EFTEM) of Ag and Ni (each labeled as "map") reveals that the nanoparticles are made up of each element equally. EFTEM provides high spacial resolution of a particle's chemical uniformity and specific distribution of chemical reactions. Color variations in particles are a byproduct of colorization.

By exposing an aqueous solution of silver and nickel salts to a large dose of gamma irradiation, they made the first-ever stable nanoparticle alloy of the two metals, an achievement that could lead to a new class of high-strength, low-corrosion metals. "With metals like silver-nickel, if you look at the thermodynamic phase diagrams you pretty much cannot make an alloy," says Tina Nenoff, lead chemist on the project. "They are considered immiscible under normal, high-temperature heating conditions. But because we are using radiolysis at room temperature, we can (now) make these alloy phases."

The key to the project is the uniform gamma irradiation dose provided by Sandia's Cobalt-60 Gamma Irradiation Facility, which delivers up to 3 x 10^6 rads an hour. The radiation split water into hydrogen and hydroxide radicals and provided a large concentration of solvated electrons that, after 18 minutes in the irradiation chamber, reduced metal ions Ag^{+} and Ni^{2+} to spherical 5-nanometer particles. The particles were a perfect mixture of 50 percent silver, 50 percent nickel, according to the group's transmission electron microscopy evidence.

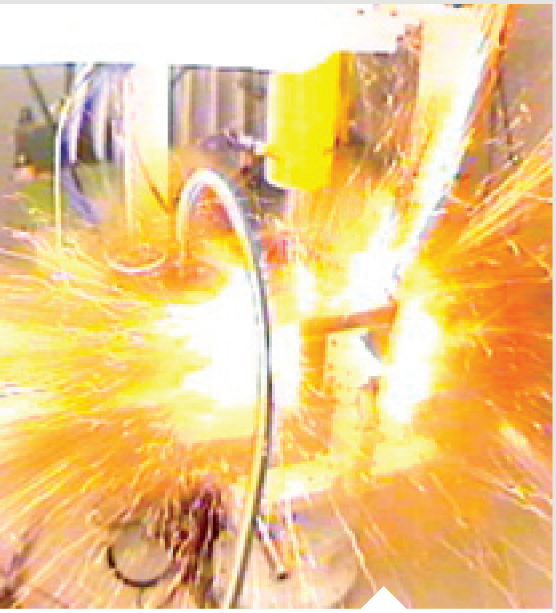
The researchers published their results in the *Journal of Physical Chemistry* in January 2009. The group is seeking a patent for its technique.

Previous attempts to create an alloy between the two metals left clusters of Tootsie Pop structures with a silver shell surrounding a nickel center – a thermodynamically stable structure but not a true alloy, Nenoff says. "The thought was if you can make these durable materials at room temperature with few defects, the potential for sintering them to bulk (for aerospace applications) or making micro-machines out of them was worthwhile."

The research team still is assessing properties of the new alloy and is working to scale up the process from a 100-milliliter flask so it can make enough bulk material to measure tensile strength, malleability and other properties.

Next, Nenoff and colleagues will turn their attention to alloys for room-temperature nuclear fuel surrogates, with the hope of producing research quantities of depleted uranium-based alloy nanoparticles.

~ Karyn Hede



BIG PICTURE

A BLAST THAT BARELY LASTS

Some of the world's strongest pulsed magnetic fields are helping scientists at the National High Magnetic Field Laboratory (NHMFL) Pulsed Field Facility at Los Alamos National Laboratory decipher the behavior of electrons in superconductors and other exotic materials. Seen here, in what is called the single-turn electromagnet design, a single copper loop is wrapped around a tube containing measurement probes and a sample of the material being tested. A 3-million-ampere current pulse creates a magnetic field as high as 240 teslas that lasts a mere few millionths of a second before the loop explodes from heat and the field's power. Researchers made the system, designed so the tube and sample survive intact, to study plutonium in a high magnetic field. The NHMFL user facility is a collaboration between LANL, Florida State University and the University of Florida, with support from the National Science Foundation and the Florida state government.

Nuclear Places of Origin

A heading warns, "the threat is real" – in red italics – on a slide that nuclear forensics expert Ian Hutcheon uses to grab audiences, as he did at the 2010 American Association for the Advancement of Science annual meeting.

A timeline begins in the early 1990s and tracks an alarming series of nuclear-material interdiction episodes, in which authorities in Europe stopped smugglers of highly-enriched uranium (HEU) and plutonium. In separate 1994 episodes in Germany, agents seized more than 400 grams of weapons-grade plutonium.

The next decade shows relative calm. Does that mean governments locked down their nuclear materials and have kept them off the black market?

Hutcheon, deputy director of the Glenn T. Seaborg Institute at Lawrence Livermore National Laboratory, wouldn't bet on it.

Since 9/11/2001, when use of radiation portal monitors surged, "there has been roughly an interdiction every two or three years. What we don't know is how much material is out there. It's similar to drug trafficking. We only know how much we interdict."

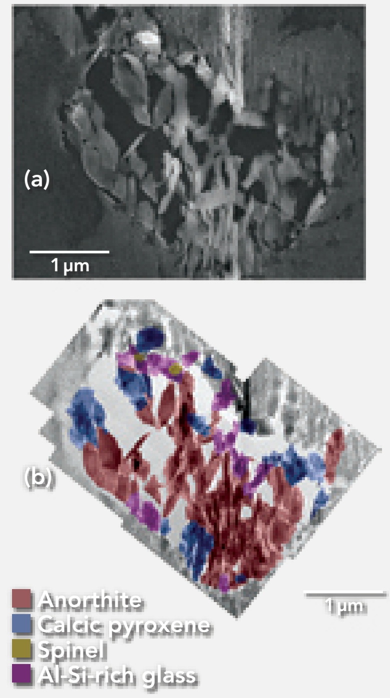
Hutcheon presides over an eclectic group of physicists, chemists, nuclear engineers and others, 30 in all, who conduct experiments on the world's most sensitive mass spectrometers to divine ridiculously small but telling differences in the chemical and isotopic compositions of uranium, plutonium and exotic materials from comets and asteroids. They're averaging a *Science* paper a year over the past decade.

Tiny differences – radioisotope and stable isotope abundance ratios, trace element impurities, molecular makeup, material age and grain size and shape – help researchers pinpoint a nuclear sample's place of origin.

The data, Hutcheon says, provide a "record (of) different signatures – plutonium and uranium isotopes and also oxygen, strontium and lead. If we combine these three factors with trace elements, we're likely to get a unique ID."

The relative abundance of trace elements such as tungsten can vary widely from uranium sample to uranium sample, depending on where it came from and how it was processed. "Uranium ore from Australia and ore concentrate (so-called yellowcake) from Kazakhstan will have very different signatures."

Those signatures change as the material changes, from ore to yellowcake and purified uranium for energy to plutonium for nuclear explosives. Hutcheon's team can measure it all and compare what they find to a database that maps the location.



Analytical techniques that may be put to use in nuclear forensics are often validated in peer-reviewed journals. Shown here: a secondary electron image (a) of a roughly 100-nanometer-thick section of a comet particle described in a Feb. 2010 *Science* paper by Ian Hutcheon's group at Livermore and colleagues from the University of Washington, UCLA and the Smithsonian Institution. The image shows mineral shards surrounded by compressed aerogel from the NASA Stardust Mission. The lower panel shows a corresponding false-color mineral map on a montage of bright-field transmission electron microscopy images.

Hutcheon notes that these and other observations that help countries comply with the Nuclear Nonproliferation Treaty and keep the black market in check are made possible by huge improvements in mass spectrometry, from ITMS (ion trap) in the early 1970s to RIMS (retarding ion) in the 1990s. With each advance, instruments could measure smaller and smaller concentrations of nuclear materials.

"I've been a geochemist for roughly 30 years," Hutcheon says, "and if you look at improvement in detection limits, it's spectacular. When I was a graduate student it was a nanogram. Now it's femto, improved by a factor of 1,000."

~ Bill Cannon

CONVERSATION

Thomas P. D'Agostino

Under Secretary for Nuclear Security and NNSA Administrator

The Obama Administration has laid out an ambitious goal of securing vulnerable nuclear material around the world within four years. How does investing in the science of nuclear security support that mission?

There is a direct link between the investments we make in our stockpile stewardship program and our effort to prevent the spread of nuclear weapons. Because we have worked for the last 65 years to maintain the safety, security and effectiveness of the nuclear stockpile, we have available the people, the facilities and the technical expertise required to tackle the challenges posed by nuclear proliferation. In fact, many of the men and women we send around the world to install radiation detection equipment, increase security at nuclear sites, and remove highly enriched uranium (HEU) work at the national laboratories and production sites that support our stockpile stewardship program.

What role does stewardship science play in addressing the issues discussed at the president's Nuclear Security Summit?

The president has said that the possibility of a terrorist getting hold of a nuclear weapon is the gravest threat facing the U.S. and the world today. The best way to prevent that nightmare scenario is to secure vulnerable nuclear material and prevent nuclear smuggling. Our laboratories have developed and deployed cutting-edge surveillance and detection technologies to key nuclear facilities, border crossings, airports and seaports around the world to detect the proliferation of nuclear and radiological material. They have also developed the technology necessary to convert research reactors from HEU to LEU (low-enriched uranium), thereby removing the most vulnerable and sought-after material for a terrorist group seeking nuclear weapons.

You told Congress that ensuring the safety, security and effectiveness of the nuclear weapons stockpile requires increased investments to sustain a depleting technical human capital base across the agency's enterprise. What does this investment in scientists and engineers who perform the nuclear-security mission involve?

As I always say, at NNSA our people are our greatest assets. If we are going to succeed in our efforts, we need to restore the invaluable cadre of experts and nuclear security professionals across the enterprise. Much of NNSA's workforce is nearing retirement age. We need to be able to recruit and retain the next generation of nuclear security professionals. To attract the best and the brightest, NNSA and the nation as a whole must demonstrate that we value the work that they do. This means giving them the basic tools and facilities they need to successfully accomplish their mission. It also means giving the workforce a challenging mission. Through the Stewardship Science Graduate Fellowship and Stewardship Science Academic Alliance programs, NNSA sends a clear message that we support basic and applied science. Our Future Leaders program brings college and postgraduate students into the enterprise for two years of intensive, hands-on learning, and our Nonproliferation Graduate Fellowship program recruits the sharpest young minds into one of our most visible areas.

Stewardship science has focused on high energy density physics, nuclear science and materials under extreme conditions. What direction is stewardship science research headed in the next few years? What areas will be the focus, what areas must be added or emphasized more?

