National Nuclear Security Administration

Stewardship Science Today

Office of Research, Development, Test, and Evaluation (RDT&E)

Volume 1 | Number 2 | June 2019

Stewardship Science Today (SST) highlights the stewardship science and academic programs supported by the Department of Energy/National Nuclear Security Administration (DOE/NNSA). SST is published quarterly by the NNSA Office of Research, Development, Test, and Evaluation. Questions and comments regarding this publication should be directed to Terri Stone via email at terri.stone@nnsa.doe.gov.

Managing Editor
Terri Stone

Technical Editors
Dr. Joseph Kindel*, Jennifer Dieudonné*

Publication Editor & Design
Millicent Mischo*

◆ ◆ ◆

Calendar

7/8-12
46th European Physical Society Conference on Plasma Physics, Milan, Italy

7/11
NNSA Job Fair, DoubleTree Crystal City, Arlington, Virginia, 8 am-5 pm

9/22-27
International Conference on Inertial Fusion and Science Applications (IFSA2019), Osaka, Japan

10/21-25
APS Division of Plasma Physics Meeting, Fort Lauderdale, Florida

Inside

*Contractor Support

Welcome to the second issue of *Stewardship Science Today* (SST). Since SST debuted in April, the Office of Research, Development, Test, and Evaluation (RDT&E) has hired three new technical staff members. We are excited to have them join the team. RDT&E has no openings at this time, but the National Nuclear Security Administration (NNSA) will host a job fair on July 11 at the DoubleTree Crystal City in Arlington, Virginia to fill positions throughout the Nuclear Security Enterprise.

This issue features three articles highlighting exciting science conducted by the highly skilled and innovative staff members at NNSA and our academic partners. The first article highlights the use of lasers to flash-freeze water into its superionic phase and then to use the technique of X-ray diffraction to identify the atomic structure. We also highlight work at the Spallation Neutron Source to understand the magnetic structures of rare earth metals using diamond anvil cells. Finally, three-dimensional visualization tools, made possible by the installation of a third neutron imaging line-of-sight diagnostic at the National Ignition Facility (NIF), are being used to close the gaps in understanding the structure of burning plasmas. This work is key to advancing progress on ignition at the NIF.

I close this issue with a farewell. After a combined 32 years of service in our DOE Enterprise at Oak Ridge National Laboratory, at Los Alamos National Laboratory, and as a federal employee, I am retiring. It has been my absolute pleasure to work with you in furthering DOE and NNSA missions. I wish all of you the best in all your endeavors.

Sincerely,

Dr. Kathleen B. Alexander
Assistant Deputy Administrator
for Research, Development Test, and Administration

New Faces in the Office of Research, Development, Test, and Evaluation (RDT&E)


Dalton


Davis


Satsangi

Join RDT&E in welcoming three senior staff members to our team. **Dr. Douglas Allen Dalton** brings his experience from the Department of Defense (DOD) as a program manager at the Defense Threat Reduction Agency, working in the Advanced Research Division of the Counter-WMD Technologies Department. There he formulated strategy and generated research activities that included energetic materials, laser-based diagnostics, and additive manufacturing. He also directed research activities in high fidelity modeling and simulation including areas such as energetics, turbulence, and Uncertainty Quantification. He earned his PhD in physics from the University of Texas at Austin and after graduate school he took a postdoctoral appointment at the Carnegie Institute of Washington within the NNSA Stewardship Science Academic Alliances program. Dalton will be working with the Dynamic Materials Properties subprogram and our Academic Alliances & Partnerships element.

