Winter 2018

Mesoscale Connections

Science and technology on the roadmap to MaRIE

INSIDE

Los Alamos NATIONAL LABORATORY EST.1943

Arianna Gleason makes final adjustments to detector positions inside the Matter in Extreme Conditions target chamber at SLAC in California.

Arianna Gleason

Harnessing high-energy x-rays to examine materials in extremes

By H. Kris Fronzak, ADEPS Communications

> *"Los Alamos's mission and national security questions are very motivating to me. I'm working on basic R&D in how materials behave under extreme conditions and linking new technology to the Lab's mission-related objectives."*

Arianna Gleason distinguished herself as a planetary scientist early. She discovered an asteroid and a comet during her undergraduate years studying extreme cosmic phenomena at the University of Arizona. Now the Los Alamos National Laboratory Reines Distinguished Postdoctoral Fellow focuses her passion for exploring the changes wrought by extreme forces by illuminating materials at the mesoscale using the Linac Coherent Light Source (LCLS).

For example, Gleason (Shock and Detonation Physics, M-9) and colleagues used the LCLS at SLAC National Accelerator Laboratory to observe for the first time how a meteor-like impact compresses silica, one of Earth's most abundant minerals, into glass. The research, published in *Nature Communications*, has important fundamental science implications, including understanding how extreme impacts deform rock. To read more about this discovery, please see page 4.

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Mesoscale Connections

is published by the Associate Directorate for Experimental Physical Sciences, which is the Laboratory's champion for the Materials for the Future science pillar. The goal of *Mesoscale Connections* is to promote awareness of mesoscale materials research relevant to the NNSA, advances in mesoscale science capabilities at user facilities, and modeling challenges and needs for big data sets in service of materials co-design. For information about mesoscale materials science at Los Alamos, please contact materials@lanl.gov. For information about the publication, contact adeps-comm@lanl.gov.

*The **mesoscale** is the spatial scale that exists between atomic structures and the engineering continuum—critical to controlling macroscopic behaviors and properties.*

MaRIE is an experimental facility concept that could address an NNSA capability gap identified in a 2016 CD-0 for simultaneous characterization of microstructure and response at the mesoscale.

Gleason cont.

The ultrafast imaging supplied by LCLS, the first free-electron laser in the world to produce very high-energy x-rays, provides an ideal way to make these observations of the mesoscale—the critical "middle scale" that greatly influences a material's macroscopic behaviors and properties.

"My work on the LCLS is a natural extension and complement to my earlier work in static compression. It timed well with the blossoming of the light source technology," said Gleason. She has used the LCLS for her high-pressure materials studies since it first went online in 2009, employing its novel capabilities to complete her PhD in earth and planetary science at the University of California, Berkeley in 2010. Gleason received a National Science Foundation Graduate Research Fellowship to study high pressure material elasticity in 2004 and joined Los Alamos in 2015, drawn by a desire to contribute to national security science.

"Los Alamos's mission and national security questions are very motivating to me," she said. "I'm working on basic R&D in how materials behave under extreme conditions and linking new technology to the Lab's mission-related objectives."

At LCLS, where Gleason is stationed, her day-to-day work involves crafting and characterizing targets for experiments on the LCLS Materials in Extreme Conditions end-station that support the National Nuclear Security Administration's (NNSA) Dynamic Materials Properties Science Campaign. She also collaborates with Theoretical Division researchers to develop kinetics models of how materials transform under extreme conditions. She has two grants; one investigating iron deformation at Earth's core conditions and another examining iron's strength over a suite of strain rates, temperature, and pressure.

Gleason, who is mentored by Cindy Bolme (M-9) and Wendy Mao (Stanford University), is an adjunct professor at Stanford University and was recently elected vice chair of the LCLS users' executive committee. Her honors include the 2016 Gordon Research Conference on High Pressure's Alvin Van Valkenburg Award and the American Geophysical Union's Early Career Award in Mineral and Rock Physics.

Gleason is actively looking to the future of dynamic materials mesoscale science using high-power light sources. Her experience at LCLS is helping to build an arsenal of knowledge that will benefit Los Alamos mesoscale research. "With a little creativity and some elbow grease we can answer questions about the next generation of light sources and optimize experiments on behalf of Los Alamos," she said.

She is particularly excited by the potential for research that could be enabled by MaRIE, the Lab's proposed capability for time-dependent materials science at the mesoscale. MaRIE would fulfill an NNSA national security need for simultaneous characterization of microstructure and response at the mesoscale. For example, it would enable researchers to make predictive models after seeing precisely how long it takes for a single atom to break a bond and reform into a new pressure phase or to tune a material's strength through the perfect combination of properties.

