STEWARDSHIP SCIENCE

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PRESSURE PLANET

Livermore team recreates deep-Earth conditions

Los Alamos: Time projection gets small

Sandia: Diamond droplets and beyond

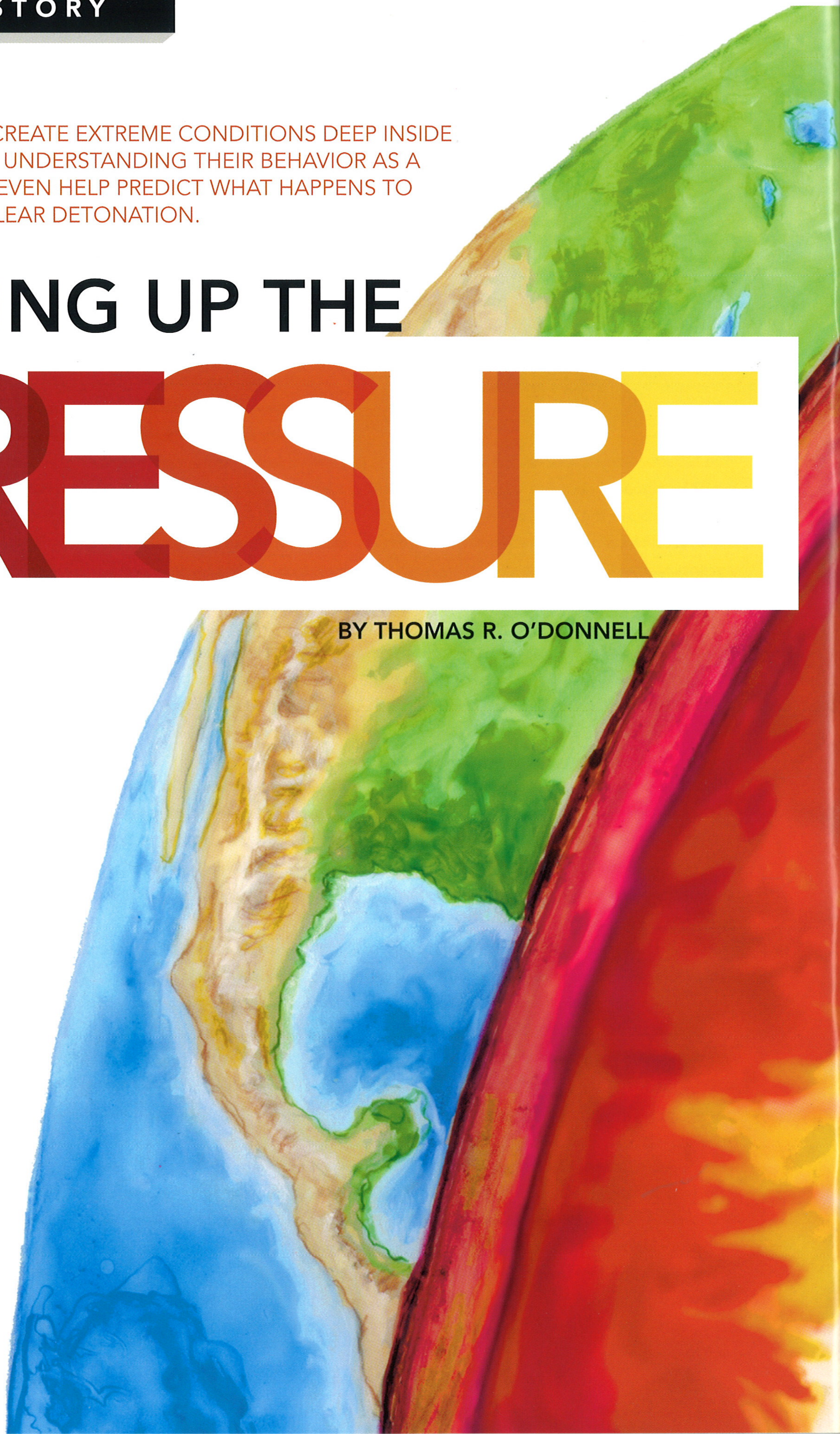
Plus: Nuclear forensics, DARHT toss, a conversation with NNSA's chief and SSGF fellows in first-person