Dr. Paul F. Davis brings his experience from DOD's Offices of Nuclear Matters and Net Assessment as an SAIC senior policy analyst focusing on nuclear strategy and survivability. He was previously a Fellow at the American Association for the Advancement of Science, working on deterrence and nonproliferation policy in the Office of the Secretary of Defense; a Legislative Fellow with the Senate Committee on Energy and Natural Resources; and a Fellow of the Stewardship Science Graduate Fellowship program. The latter was while he attended the University of California, Berkeley and conducted high energy density (HED) physics research at Lawrence Livermore National Laboratory. Davis earned his bachelor's degrees in engineering physics and political science from the University of British Columbia. He earned his PhD in Applied Science and Technology from the University

(continued on page 3)

X-ray Diffraction Reveals the Structure of Exotic Water Supersonic Ice

by Marius Millot and Federica Coppari (Lawrence Livermore National Laboratory)

Scientists from Lawrence Livermore National Laboratory (LLNL) used giant lasers to flash-freeze water into its exotic superionic phase and to record X-ray diffraction patterns to identify its atomic structure for the very first time–all in just a few billionths of a second. The findings are reported in *Nature*[1] and follow the team's first experimental evidence[2] for superionic water ice, an exotic state of matter characterized by the coexistence of a solid lattice of oxygen and liquid-like hydrogen ions. These experiments were carried out at the Omega Laser Facility at the University of Rochester Laboratory for Laser Energetics under the Laboratory Basic Science program.

The team led by Drs. Marius Millot and Federica Coppari (see Figure 1), both in the Physics Division at LLNL, managed to recreate the extreme pressure and temperature conditions required to transform water into its superionic ice using laser-driven shockwaves and record *in-situ* X-ray diffraction. The X-ray diffraction shows the nucleation of a crystalline lattice of oxygen in a few billionths of a second and reveals, for the first time, the microscopic structure of superionic ice (see Figure 2).

The researchers used six laser beams to generate a sequence of shockwaves of progressively increasing intensity to compress a thin layer of initially liquid water to extreme pressures (100-400 gigapascals (GPa) or one to four million times Earth's atmospheric pressure) and temperatures (3,000-5,000 degrees Fahrenheit) that are typical of the deep interior of giant planets such as Uranus and Neptune.

To document the crystallization and to identify the atomic structure, the team blasted a tiny iron foil with 16 additional laser beams to create a hot plasma which generated a flash of X-rays precisely timed to illuminate the compressed-water sample in the predicted stability domain of superionic ice.

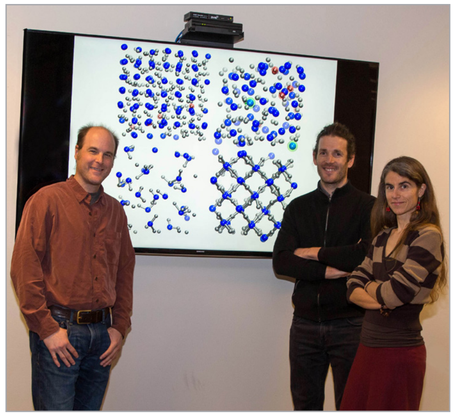

Figure 1. (From Left to right: Sebastien Hamel, Marius Millot, and Federica Coppari). The LLNL Team of scientists documented for the first time the existence of a solid lattice of oxygen with a face-centered-cubic (f.c.c.) structure in superionic water ice. The molecular dynamics simulations results shown on the screen illustrate that water can assume many different forms depending on the pressure/temperature conditions: top-left: superionic, top-right: plasma, bottom-left: ionic fluid, bottom-right: solid ice X. Credits: Millot, Coppari, Hamel (LLNL), and photo by Julie Russell.

The X-ray diffraction data provide characteristic evidence for a solid crystalline lattice formed by the oxygen ions. Tuning the intensity and timing of the series of laser pulses allowed the team to explore 10 different conditions of pressure and temperature. Analyzing how the X-ray diffraction patterns varied for the different experiments, the team identified a phase transition to a previously unknown f.c.c. atomic structure for dense water ice that they named water ice XVIII.

Because the new ice XVIII is found to be stable at pressure and temperature conditions similar to those at which superionic conduction was evidenced in the 2018 study,[2] water ice XVIII most likely is superionic, with hydrogen ions diffusing through the f.c.c. lattice of oxygen.

The team's new data represent a stringent test of quantum simulations of material properties at extreme conditions, an important mission for the Stockpile Stewardship Program (SSP). This research also has broad implications for planetary science: because superionic water ice can sustain high temperatures without melting, it may dominate the interior of water-rich icy giant planets such as Uranus and Neptune as well as all their numerous extrasolar cousins.