With the completion of the National Ignition Facility (NIF), high energy density physics is entering a vital and exciting new phase of investigation. New regimes of extreme conditions – in temperature, density and pressure for example – will now be accessible. This will enable experiments that are extremely valuable to stockpile stewardship and will be of considerable interest in basic science such as astrophysical investigations. The NIF (Lawrence Livermore National Laboratory), OMEGA (University of Rochester) and Z machine (Sandia National Laboratories/New Mexico) all provide exciting venues for research on materials that will continue for a considerable time.

Hydrodynamics and computational sciences will also be critical for the foreseeable future, as will material sciences. We need to continue to develop our skills in those areas, which is why it is so important to attract and retain the next generation of scientists and engineers.

EXPERIMENTS TO RECREATE EXTREME CONDITIONS DEEP INSIDE PLANETS ARE KEY TO UNDERSTANDING THEIR BEHAVIOR AS A WHOLE AND COULD EVEN HELP PREDICT WHAT HAPPENS TO MATERIALS IN A NUCLEAR DETONATION.

RAMPING UP THE PRESSURE

BY THOMAS R. O'DONNELL

NO ONE'S QUITE SURE what's happening deep inside our planet, where extreme pressures and temperatures change minerals' structures in unexpected ways.

And if it's tough understanding what goes on deep in the Earth, imagine how difficult it is to figure out conditions in more massive planets inside – and outside – our solar system. It's estimated core pressures in these bodies are more than four times those at Earth's core.

"We want to understand how the high pressures and temperatures in these planets affect the crystal structure – the arrangement of atoms and whether they are solid or liquid," says Thomas Duffy, a professor in the Princeton University Department of Geosciences. Researchers also want to know how those conditions affect "a host of physical properties: how dense these materials are, whether they are insulators or metals" and others.

Deciphering interior structure is key to understanding a body's behavior as a whole, Duffy says. "Yet they are very hard to probe because by definition they are under the surface," and the consequences on materials are difficult to predict theoretically.

It's possible to create such extreme pressures in the laboratory, but the available techniques have limitations. Now Lawrence Livermore National Laboratory researchers have added a new method to the experimental arsenal. Laser-driven ramp compression – also called ramp-wave compression, quasi-isentropic compression and other names – is opening new horizons in materials research.

Laser-driven ramp compression "is giving us a new tool to expand to pressures far beyond the range of what we could before," says Duffy, who is collaborating with the LLNL group. "It's the only game in town for sufficiently high pressures." And soon the researchers will tap pressures far beyond anything possible before, thanks to the recent completion of the world's most powerful laser facility at LLNL.

Although this isn't weapons work, such experiments may have stewardship science applications. Techniques that the LLNL group use could help scientists better understand and predict what happens to materials under the extreme pressures and temperatures of a nuclear detonation.

Until recently, scientists who wanted to understand what happens to materials under great pressures generally had to choose between two experiments: Diamond anvil cell (DAC) or shock compression.

A DAC squeezes the target material between the flattened tips of two diamonds. It compresses materials for a long time, but its peak pressure is limited to around 300 gigapascals (GPa). That's 300 billion pascals, compared to normal Earth atmospheric pressure of about 100,000 pascals. It's close to the 350 GPa found at Earth's core,

Senior Science Editor Thomas R. O'Donnell covers science at the DOE national laboratories for the Krell Institute. He is a former science reporter for the Des Moines Register.

Ramp compression recreates, in the lab, deep-planet conditions.

UPPER MANTLE
24 GPa | 660 km

LOWER MANTLE
24 GPa - 125 GPa | 660-2,700 km

POST-PEROVSKITE REGION
125-135 GPa | 2,700-2,890 km

OUTER CORE
135-330 GPa | 2,890-5,150 km

INNER CORE
330-350 GPa | 5,150-6,370 km

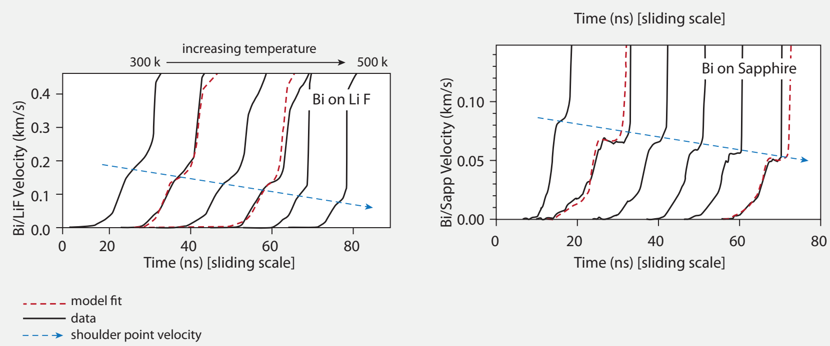
but nowhere near the pressures found inside gas giant planets like Jupiter or huge "super-Earth" planets orbiting other stars. A DAC also doesn't provide time-dependent data related to the dynamics of material compression, such as changes in strength.

A HOT SHOCK

Shock compression, produced with gas guns, powerful lasers and other devices, generates pressures in the trillions of pascals, but the increase is instantaneous – like a punch in the face.

"When you shock compress a material there's a lot of heating involved. You get a high state of pressure but also high temperature," says Raymond Smith, a physicist in LLNL's Physical and Life Sciences Directorate who leads the lab's ramp-compression research. That high temperature often melts the target material, stymieing efforts to understand solid-state materials under great pressures.

These plots compare the velocities of compression waves in bismuth heated to various temperatures and mounted on either a lithium-fluorine or sapphire window. Both show a shoulder point at which the wave slows, indicating a structural phase transformation. The tests show the shoulder point falls as initial temperature increases.



Ramp compression gets around the melting problem by ramping up pressure over time, like a steadily increasing shove. "In our experiments we compress over maybe 10 nanoseconds," Smith says. "When you compress with a ramp, you keep the materials a lot cooler," so they stay solid. Ramp compression generates conditions more like those in planetary interiors, where materials typically lie along an isentrope – a line of constant entropy.

The time-dependent approach also lets scientists detect and track phase changes – the points during compression when atoms reorient into a different crystal lattice or state of matter. Ramp compression creates conditions that fall between the dynamic high pressures of shocks and the static pressure of a DAC, Duffy says. "We're always trying to look at shock data and static data and bridge that gap between them." Ramp compression "will make that a little bit easier." Early ramp compression experiments used the magnetic driver of Sandia

The target transforms from an ambient crystal atomic arrangement to a new phase, with atoms flowing and reorienting in a new crystal structure.

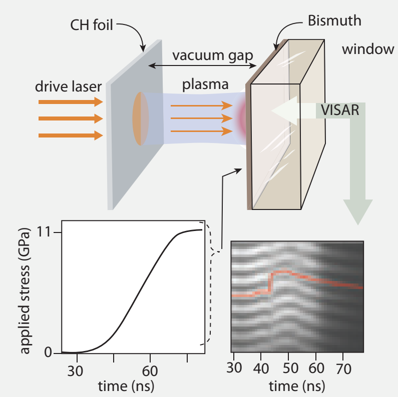
National Laboratories' Z machine. Really fast ramp compression, however, requires powerful lasers, like Livermore's Janus, a system with two beams rated at 1 kilojoule each.

In an early experiment, Smith and his LLNL colleagues subjected bismuth to Janus's power. The group chose bismuth because previous work found its phase changes at relatively lower pressures. That meant the group could test its technique on a comparatively small laser facility before trying more powerful devices and more challenging materials.

A single Janus beam delivered 150 to 200 joules to a polyimide foil, rarefying it and driving plasma across a vacuum gap and into the sample. The bismuth was mounted on a window (made of either lithium-fluorine or sapphire), allowing a line-imaging velocity interferometer system for any reflector (VISAR) to capture the time history of the compression wave. VISAR bounces a beam off the back of the sample, Smith says, producing a Doppler shift that gives an accurate measurement of movement as a function of time. Thermal emission emanating from the target also is collected to measure temperature.

All of this took place on a relatively tiny scale, both in space and time. The polyimide foils were just 125 microns thick, while the bismuth samples had a grain size of about 5 microns in the direction of the load. The laser pulses lasted just 4 nanoseconds, but generated ramp waves with rise times ranging from 15 to 35 nanoseconds and peak pressures of about 11 GPa.

The researchers also preheated the bismuth sample to six different temperatures, ranging from 296 to 495 K, letting them explore different regions of phase space.



In the Livermore group's ramp compression experiment, the Janus laser hit a polyimide foil, driving plasma across a vacuum gap and into the bismuth sample. A ramped pressure wave applied increasing stress to the sample over many nanoseconds. A line-imaging velocity interferometer system for any reflector (VISAR) calculated the velocity of the wave as it moved through the material. The VISAR data at lower left shows a shoulder where the compression wave stalled briefly, indicating a phase transformation.

SHOULDERING A RESULT

At each temperature, graphs tracking velocity over time showed a "shoulder" – a point at which the compression wave stalled slightly before picking up speed again. That reflects the bismuth target transforming from an ambient crystal atomic arrangement, with atoms squeezing together, to a new phase, with atoms flowing and reorienting in a new crystal structure.

"When you go from one phase to another phase there's a drop in the sound speed associated with this mixed phase," Smith says. "Our experimental design compresses the bismuth sample with a linear ramp in time, but the VISAR detects a very structured transmitted pressure wave profile with shoulders." That phase-change signature isn't visible under conventional laser shocks, the researchers say. "The main thing we found is that there's a lot of kinetics in the transformation," with phase change occurring over a range of times and pressures, Smith says. Slow ramp waves led to phase transitions similar to those produced over the longer time-scale compression of a DAC. Fast ramp compression led to fast transformations. Data from the experiments and from past research suggest a logarithmic dependence of transformation time on the material's strain, or deformation, rate.

"This kind of strain rate kinetics is common across a host of other materials – in iron, water, titanium and ytterbium. If you compress faster than the material has time to respond you are going to overshoot equilibrium phase map boundaries" to the point they may no longer apply, Smith says.

Pressures generated in the bismuth experiment still are unlike the 360 GPa at Earth's center, the more than 1 trillion pascals (1,000 GPa) likely to exist at the core of gas giants like Jupiter, or the 3 trillion to 5 trillion pascals (3,000 to 5,000 GPa) predicted deep inside huge "super-Earths" detected orbiting other stars in our galaxy. They're also nothing like the 1,400 GPa peak pressure the group achieved in later experiments using the University of Rochester's OMEGA laser. The facility can focus as many as 60 beams with a combined power of up to 30 kilojoules onto targets less than a millimeter in diameter.

The researchers tweaked their experiment design to use that power effectively in the ramp compression of a pure diamond target. The direct laser ablation ramp compression approach replaces the polyimide foil with a 2 mm-diameter gold hohlraum. Multiple laser beams fire into the hohlraum, generating a spatially uniform distribution of thermal X-rays that increase steadily over several nanoseconds to a peak radiation temperature. The X-rays directly ablate the diamond target's front surface to launch the ramp compression wave.