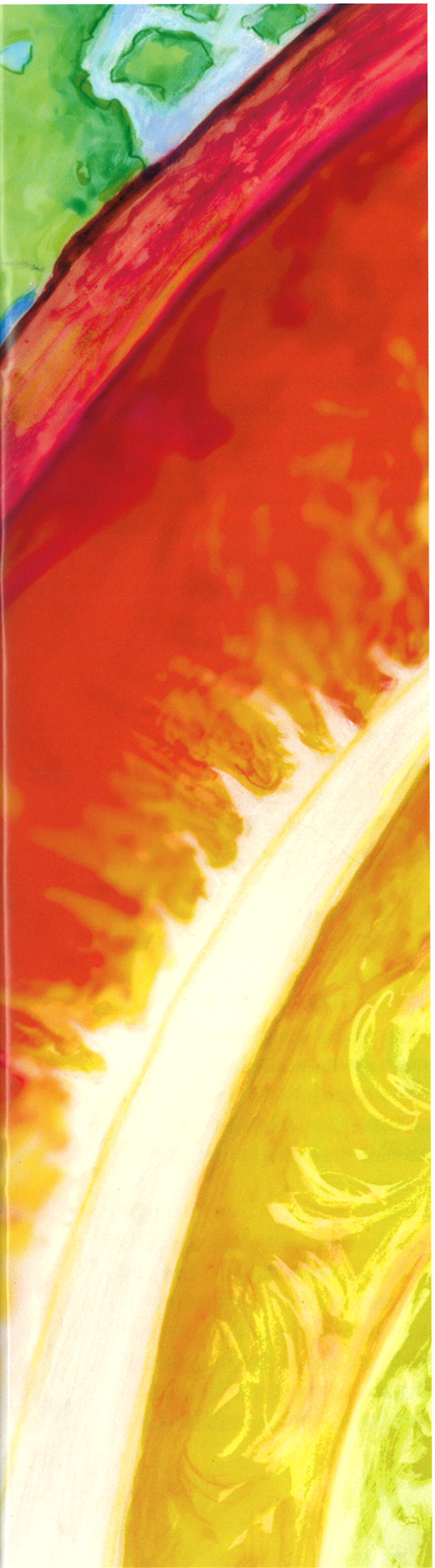
COVER STORY

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

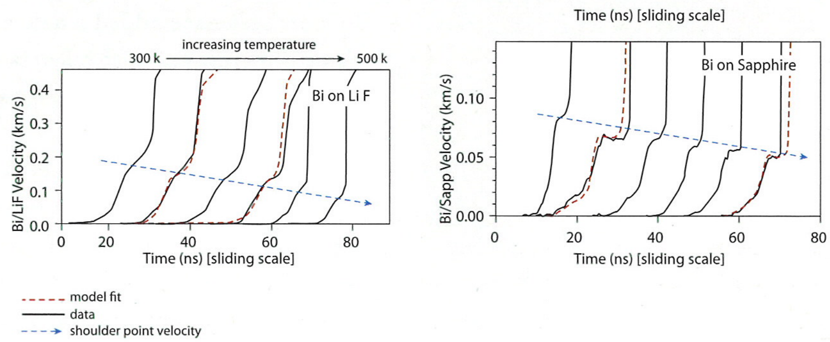
but nowhere near the pressures found inside gas giant planets like Jupiter or huge "super-Earth" planets orbiting other stars. A DAC also doesn't provide time-dependent data related to the dynamics of material compression, such as changes in strength.

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.

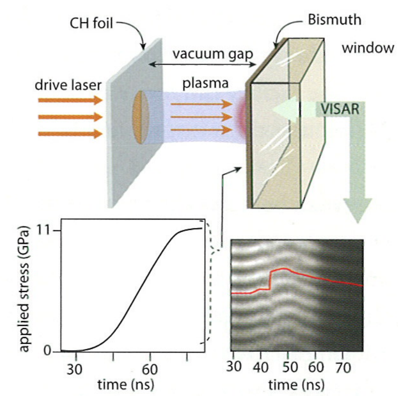
National Laboratories' Z machine. Really fast ramp compression, however, requires powerful lasers, like Livermore's Janus, a system with two beams rated at 1 kilojoule each.

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.

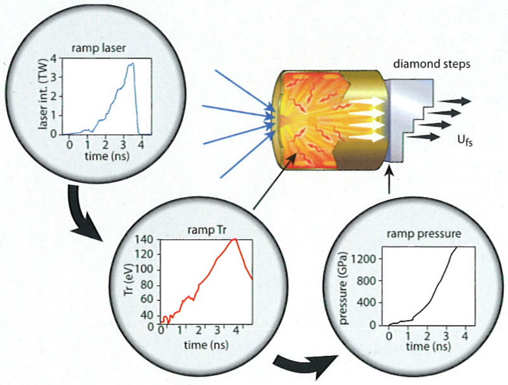
OUTRUNNING A WAVE

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." SS