Figure 2. Artistic rendering of the laser compression experiment. High power lasers focused on the surface of a diamond generate a sequence of shock waves that propagate throughout the sample assembly (from left to right) and simultaneously compress and heat the initially liquid water sample forcing it to freeze into the superionic water ice phase. Credits: Millot, Coppari, Hamel (LLNL), Image by Liam Krauss (LLNL).

Finally, demonstrating the use of X-ray diffraction under shock compression for low atomic number materials and the nucleation of crystalline grains from initially liquid samples in nanosecond timescale, this study opens a broad range of possibilities for future SSP programmatic research to investigate phase transformations and to provide new benchmarks to theory and large-scale computer simulations.

This research was initiated with the support of the joint DOE Office of Science/National Nuclear Security Administration (NNSA) High Energy Density Laboratory Plasmas program when Dr. Millot was a postdoctoral researcher at the University of California, Berkeley. It built on the work by Dr. Coppari and others at LLNL to develop X-ray diffraction of dynamically compressed planetary materials which was, in part, supported by the National Laser Users' Facility program.[3] This work now involves a new generation of postdoctoral researchers and students who recently joined the project, such as Dr. Yong-Jae Kim (LLNL) and NNSA Stewardship Science Graduate Fellow Michael Wadas (University of Michigan).

References

[1]M. Millot, F. Coppari et al., "Nanosecond X-ray Diffraction of Shock-compressed Superionic Water Ice," Nature 569, 251–255 (2019).

[2]M. Millot et al., "Experimental Evidence for Superionic Water Ice Using Shock Compression," Nat. Phys. 14, 297–302 (2018).

[3]F. Coppari et al., "Experimental Evidence for a Phase Transition in Magnesium Oxide at Exoplanet Pressures," Nat. Geosci. 6, 926-929 (2013). ◆

Rare Earth Metals under Extreme Conditions at the Spallation Neutron Source

by Christopher Perreault[1], Antonio M. dos Santos[2], Jamie J. Molaison[2], and Yogesh K. Vohra[1]

Rare earth elements are materials of strategic national importance due to their widespread applications in computers, cell phones, electric vehicle batteries, and catalysts and for their use in defense industries. They are 17 elements consisting of yttrium, scandium, and 15 lanthanide elements. The high pressure phase transformations, magnetic properties, and equation of state of rare earth metals are significant because of their similarity with the behavior of actinide elements under extreme conditions that are critical to the Stockpile Stewardship Program. The structural phase transformations and equation of state of rare earth elements have been documented to pressures as high as 200-300 GPa using X-ray diffraction at synchrotron facilities. However, the magnetic structures of rare earth elements under extreme conditions remains largely unexplored. Neutron diffraction experiments are necessary to reveal details of magnetic structure at high pressures that are not revealed by the X-ray diffraction, electrical transport, and magnetic susceptibility measurements.

Owing to the traditional pressure and temperature limitations of high pressure neutron scattering, the determination of the magnetic structure of the high pressure phases of rare earth metals still is lacking. Recent advances have been made to reach higher pressures at the Spallation Neutron Source (SNS) using a new large-volume diamond anvil cell shown in Figure 1a. Studies on rare earth elements under extreme conditions at SNS were initiated under support from the Stewardship Science Academic Alliances program. The rare earth metal dysprosium (Dy) was chosen for initial investigations, as it has one of the highest intrinsic magnetic moments among the heavy rare earth elements with a value of 10.6 Bohr magneton (μB) leading to a complex phase diagram under high-pressure and low-temperature conditions.