The design is a key advancement in ramp compression experiments, Smith says. By tailoring the power, "we put a ramp in the laser pulse, and it puts a ramp in the compression wave." The 1,400 GPa it created in the diamond is "the highest pressure solid ever created in the lab," but "if it were a shock compression, it would have melted the material."

COMPUTATIONAL DEMANDS

High-performance computers could calculate and predict the phase changes ramp compression is designed to create, but experiments still are necessary to ensure the models are accurate.

"Computational calculations have grown in the scale and scope of the problems they can address, and the accuracy (of the models) has improved," Princeton University's Thomas Duffy says. "Nevertheless, they still are estimations," and experiments must provide data for validation and verification.

Lawrence Livermore National Laboratory researchers, for instance, used a one-dimensional hydrocode with a rudimentary kinetics package to model the velocity of a ramp compression wave moving through a bismuth sample, simulating an experiment on the Janus laser. The model agreed well with data from the VISAR diagnostic, generating a "shoulder" (see "Shouldering a result," main story) in the velocity curve that indicates a phase transformation.

The group now is trying molecular dynamics simulations of the experiments, LLNL's Raymond Smith says. "That will give us an idea of what's going on – how fast or the mechanism of this dependence we saw in experiments." But the models are so computationally demanding they can simulate a sample of only about a micron in size for only about a nanosecond.

Even at that tiny temporal and spatial scale, computational models still are important, Duffy says. "As we go into new regimes that we couldn't explore with experimentation before, we also will work with colleagues who carry out computational modeling. This will work hand in hand – experiments will help us figure out the strengths and weaknesses of the calculations" while modeling suggests new areas for experiments to explore.

The lasers fired for about 3.5 nanoseconds, delivering as much as 5,700 joules of energy.

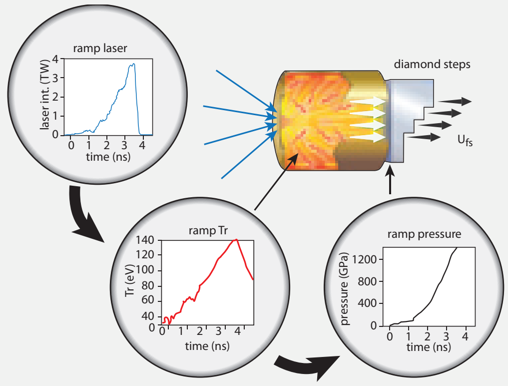
OUTRUNNING A WAVE

It's not that the direct-laser technique doesn't produce heat capable of melting diamond. It's that the compression wave outruns the thermal wave, Smith says, and "we're making our measurements before the heat wave hits."

In one experiment the target was a 2 mm-square piece of diamond, flat on the laser-facing side but with four steps of about 15, 30, 45 and 60 microns each on the opposite side. The lasers fired for about 3.5 nanoseconds, delivering as much as 5,700 joules of energy.

VISAR recorded the free-surface velocity history for each 15-micron step as it accelerated into space. "Each step experiences the same input from the hohlraum. We measure the time history from one step to the next step to calculate how fast the compression wave travels over an increment. That gives us a measure of the compressibility of the material," Smith says. Instruments calculated a single step in the diamond target at peak pressure, but because researchers need to compare data from at least two steps to measure pressure, or stress, versus density, they calculated diamond's properties only up to 800 GPa.

In direct laser ramp compression, lasers (blue arrows) are fired into a gold hohlraum (center), generating thermal X-rays (red squiggles) that directly ablate a target. Tuning the laser to ramp up in power over time creates a corresponding ramp in compression.



The results suggest diamond lives up to its legendary billing as the world's hardest substance. Data detected no signs of a phase transition, indicating that diamond's structure is stable up to at least 800 GPa. The material also seemed to retain its strength up to that pressure level, the researchers reported. Although the experiment provides valuable data on materials under extreme pressure and on an important material in science and technology, the experiment design itself may be most important, Smith says.

"We have this technique now that allows us to keep the materials solid under these high-pressure conditions. This is really the basis for all our high-pressure work we're going to be doing."

The LLNL researchers are conducting more OMEGA experiments on other materials. Besides Princeton, they're also collaborating with researchers from Washington State University and the Carnegie Institution of Washington. Another participant is University of California, Berkeley, graduate student Dylan Spaulding, a Department of Energy National Nuclear Security Administration Stewardship Science Graduate Fellowship recipient.

Besides higher pressures, OMEGA's multiple beam lines also give the group access to tools, like X-ray diffraction, that reveal more about what's happening in the sample.

"With more beams you have more flexibility in the diagnostics you can field," Smith says. "Peak pressure is a main component (of using OMEGA), but also being able to look more closely at what's happening in the target at those pressures." VISAR, for example, can detect when a phase change happens. X-ray diffraction can tell just how the atomic structure changed.

The group already has ramp-compressed iron up to 300 GPa and quartz up to 250 GPa. "In both cases we found phase transformations along the ramp that you wouldn't see with a laser shock," Smith says.

Higher-pressure shots are coming on OMEGA, but the major goal is to fine-tune the experiment for the really big time: LLNL's National Ignition Facility (NIF).

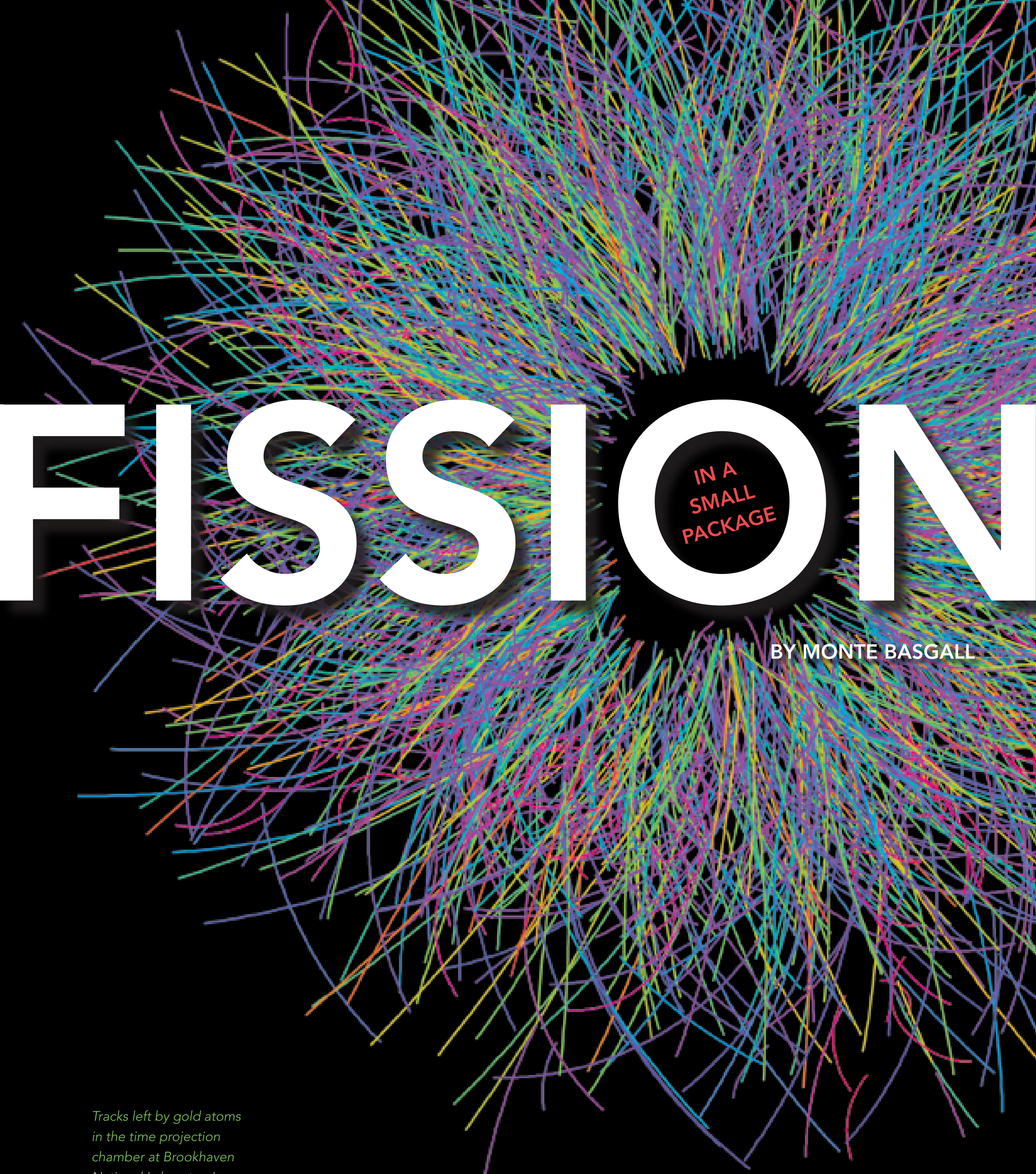
Housing the world's most powerful laser system, NIF can focus as many as 192 beams and 2 megajoules on targets measured in millimeters and microns.

"OMEGA has been very important," Duffy says. "You can do really good experiments and reach pressures and compression states that are beyond what we can achieve with diamond anvil cell and other static techniques." At the same time, "we're able to do a lot of testing of shots and configurations and sort of work out what the problems are as we prepare for extending to NIF."

Starting this fall, the ramp compression group will use 128 NIF beams to subject materials like tantalum, iron and diamond to thousands of gigapascals. The researchers hope the experiments give them an idea of not just when phase changes but also where nucleation, the initial step in a phase shift, begins.

Smith acknowledges the group's experiments can't completely recreate conditions beneath a planet's surface. They apply compression along only one axis, for instance, and for only a few nanoseconds. Nonetheless, the research is providing important data about the material physics accurate enough for quantitative comparisons with that gathered in DAC, shock compression and Z-pinch compression.

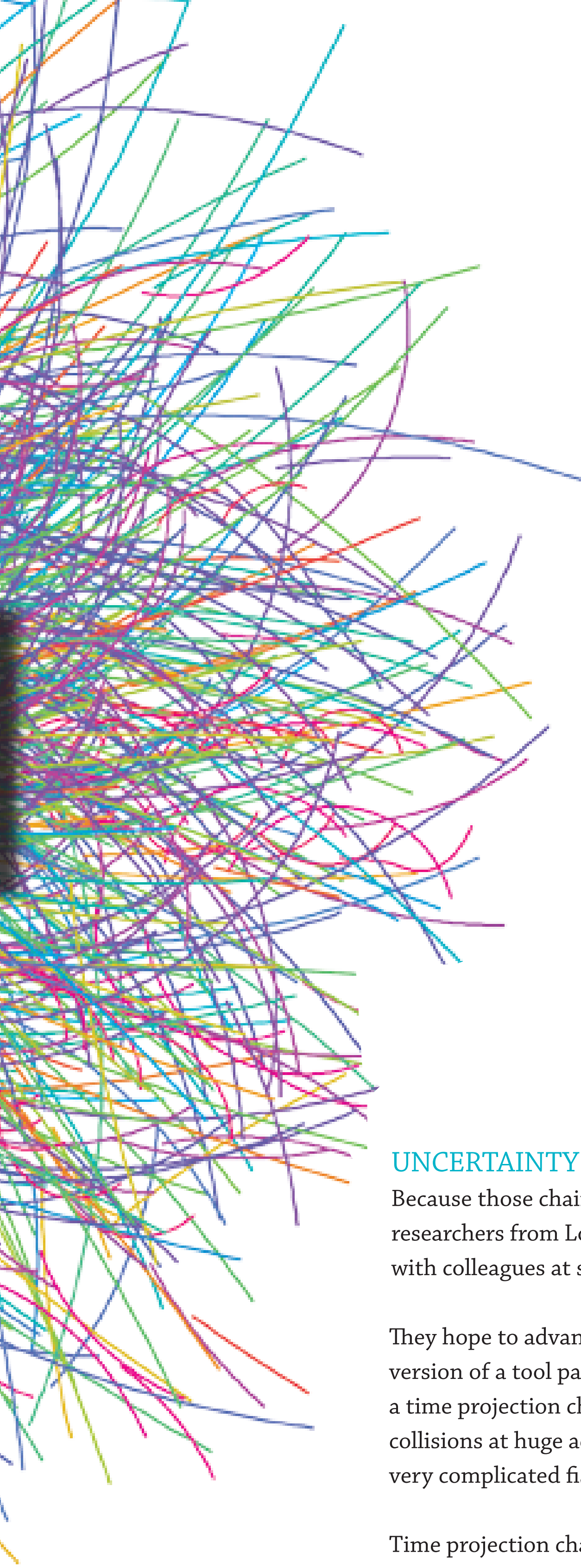
"They're complementary," Smith says. "You're trying to understand the time dependence of the material. The best way is to gather data over a long range of time scales."



FISSION IN A SMALL PACKAGE

BY MONTE BASGALL

Tracks left by gold atoms in the time projection chamber at Brookhaven National Laboratory's Relativistic Heavy Ion Collider. (Image courtesy of the STAR collaboration.)



RESEARCHERS AT LOS ALAMOS AND ELSEWHERE HOPE THAT A SCALED-DOWN DEVICE FROM PARTICLE PHYSICS WILL PUT FISSION – AND ASSOCIATED WEAPONS, ENERGY AND WASTE – IN SHARPER FOCUS.

UNCERTAINTY LINGERS IN THE fleeting moments after nuclei split in reactors and weapons. Because those chains of events affect everything from energy production to waste generation, researchers from Los Alamos National Laboratory and two other national laboratories are working with colleagues at six universities to better their understanding of fission.

They hope to advance their observational and forecasting precision with help from a miniaturized version of a tool particle physicists use to recreate conditions of the early universe. The tool, called a time projection chamber, or TPC, is used to identify charged particles created in high-energy collisions at huge accelerator facilities. The downsized TPC will instead reveal details about the very complicated fission process.

Time projection chambers at places like Brookhaven National Laboratory's Relativistic Heavy Ion Collider, measuring about 14 feet long and wide, would fill the lane of a basketball court. The scaled-down TPC, no bigger than a coffee can and only 15 centimeters across inside, is a hydrogen-filled aluminum cylinder charged with high voltage and crammed with enough high-speed, high-capacity electronics to process half a trillion bytes of data a second.

Monte Basgall is a freelance writer and former reporter for the Richmond Times-Dispatch, Miami Herald *and* Raleigh News & Observer. *For 17 years he covered the basic sciences, engineering and environmental sciences at Duke University, leaving in early 2010.*

"There are all kinds of technical challenges," says Fredrik Tovesson, a nuclear scientist who heads TPC efforts at LANL, where the first working prototype will be installed summer 2010 on a neutron beam line at its Neutron Science Center. "We're doing something that is pretty hard and really hasn't been done before," says Tony Hill, the director of nuclear data efforts at Idaho National Laboratory's Technical Integration Office and co-scientific director of the project.

In a typical U.S. nuclear reactor, substances called moderators slow down neutrons so they interact with fuel largely composed of uranium-235 with a small fraction of plutonium-239. U-235 and Pu-239 easily undergo fission, splitting into at least two fragments, many gamma rays and several neutrons and releasing large amounts of energy. Neutrons from this reaction continue a chain – fission, moderation, fission – controlled by neutron-absorbing rods.

Pu-239 is a byproduct of neutron-capture reactions in U-238 and is therefore bred into reactor fuel. Some reactors burn higher fractions of plutonium, which can be harvested from former nuclear weapons or spent nuclear fuel.

The project targets these fissile isotopes, along with many others further down the periodic table. The commercial product of these fission processes is heat that drives the steam turbines to generate electricity. What remains presents an international predicament: highly radioactive wastes that must be safely secured for far longer than the lives of those who made them.

Experts base reactor and weapon designs on a combination of experiment and theory. One important goal is to determine, as reliably as possible, "cross sections" for the different isotopes in nuclear fuel. Cross section translates to "reaction probability," Tovesson says. "You need to know the probability of different nuclear reactions, such as fission, in the fuel."

FISSION'S BLACK BOX

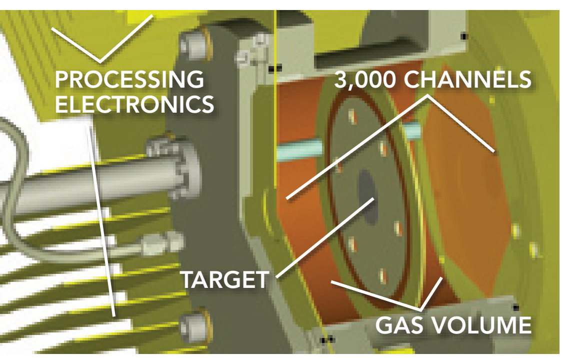
For 50 years experimenters have measured cross sections by methodically detecting fission fragments in fission chambers placed in neutron beams. "Previous measurements on these things tend to be black boxes," Hill says. "You're getting very little information."

Over time the nuclear community has used these traditional methods to develop a good but imperfect standard for what to expect from U-235, the most widely used fuel. With the uranium results as a guide, experimenters and modelers then try to determine how the fission behavior of other fuel components, such as plutonium, may differ.

"They inherit all of the uncertainties associated with U-235," Hill says. Such cross-section knowledge gaps "propagate into uncertainties in reactor performance parameters," says the 2009 annual report for the new TPC project, funded by the Department of Energy's Office of Nuclear Energy and National Nuclear Security Administration.

Those uncertainty parameters, the report continues, include "criticality, peak power, temperature, reactivity, transmutation potential, radiotoxicity and decay heat in a repository" – every aspect of how the fuel behaves and morphs during fission. As a result, the nuclear community must perform integral tests designed to provide best estimates of operating parameters when it starts up a reactor, Tovesson says.

"Since there are large uncertainties in specific quantities, and the reactors want to operate in the safest fashion possible, they don't worry about the details of the



TARGETING FISSION

A fissile target is mounted on the time projection chamber's central cathode plane between two anodes, each with 3,000 small hexagonal pads to register an ionization charge that drifts through gas. The signals from each of the 6,000 channels are routed to the processing electronics mounted just outside the TPC gas vessel. The processing electronics consist of 192 pairs of specialized boards – preamplifiers that boost and shape the raw signals and analog-to-digital boards that convert and process the signals into a computer-friendly format and export it to data-acquisition computers.

IN THE CAN

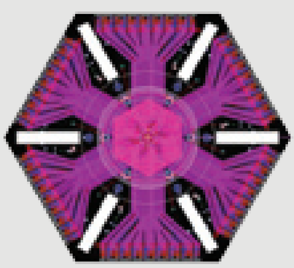
The Department of Energy's fission Time Projection Chamber, with its metallic cylinder and two extended hexagonal planes on each end, resembles a model of a Star Wars fighter ship.

But in this case, its central, coffee-can-sized space will serve as an arena for particles emerging from nuclear fission reactions. The two pad planes contain massive amounts of highly miniaturized electronic circuitry that will calculate and reconstruct particle tracks in three dimensions.

When positioned in experimental neutron beams, initially at Los Alamos National Laboratory's Neutron Science Center, this powerful diagnostic tool will harbor elaborate displays of nuclear fireworks.

Incoming neutrons will induce fission in ultrathin central targets made of heavy fissionable isotopes called actinides – principally nuclear fuels such as uranium-235 or plutonium-239 – inserted into the aluminum pressure chamber's center. The array of charged particles that fission creates will pass through hydrogen gas compressed to several atmospheres in the almost 6-inch-wide chamber, knocking away protons and liberating electrons.

Because the chamber is charged to several thousand volts, an internal electric field will cause freed electrons to drift. The electrons and charged products of neutron-proton scatterings will leave ionization trails through the gas, much like jet airplanes leave vapor trails high in the atmosphere. The TPC's computerized detection system will store those 3-D ionization trails for visualization.

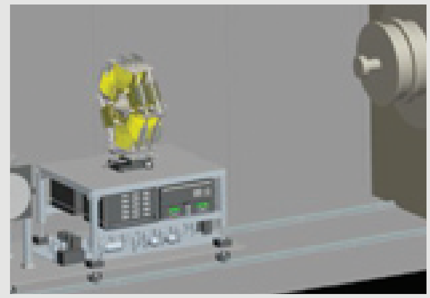


The TPC pad plane design.

Mike Heffner, the project's co-scientific director at Lawrence Livermore National Laboratory, says preparing and maintaining the electronics and software is labor-intensive. "There are lots of person-hours that go into processing and writing codes for that much data, plus getting the electronics built and getting the TPC to work in this miniaturized state."

The TPC will move up to half a trillion bytes of information a second over about 6,000 separate channels, funneled and processed in thin dual pad planes that not only span the pressure vessel's end walls but also jut outside even further. That forms two six-sided working surfaces of about 20 inches – each made of 12-layer circuit boards.

The ionization charges will drift along the electric field to either plane, where analog amplifiers in the pads will read them. Arriving charges will be time-stamped and the analog voltage will be converted to a digital number. These assembled data packets will be passed along those 6,000 channels, which will operate in parallel to save time, and will allow researchers to reconstruct a given ionization trail's original location in the chamber.