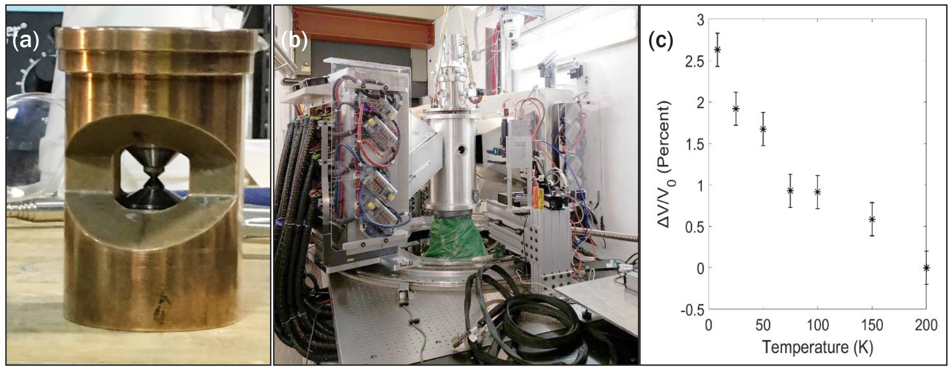

Figure 1. (a) Large volume diamond anvil cell used for neutron diffraction studies at high pressures (b) cryostat mounted on beamline BL-3 at the Spallation Neutron Source (c) the measured relative change in atomic volume for dysprosium at various temperatures at 7.7 GPa illustrating a negative thermal expansion due to magnetic ordering.

Neutron diffraction studies on Dy at high pressure and low temperature to 10 K were conducted at the SNS Spallation Neutrons and Pressure Diffractometer (SNAP) BL-3 as shown in Figure 1b. These studies have revealed both antiferromagnetic and ferromagnetic ordering in Dy under compression. In addition, we have documented negative thermal expansion in Dy at high pressures and low temperatures due to magnetic ordering. Figure 1c reveals a negative thermal expansion of Dy where atomic volume at various temperatures has been measured by neutron diffraction at a pressure of 7.7 GPa. This phenomenon of negative thermal expansion was observed in both the low pressure, hexagonal, close-packed phase and the high pressure alpha-Samarium phase of Dy. Thus, neutron diffraction studies using high-flux spallation neutron sources provide direct observation of magnetic ordering and negative thermal expansion in rare earth metals under extreme conditions of pressures and temperatures. There is a potential to extend the neutron diffraction studies in the 50-100 GPa pressure range where the magnetic ordering in Dy is expected to reach near ambient temperature.

This material is based on work supported by the Department of Energy/National Nuclear Security Administration under Award Number DE-NA0002928. A portion of this research used resources at the Spallation Neutron Source, a DOE Office of Science User Facility operated by the Oak Ridge National Laboratory. ◆

[1]Department of Physics, University of Alabama at Birmingham, Birmingham, Alabama

[2]Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee

New Faces (continued from page 1)

of California, Berkeley. He will be working with the HED & Ignition Science for Stockpile Applications element.

Ms. Ann J. Satsangi is a federal program manager specializing in broad vision, strategic planning, and leading with integrity. She has extensive expertise in scientific research program management, coordinating interagency programs, and balancing cross-cutting research objectives with a focus on future strategies for the most effective federal investments. Prior to her time with the Office of Science, Ann worked in the Office of Inertial Fusion and the National Ignition Facility, and she was key in contributing to the start of the Academic Alliance Program. As a program manager in the Office of Experimental Sciences, Satsangi will be working closely with the Laboratory for Laser Energetics, the Naval Research Laboratory, our academic partners, and our Facility Operations site managers. ◆

New Era of Three-Dimensional Visualization of Compressed Burning Plasmas

by Petr Volegov (Los Alamos National Laboratory)

Until now, the full complexity and three-dimensional (3D) interplay between processes impacting the performance of fusion implosions has been hidden from researchers. Like the world around us, implosions are inherently 3D in nature with energy flowing into a previously hidden third dimension. For decades, inertial confinement fusion (ICF) and high energy density (HED) physics studies have been challenged, as measurement and computational modeling tools have been limited to capturing 1D and 2D representations of inherently 3D implosions.

It is well understood that 3D effects or perturbations can significantly change the interpretation of 1D and 2D data and can make comparisons of simulations difficult, challenging our ability to validate computational models.

In recent years, advances and investments in high performance computing (HPC) tools and codes have begun to enable full-scale, 3D modeling of capsule implosions. Unfortunately, such “hero” calculations are both challenging and expensive, limiting the number that can be delivered within a reasonable time frame.