The Time Projection Chamber, depicted here on a stand that can move on rails.

Inside each channel, nimble computational devices called field programmable gate arrays and associated algorithms will be able to weed out unnecessary information to reduce the computer-processing volume. The data flow may thus be reduced to mere megabytes per second.

The targets also have challenged TPC builders. Highly skilled teams must deposit the actinides in extremely thin layers using processes like evaporation. The thicker the target, the more fission will occur inside rather than on its surface, where a detector can log the results. The current standard is a wispy 100 millionths of a gram of material per square centimeter.

The actinides are deposited onto foils of backing materials such as carbon. Those also must be equivalently thin yet tough enough to withstand radiation damage during operation or tears during deposition.

Researchers have experimented with backings as thin as 30 millionths of a gram of material per square centimeter.

Says Tony Hill, a co-scientific director working at Idaho National Laboratory: "It's unclear these will be reliable enough to use. But certainly we've gotten down to 100, which is borderline negligible."

data. Instead, they run the reactor once and map out much of the parameter space in an integral fashion and look at the results in the fuel. Now they know approximately what happens, but they can't really say why.

"That works well with current nuclear reactors. But now try and design an advanced reactor. You only know how the current system works, but you can't really predict something unknown."

Partly driving the TPC project is DOE's Fuel Cycle Research and Development program, which needs to come up with cleaner, less waste-producing and better-known fuels to support next-generation reactor designs. It also seeks increased control of such materials to ease concerns about nuclear proliferation.

OLD PROBLEM MEETS NEW TECHNOLOGY

The fission TPC project started about six years ago at Lawrence Livermore National Laboratory (LLNL), says Mike Heffner, an LLNL staff physicist and the TPC project's other scientific leader.

The original focus, Heffner says, was to provide the cross sections needed for NNSA's Stockpile Stewardship program, which aims to preserve weapon reliability without underground testing. "Then we realized there was also an application for the nuclear power industry."

Heffner notes that researchers have exhausted current techniques' ability to study cross-section/reaction probability measurements. TPC throws a new technology at an old problem, he says.

Elastic scattering triggers 'a contrail of ionization in the gas, much like a jet airplane leaves a vapor trail.'

The TPC overcomes old methods' limitations with a data-acquisition system that can process the vast information that pours from what amounts to a 3-D movie camera. Large TPCs offer massive signal processing and computerization. Particles from reactions in or near them are identified by the way they respond to gas and electric and magnetic fields inside.

Heffner and colleagues can track particles in three dimensions because the particles leave an ionized trail in the electrified gas. That information is then read out by copper pads and charge-sensitive preamplifiers and quickly piped along channels for digital processing. "The biggest TPCs have hundreds of thousands of channels," Heffner says.

"The real complication is downscaling," he says. "The challenge of building a small TPC is doing all that processing in a very small volume. And the techniques that will allow this to happen have only been developed in the last five to 10 years."

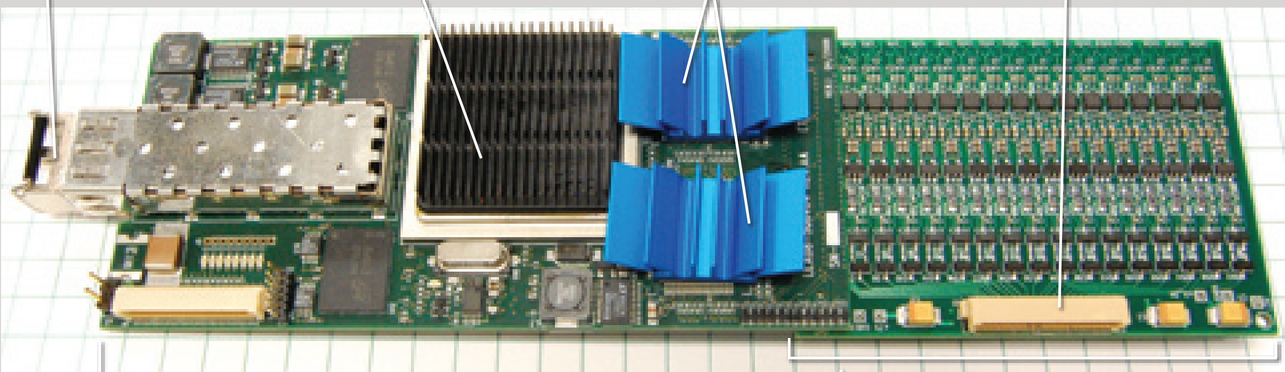
The TPC design will allow researchers to use pure hydrogen to make use of "a different nuclear reaction that is better known than U-235's," Tovesson says. That's because the hydrogen gas in the chamber is not just for ionization. An incoming beam of neutrons will also initiate what is called elastic scattering with the protons in the hydrogen. Elastic scattering is much better understood than the U-235 fission cross section typically used in these types of experiments to develop standards. Removing the U-235 fission cross-section liability is key to reducing uncertainties to less than a single percentage point.

In elastic scattering, each fission fragment and scattered proton is charged and will ionize the hydrogen gas to "leave a contrail of ionization in the gas, much like a jet airplane leaves a vapor trail," Hill says. The cloud of electrons liberated from the hydrogen gas then moves along the precision electric field maintained within the chamber.

Because this neutron-proton elastic scattering reaction is much simpler than uranium reaction probability measurements, researchers can measure and calculate it much more accurately compared to actual nuclear fuels such as U-235 – "a factor-of-10-difference in precision," Tovesson says, over cross sections.

U-235 is typically included in measurements of other fission cross sections to understand the energy structure of the incoming neutron beam, but researchers can improve precision by looking at the interaction of neutrons elastically scattered off hydrogen.

AMPING UP FISSION SIGNALS



The fission TPC electronics maximize the signal processing available while minimizing the space required, each card being about the size of a business card. The complete electronics chain consists of two boards that can process 32 independent channels. The signals enter through a small connector that attaches directly to the TPC. The first board is a set of independent preamplifiers that increase the raw analog signals and prepare them for digitization, which occurs on the second board. The digital board converts the analog signals. A field-programmable gate array then performs calculations on the data to minimize the output stream, which is fed to a local network. Data from the 192 identical systems are reconstructed at a remote computer for analysis. The boards were designed at Lawrence Livermore National Laboratory.

FISSION MOVIES IN 3-D

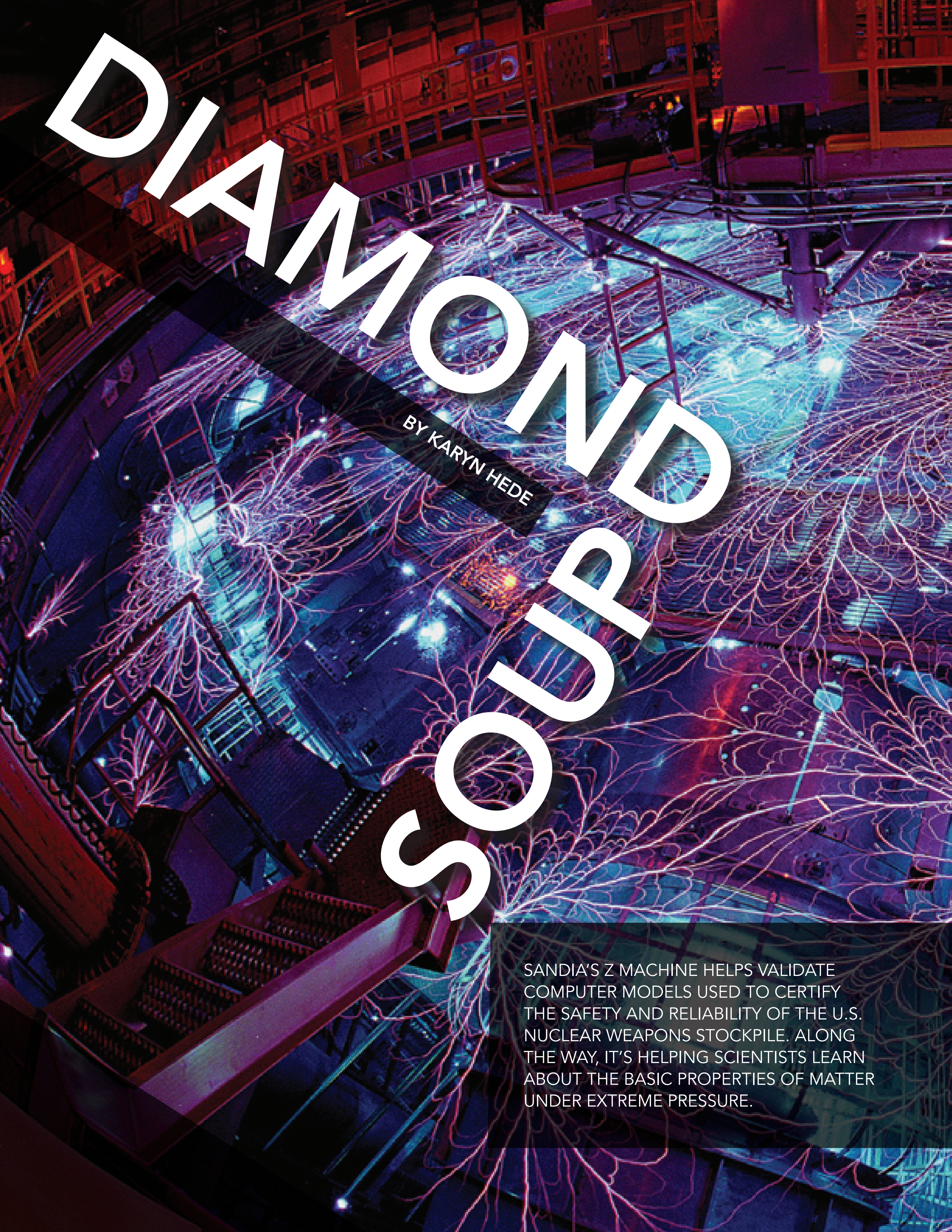
Because many fission products are electrically charged, the TPC will act like a 3-D movie camera that can capture and record every unfolding cross-sectional event rather than the previous few, Hill says. After neutrons pass through both the gas and ultrathin targets of fissionable materials called actinides, electronic readouts of all resulting ionizations will be processed by about 6,000 parallel computational channels within a volume measured in inches. So "everything that happens in that chamber can be identified."

Says Heffner, "I would say the ultimate goal is to make a measurement of the neutron-induced fission of Plutonium-239 as accurately as we can." The researchers aim to reduce measuring uncertainties from 2 to 3 percent to less than 1 percent. That will take time, they caution. "We're shooting for 2014 or 2015 at this point," Heffner says. They also hope for similar improvements in understanding other fuel types and some of their breakdown products.

A prototype TPC is in early testing at LLNL. Plans call for shipping it to the Los Alamos Neutron Science Center by late summer for insertion into an intense neutron beam.

More elaborate testing will follow at more than one neutron site to eliminate any bias. "There is one goal in the end, but there will be many, many steps," Heffner adds. The TPC collaboration includes 23 active members working at the three national labs plus Abilene Christian University, California Polytechnic State University, the Colorado School of Mines, Georgia Institute of Technology, Ohio University and Oregon State University.

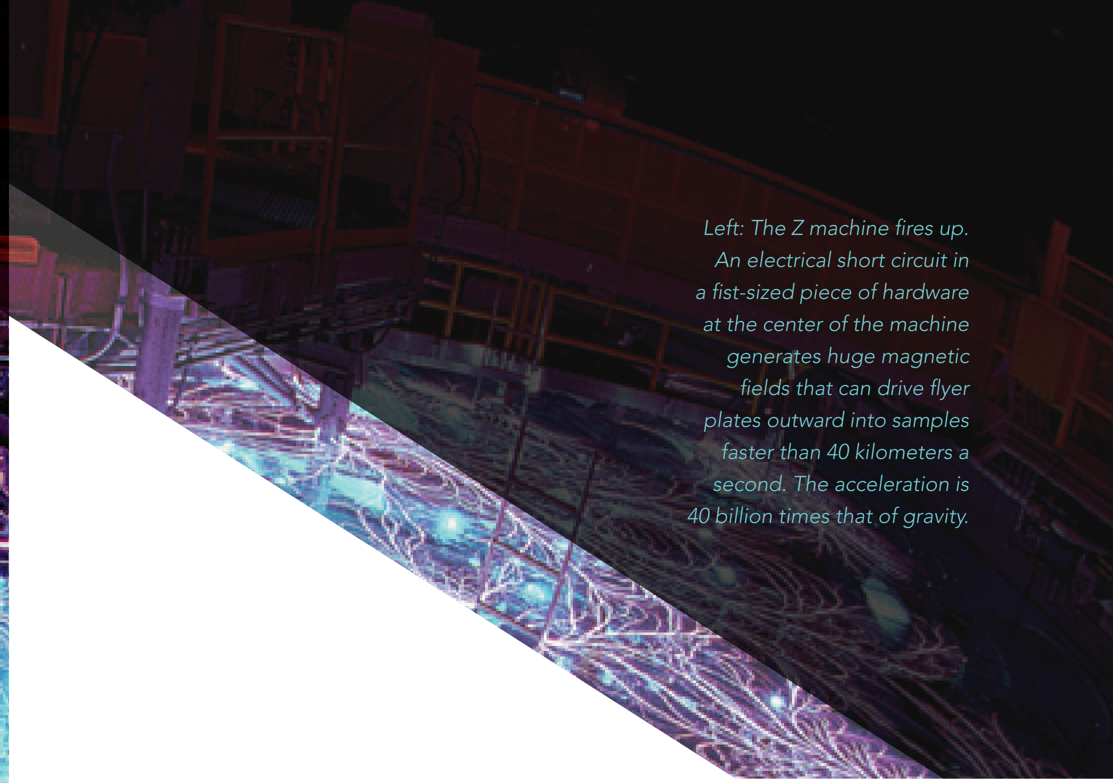
"There are students and post-docs involved, so we have a fairly young crowd as well as people who have spent a number of years doing this," Heffner says. "We're hoping to develop the next generation for this kind of work." SS



DIAMOND SOUP

BY KARYN HEDE

SANDIA'S Z MACHINE HELPS VALIDATE COMPUTER MODELS USED TO CERTIFY THE SAFETY AND RELIABILITY OF THE U.S. NUCLEAR WEAPONS STOCKPILE. ALONG THE WAY, IT'S HELPING SCIENTISTS LEARN ABOUT THE BASIC PROPERTIES OF MATTER UNDER EXTREME PRESSURE.



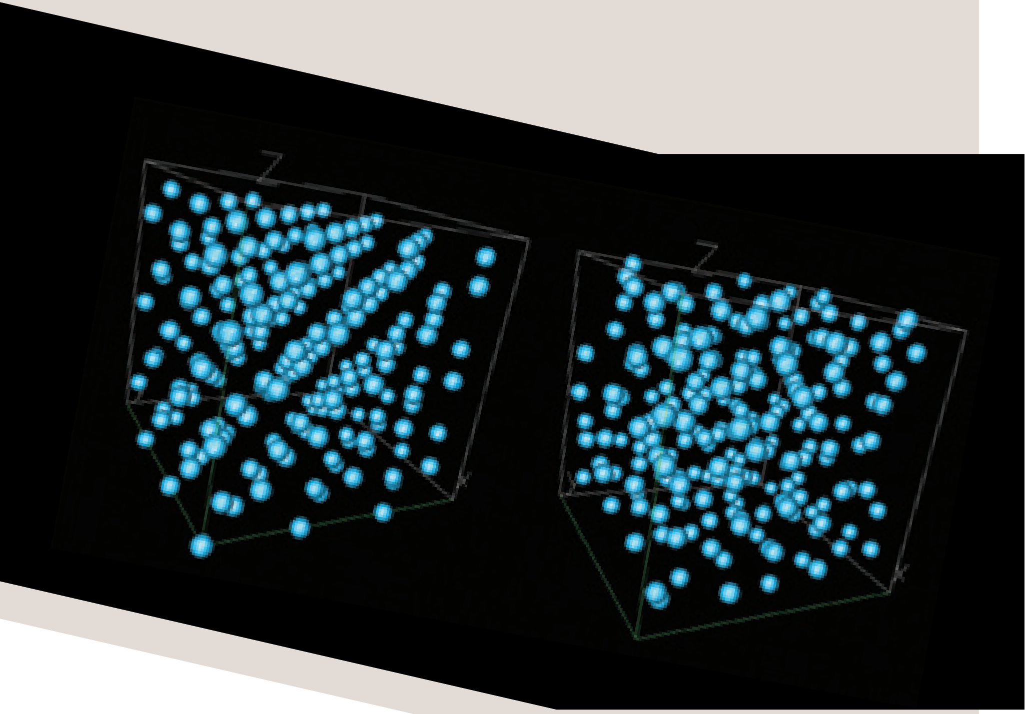
Left: The Z machine fires up. An electrical short circuit in a fist-sized piece of hardware at the center of the machine generates huge magnetic fields that can drive flyer plates outward into samples faster than 40 kilometers a second. The acceleration is 40 billion times that of gravity.

TO ENTER THE WORLD of Sandia National Laboratories' Z machine is to journey to a world where matter shrinks and swells, bends and breaks, expands and contracts in ways reminiscent of Alice's fantastical trip through the looking glass. Here, at temperatures and pressures found only inside celestial bodies or in the core of a nuclear reaction, matter deforms in ways never before observed on earth. Diamonds melt into liquid droplets, and water becomes metallic.

If Alice peeked inside Sandia's Z machine, the pulsed-power laser system that makes it all happen, she would see a facility the size of a sports arena supporting experiments that occur in nanoseconds inside a container that could fit in the palm of her hand. But the Z-machine's mission is far from fanciful; it allows scientists to explore the high energy density physics of plastics, foams, metals and other materials to determine how they might react in a nuclear detonation.

Data obtained from Z, located at Sandia's Albuquerque, N.M., site, helps validate computer models used to certify the safety and reliability of the U.S. nuclear weapons stockpile, obviating the need to conduct actual tests. In addition, scientists are gaining valuable information about the basic properties of matter under pressure extremes that can exceed 1,000 gigapascals – 10 million times atmospheric pressure – and temperatures that soar to tens of thousands of degrees Kelvin, hotter than the sun's surface. Such experimental conditions have been achievable only in the last decade at only a handful of

Karyn Hede is a freelance science journalist who writes regularly for Science *and the* Journal of the National Cancer Institute. *Her work has appeared in* Technology Review, Scientific American *and* New Scientist.



To tease out behavior of diamond on the Hugoniot – a function that specifies the locus of possible material states after shocking – researchers perform *ab initio* calculations with density functional theory for various shock conditions. Left: carbon in its initial room temperature diamond configuration. Right: diamond (now, technically speaking, liquid carbon) after it has shock-melted.

> *'You are trying to get these capsules to 300 times normal density and that's a huge compression. So it's a delicate process.'*

facilities worldwide. The physics that has emerged is truly at the far reaches of what is measurable, with surprises for all involved.

"We are dealing with conditions that are far from ordinary," says Mike Desjarlais, a computational physicist who collaborates with the experimental team. "There may have been speculations over the years as to how a material might behave, but one of the main drivers for doing the experiments is to find out how they actually do behave."

In recent years, one of the biggest questions facing the Sandia team is how to make a container to hold the hydrogen fuel in a nuclear inertial fusion reaction, a potential clean energy source. To turn that potential into reality, the fusion reaction must release more energy than it takes to initiate. For practical fusion energy, researchers must find a material that will hold the hydrogen in place under extreme pressure and temperature, and then cleanly implode just as the fusion reaction begins. Desjarlais and fellow Sandia physicist Marcus Knudson are working with colleagues at Lawrence Livermore National Laboratory's National Ignition Facility (NIF) to help identify the best coating choice for this inertial confinement fusion (ICF) capsule.

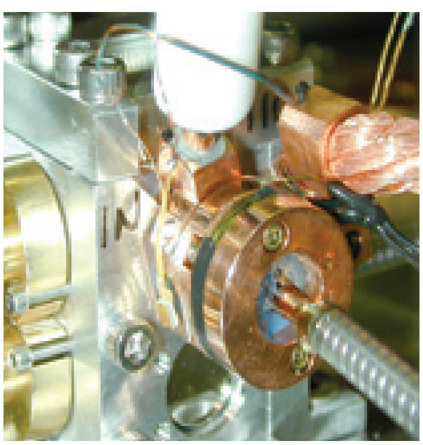
"If you have small perturbation as the capsule implodes those are going to grow and if they are too large they can actually rip the capsule apart before you reach the necessary density condition," Knudson says. "You are trying to get these capsules to 300 times normal density and that's a huge compression. So it's a delicate process. Any potential source of instability is of concern. (NIF scientists) are concerned about having a shock wave that lands in the coexistence region, where you've got some mixture of solid and liquid. Then the second shock that comes in is going to be going through a fairly heterogeneous material and that would be enough to cause this instability growth."

Knudson, an experimental physicist, has been working with a short list of materials that could make suitable capsule components. The research team has tested diamond and beryllium, a rigid, lightweight metal with a high melting point – a desired capsule property. The goal is to find out how the elements behave as a series of laser pulses raises the pressure and temperature of the capsule to the cusp of nuclear fusion. What they've learned is rewriting our understanding of high-density physics.