The recent installation of a third neutron imaging line of sight at the National Ignition Facility at Lawrence Livermore National Laboratory, is a potential game changer for improving fusion performance. The additional line-of-sight measurement enables researchers to observe 3D structure and effects in fusion implosions for the first time. The ability to produce 3D tomographic images of the burning fuel during the thermonuclear burning phase of an implosion is an exciting development, enabling the visualization of performance-limiting asymmetries and hydrodynamic mix in fusion implosions.

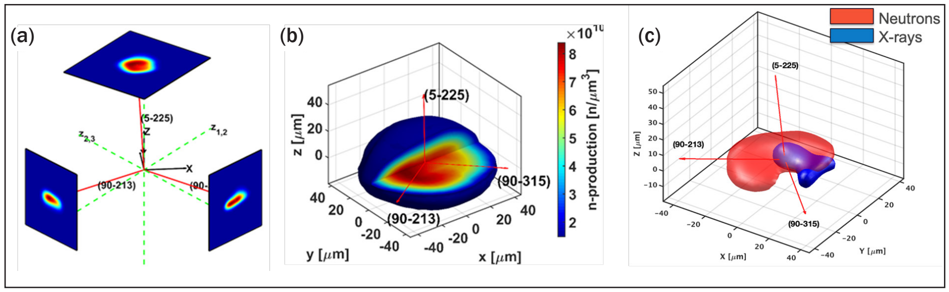

Figure 1. (a) Images of neutron flux density along three orthogonal lines of sight. (b) Reconstructed 3D density map of hot spot neutron production. (c) Combined neutron and X-ray (using two lines of sight) image showing the fill tube quenching fusion burn.

Figure 1 shows neutron measurement images from three independent lines of sight (a) along with the 3D reconstructed density map of neutron production (b). Even more spectacular is the image in (c) showing the 3D iso-contour of neutron production (red) along with a reconstruction of X-ray emission (blue) believed to be a jet of energetic material from the capsule’s fill tube. This image, correlating the 3D structure of the neutron production with X-ray data, provides direct evidence supporting the hypothesis that a portion of the fusion burn region is quenched by a jet of fill tube material resulting in the observed half-moon shape of the hot spot. More effort in co-registering the neutron and X-ray images is required in order to establish a more quantitative determination.

What does this mean for stockpile stewardship?

The image reconstruction algorithms being developed to recover 3D neutron images also can be applied to X-ray imaging, a work horse diagnostic for HED stockpile stewardship applications. This, combined with the development of single line-of-sight X-ray sensors, placed along three orthogonal lines of sight, will enable the eventual 3D reconstruction of critical experimental measurements. As a result, researchers will be able to account for 3D effects when comparing data from a single line of sight with numerical simulations. This will deliver tighter data constraints supporting model validation. For ICF, the ability to isolate the 3D character and structure of the hot spot will aid in distinguishing and quantifying performance degrading mechanisms, enabling researchers to design mitigation methodologies to improve implosion performance. Lastly, this new capability stands to provide critical quantitative measurements of mix in the presence of fusion burn, directly supporting stockpile stewardship.

Researchers include Petr Volegov, Christopher Danly, Verena Geppert-Kleinrath, Frank Merrill, Carl Wilde (all Neutron Science and Technology, P-23), Valerie Fatherley, Steve Batha, Michael Springstead, John Oertel (Plasma Physics, P-24), Derek Schmidt, Lynn Goodwin, John Martinez (Engineered Materials, MST-7), Justin Jorgenson (Process Automation & Control, E-3), Doug Wilson (Plasma Theory and Applications, XCP-6), and David Fittinghoff, Gary Grim, Robin Hibbard, Cory Waltz, Sebastien Le Pape, Arthur Pak, Laurent Divol, Laura Berzak Hopkins (Lawrence Livermore National Laboratory).

For more information, contact Petr Volegov at volegov@lanl.gov or 505-665-1029.

This work was funded by the National Nuclear Security Administration Office of Experimental Sciences under the Los Alamos National Laboratory Inertial Confinement Fusion Program. ◆