CURIOUSER AND CURIOUSER

Each Z machine experiment is an expensive proposition, so before firing up the accelerator, Knudson and Desjarlais spend a lot of time ensuring they will get the biggest experimental bang for the buck. Desjarlais' role is to narrow the field of play to an area that will yield useful information. "We are simulating in a very high fidelity way how these experimental loads are going to respond on the Z machine to be able to extract the data that we need," Knudson says.

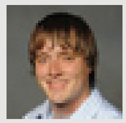
In the case of diamond, which is pure carbon formed into a perfect cubic lattice, the researchers wanted to draw a detailed picture of the conditions required to convert it from solid to liquid. It's difficult to imagine a droplet of diamond (and technically it's not a diamond until it hardens) but it's the intense conditions like those in the Z machine that rearrange carbon atoms into gemstones within the earth's mantle. No, making gems in the Z machine isn't realistic, but understanding how diamond is formed and deformed is.



High magnetic fields on the aluminum side of this magnetically launched aluminum/copper flyer drive it into diamond targets at tens of kilometers per second, generating enormous pressures and shock waves in the diamond. The flyer is the size of a gum stick.

HEAVY HYDROGEN UNDER PRESSURE

There are few places to turn for advice if you're a physics graduate student trying to decide how best to design an experiment to capture elusive photon signals generated from pressurized, liquid hydrogen. High-density physics is a specialized field, and those with a deep theoretical understanding of how hydrogen behaves at these physical extremes are few and far between.



That's why when Paul Davis, a Department of Energy National Nuclear Security Administration Stewardship Science Graduate Fellow, needed a place to do his summer practicum, one name quickly emerged: Mike Desjarlais.

"He's written several theory papers on the properties of hydrogen under high pressure and high temperature," Davis says. "That's interesting to me. I'd heard him speak at conferences and his work relates to my work, so it was an easy choice for me."

Davis will spend the summer of 2010 at Sandia National Laboratory in New Mexico learning the intricacies of *ab initio* molecular dynamics simulations as they pertain to his experimental system of choice, the hydrogen isotope deuterium. Davis, a graduate student in the University of California, Berkeley, applied science and technology program, is trying to detect temperature and density changes in deuterium under pressurized conditions. To conduct the experiments, he works closely with Siegfried Glenzer's plasma physics group at Lawrence Livermore National Laboratory. Glenzer is a leader in the effort to harness hydrogen fuel for fusion energy. In the big picture, gaining a better understanding of deuterium's properties could help design better fusion systems for power generation, but Davis' system operates at much lower pressures than would be required for energy production.

He hopes to show it's possible to use X-rays to detect photons scattered by deuterium under laser excitation. LLNL and other groups have already successfully used X-rays, but with material that is much denser to begin with. Hydrogen and its isotope deuterium contain but one electron per atom and even when condensed into a liquid, the material is much less dense than, say, boron, which deflects X-rays quite nicely. Just getting a reliable signal with a deuterium sample would be an achievement, Davis explains.

"We are constantly fighting background noise in the system," he says. The payoff would be a way to directly measure temperature, a variable that must be derived indirectly using today's detection systems. In addition, X-ray diffraction gets at *how* the internal structure of materials changes, not just *when* it changes. The work is fundamental physics, but if Davis is successful in getting a signal, it would create a whole new detection system to extract information about hydrogenic systems – the various forms hydrogen can assume. And those systems are more complex at high pressure and temperature.

Another goal is to combine the laser excitation work with computational simulations that could add theoretical heft to his experimental results. "I want to get a feeling for how these codes work and kind of get my feet wet in the field of simulations of warm, dense matter," he says. For him, there's no better place to do that than side-by-side with Sandia's Mike Desjarlais.

The path through phase-space that shock-wave physicists want to locate is called a Hugoniot, a locus of material states that can be reached through strong shock-wave compression. At these very high densities, diamonds can, in fact, liquefy. But not all at once, and therein lies the conundrum.

"The capsule designers really wanted to understand the melt properties of diamond along the Hugoniot so they can try to design around it," Knudson says. Using magnetically accelerated copper plates the size of a gum stick driven into milligram-sized samples of diamond, the physics that emerged did, in fact, determine the onset and completion of diamond melt. That in itself was useful, but more interesting was the discovery of the simultaneous existence of two solid lattice forms of diamond: the conventional cubic gem form and a theoretical configuration called bc8 (body-centered, 8 atoms per cell) that had never been observed to form on earth, along with the liquid form in what's called a "triple point."

The discovery was hidden among the mountains of data that emerge from each experimental run. It took the combined efforts of Knudson's experiments and Desjarlais' computational models to find it.

Desjarlais specializes in predicting what will happen in high-density physics experiments by using a computational approach that calculates subatomic behavior using quantum mechanical theory. The models that emerge are predicted *ab initio* – "from first principles."

"The region of phase space we are sampling – warm, dense matter – doesn't yield to simplifying approximation," Desjarlais says. Instead, he and his colleagues use density functional theory, a powerful computational approach that allows them to model hundreds of atoms using *ab initio* methods. In the past, such calculations had to account for each electron-electron interaction, but doing so made any realistic modeling computationally prohibitive. Density functional theory, along with inputs on the physical characteristics of the material being modeled, allowed Desjarlais to predict the existence of the diamond "triple point."

"My calculations said, 'Hey, if the bc8 phase is there, we ought to see an abrupt change in the shock velocity when we go through the triple point,'" Desjarlais says. Sure enough, the research team found the velocity changes just where Desjarlais had predicted, providing empirical evidence for the triple point. The result was a wholly new diamond phase diagram, a plotting of the curve along which diamond melts at extreme temperature and pressure.

"Because we were able to make such high-precision measurements, we actually had the fidelity in the experiments to make a quantitative comparison with these *ab initio* models and extract evidence for the triple point," Knudson says.

This first-ever experimental evidence for a triple point in diamond, along with the theoretical framework to support the findings, garnered a Dec. 18, 2008, publication in the journal *Science*. The results give valuable guidance to the NIF experimental team as it continues work on the first fusion experiments. For the fusion application, the relatively high melting point of diamond, along with its complex melt behavior, may push it down the list of capsule materials. But for the Sandia team, the excellent agreement between experiment and model in the diamond work gave them confidence to create phase diagrams for other materials under extreme conditions.

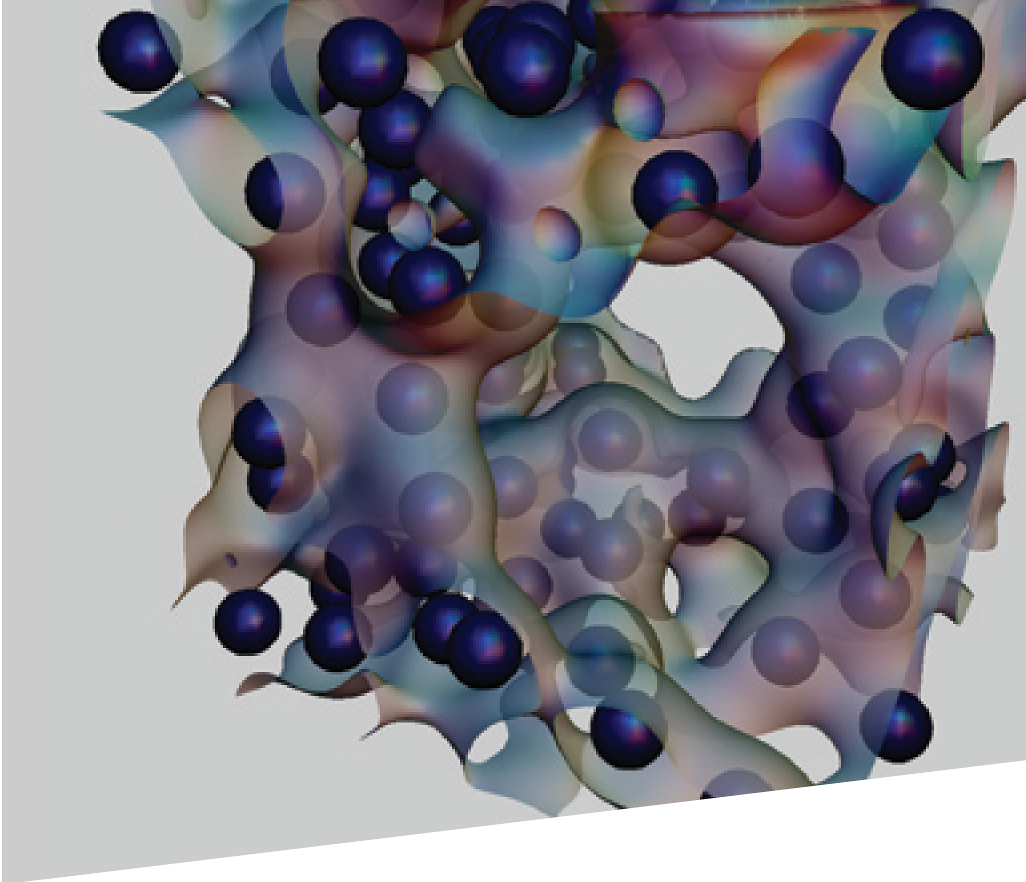
THROUGH THE LOOKING GLASS

"We followed up the diamond work with some work on quartz," Desjarlais says. "Quartz is interesting because it is used as a standard in these shock experiments. What we discovered, again using the combination of the theoretical calculations and the data, was that the existing models for quartz were incomplete."

Quartz is an ordered form of silica – a clear solid that becomes conductive when it liquefies, allowing scientists to aim a laser through it and measure the shock velocity of the flyer plates as they strike samples through a technique called velocity interferometry. Experimental results are compared to this quartz standard to ensure accuracy.

In a *Physical Review Letters* paper published Nov. 27, 2009, the researchers described a zone of disordered melting at up to 1,000 gigapascals, well within the pressure range used in many shock-wave experiments. The findings suggested a revised standard Hugoniot curve for quartz, which, by definition, will

'The existing models for quartz were incomplete.'



Like its target, the flyer plate itself can morph under extreme conditions, and researchers need to account for this. A density functional theory illustration of hot, expanded aluminum (the magnetically-driven side of the plate) depicts ions as blue spheres, surrounded by a surface of constant electron density that flows broadly through the system. This allows for high conductivity but also hints at early signs of electron-density localization, or electron bunching, as the material expands, which can reduce conductivity.

change estimations of the density of materials that rely on the quartz standard, at least within the disordered quartz melt zone.

THE BIG SQUEEZE

Sandia shut down the Z machine for an upgrade in 2007. Knudson and Desjarlais used that downtime to conduct simulations and predictions to even more closely align the experimental and theoretical work. By 2009, the team was using Z to conduct ramp wave experiments, in which the magnetic drivers steadily increase pressure, rather than delivering it as a shock wave.

The new work opens up a different region of the phase space to experimental work, Knudson says. For example, in shock wave experiments beryllium liquefies at 300 gigapascals pressure. In a ramp wave experiment, it remains a solid at that pressure. The difference is that ramp waves increase the sample temperature to a few hundred degrees Celsius, which is "cool" compared to shock wave experiments.

Other groups are using lasers to do ramp wave experiments at similar pressures, Knudson says. (See cover story this issue, "Ramping Up the Pressure.") But the Z machine can handle thicker samples and can make measurements in the hundreds of nanoseconds, versus 10 to 20 nanoseconds for laser-based systems. "We know less about material strength than we do about these other quantities," Desjarlais says. "That has a lot to do with the meso-scale structure of the materials. There are defects and grain boundaries, there are vacancies, and all of these things contribute to a material's real strength. The (National Nuclear Security Administration) community is very interested in the strength of materials at higher pressures." Ramp wave compression can probe phase boundaries to test the strength of complex materials with inherent imperfections – things like plastics and metal alloys.

"Our ramp compression wave can be 600 nanoseconds, which allows us to propagate through thicker materials that might be more relevant to studying grain structure and things like that," Knudson says. "There are complementary experiments that can be done on these different platforms. Each one has its strengths."

In addition, the downtime with Z allowed the researchers to practice simulating how materials could be expected to deform depending on the curvature of the pressure rise. Each material has characteristics that require changes to the steepness of the pressure wave, and that's an area where Desjarlais' simulations and material models have saved valuable experimental time.

"We spent a good year or so trying to refine our simulations to get to predictive capability," Knudson says. "I would say in the last six months or so we've gotten there." SS

Final-year Stewardship Science Graduate Fellows recount their research experiences at the national laboratories.

Miguel Morales
University of Illinois, Urbana-Champaign
Practicum: Lawrence Livermore National Laboratory

Mixing It Up Inside Gaseous Planets

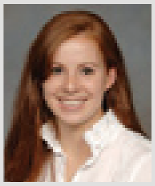
I chose planetary science when Eric Schwegler in the Quantum Simulations Group at Livermore presented me with different research options. We were interested in materials that are important for planetary interiors, and my original project was related to understanding the ionic component of the electrical conductivity in dense molecular mixtures near dissociation. But as Dr. Schwegler and I started learning about each other's work, the problem of the miscibility of hydrogen-helium mixtures at high pressures and intermediate temperatures came up, and that eventually became my main project.

The challenge was whether we would have enough computer time to do it during my practicum. There was an opportunity, though, and I had a week to get the model ready to run on a big cluster that would be available for a month. I did a lot of coding in a short time, but we were able to get close to 4 million hours.

We found quite an interesting result: that hydrogen and helium become partially miscible in a large region of the interior of giant gas planets. That accounts for the energy source needed to explain why the surface temperature of these planets is considerably higher than planetary models predict.

The hydrogen-helium problem was something I had planned to do in my thesis research, but I was going to use a different method: quantum Monte Carlo. Density functional theory was where I ended up.

Since fall 2009, when I became the first SSGF recipient to graduate, I've been on a postdoc at Rice University, working mainly on numerical simulations of actinide systems to better understand elements important for nuclear fuels and to try to push the boundary on the accuracy we can achieve.

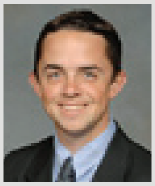


Laura Berzak
Princeton University

Practicum: Sandia National Laboratories, New Mexico

LIQUID LITHIUM DIVERSION

Under Richard Nygren, I worked on materials testing for the liquid lithium diverter, or LLD, to be installed on the National Spherical Torus Experiment at the Princeton Plasma Physics Laboratory, a fusion reactor based on a spherically shaped plasma design. The LLD will provide density control and a high heat-flux handling capability. I did initial infrared temperature gradient tests and scanning electron microscope analysis on a novel molybdenum mesh for LLD solid components. These components will provide a constant wicking surface of lithium to the plasma. I also designed a vacuum chamber and diagnostics to test the material with lithium. The test stand was completed after my practicum and is being used. The LLD design changed and this material wasn't used, but it's under consideration for the next design iteration. The experience I gained in my dissertation research helped in engineering the test stand. My practicum, meanwhile, helped me better understand the physics behind the LLD design and whether the molybdenum material has potential for plasma-facing components.

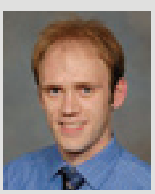


Dylan Spaulding
University of California, Berkeley

Practicum: Lawrence Livermore National Laboratory

VISIBLY SHOCKED

My project under Bruce Remington was to propose a diagnostic for laser-driven shock experiments. The diagnostic would do white-light spectroscopy of the shock front to better constrain emissivity for temperature measurements and to understand absorption and band structure in shock-compressed materials. It also set out to better characterize the optical properties of tamping windows often used in high energy density experiments and determine the windows' effects on optical measurements of the underlying sample. It's like looking through a colored window: If you don't know the properties of that window, you can't with certainty explain what's on the other side. Since my practicum, we've run tests showing the diagnostic technique we chose may not be the best way forward. I hope to go back later this year and experiment with different techniques. It was a valuable project because it also applies to my research measuring shock temperatures for geophysical experiments.



Forrest Doss
University of Michigan

Practicum: Lawrence Livermore National Laboratory

'A GOD'S-EYE VIEW' OF SUPERNOVAE

My main goal during my practicum under Larry Suter was learning HYDRA, Livermore's radiation hydrodynamics code. I wanted to simulate things that looked like my experiment – a laser-driven shock tube designed to recreate high energy density processes like those driving supernovae and other phenomena. Simulation helped explain a somewhat mysterious result: a deflection in the primary shock. Diagnostics could see it, but the mechanism was invisible. In the simulation, everything is visible – you have a God's-eye view. What's happening is the shock heats the tube walls and vaporized material streams inward to meet the primary shock. The simulations explained similar data from Early Light experiments at NIF (Livermore's National Ignition Facility). My practicum was planned to complement my dissertation research. I'm not primarily a computational student, and the work I've done or learned to do at the practicum is where the computational support really comes from. It added a very useful tool.

NNSA SSGF FELLOWS DIRECTORY

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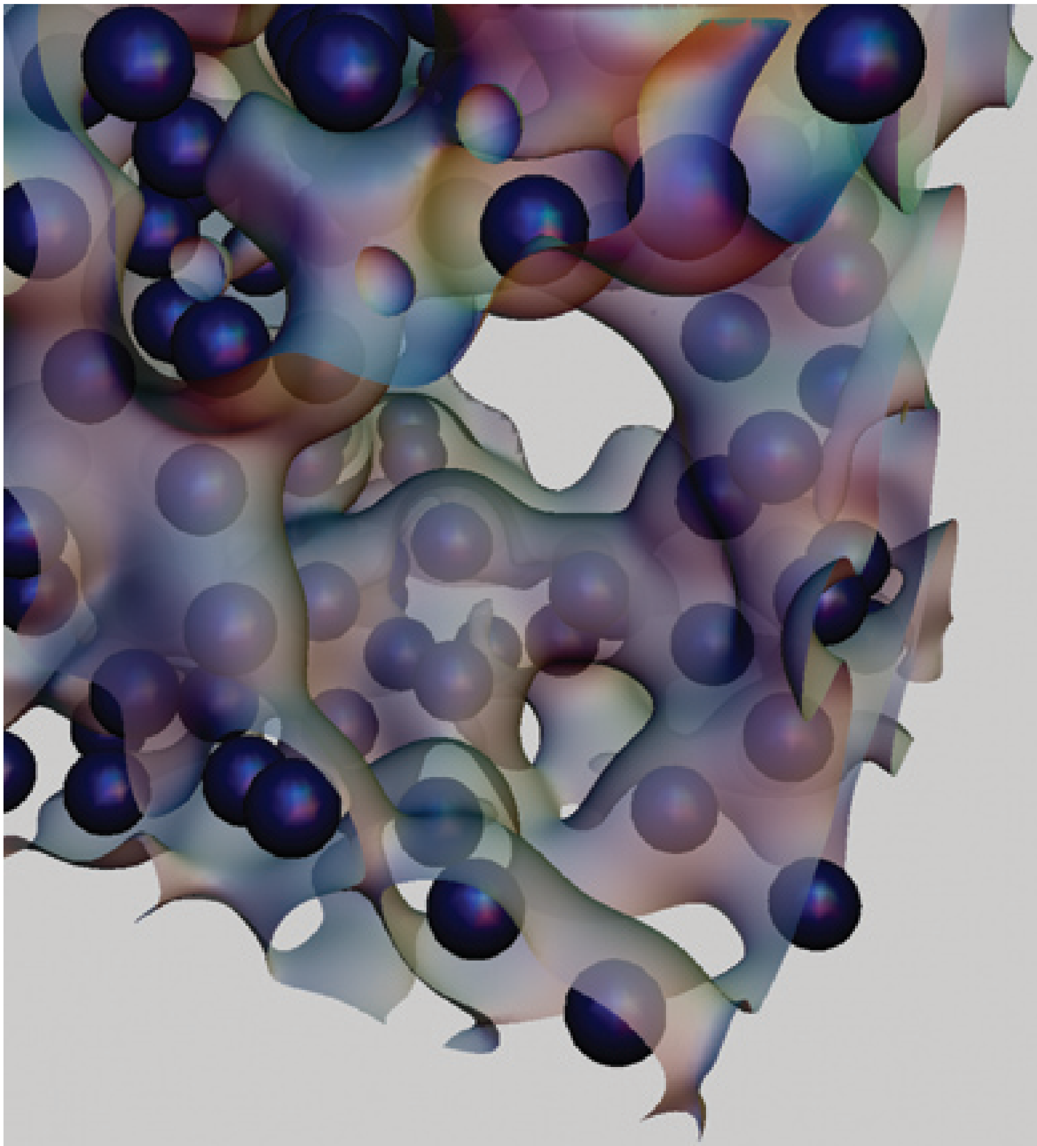

CONDUCTING HIGHLY CONDUCTIVE EXPERIMENTS

Detail from a rendering of electron density in hot, expanding aluminum put under the extreme heat and pressure of the Sandia National Laboratories Z machine in New Mexico. The distribution of ions (the blue spheres) in an electron-density flow (the surrounding cloudy material) determines the degree of aluminum's conductivity. For more on the strange things that happen to aluminum and other materials under the shocking magnetic thrall of the Z facility, look inside ("Diamond Soup," starting on page 18).

KRELL institute

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