"MaRIE is the next big thing in visualizing materials changes," she said, adding it would enable work critical to the nation's national security needs "and help people in many disciplines to do outstanding science."

Mesoscale science's essential role in maintaining a safe, secure nuclear deterrent

The nation's Stockpile Stewardship Program is designed to provide predictive capabilities for weapons performance in the absence of nuclear testing. More than 20 years of effort have dramatically expanded understanding of weapons physics and the materials that make up the stockpile. However, as we look at future challenges in the stockpile it is clear we must make continued progress to understand many areas of weapon science that remain poorly understood. As weapons continue to age and as new manufacturing processes are employed, we must continue to assess the impacts on weapons performance.

This is where mesoscale materials science is critical. This "middle scale," between the atomic and integral scales, is key to understanding and controlling many of a material's properties and its performance. To date, there is a "knowledge gap" in stockpile stewardship science at the mesoscale.

Many of the key uncertainties that remain in understanding weapon safety and performance are related to our lack of understanding certain material properties, especially dynamic properties. Examples include material strength, compressibility, and explosive initiation and burn. Understanding how these properties change, especially in either aging materials or as a result of alternate manufacturing processes, is a critical element of certification in the era of stewardship. These properties derive from the response of materials at the mesoscale: the scale larger than the unit cells of atoms in a crystal but below the bulk scale where integrated experiments are conducted. It is at the mesoscale where microstructure, defects, interfaces, and inhomogeneities in materials manifest, and these same features are responsible for such material properties as strength and dynamic response. Microstructure is important because it determines the material's macroscopic engineering properties, such as strength and stability under heat and pressure as well as the elastic properties in engineering components and how they stand up over time.

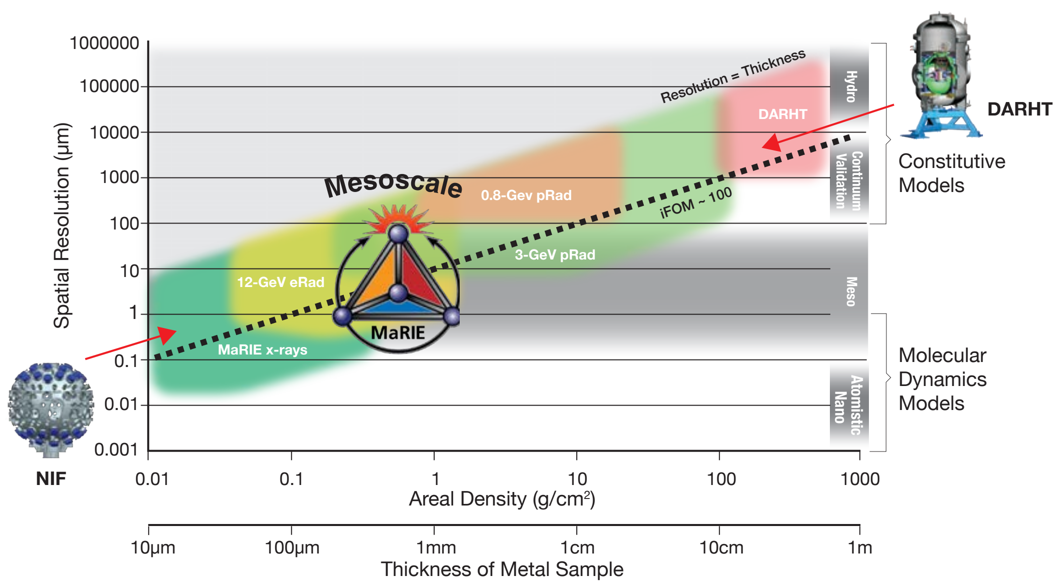
This scale lies between the integral scale measured at facilities such as the Dual-Axis Radiographic Hydrodynamic Test Facility (DARHT) at Los Alamos National Laboratory and the atomic scale, which is evaluated on facilities such as the National Ignition Facility (NIF) at Lawrence Livermore National Laboratory or the Z Pulsed Power Facility operated by Sandia National Laboratories. We currently lack an experimental capability to resolve materials response at this scale with the ability to characterize interfaces, defects, and microstructure between the spatial scales of atomic structures and those of the engineering continuum.

Our models in materials science, and especially those in stockpile stewardship, have largely been based on bulk or homogeneous properties of materials. They have been fitted to available test data and are only known to be valid within narrow ranges of parameters and regions of physical behavior. The development of predictive models requires that the physics of microstructural heterogeneities at the mesoscale be included. Many physical responses, such as phase transitions and deformation, remain exceedingly challenging to model with this approach. They require much more data and imaging of materials, especially under dynamic conditions, to elucidate the actual mechanisms

To address these challenges of understanding—and ultimately controlling—materials behavior under extreme conditions requires the ability to observe mesoscale phenomena under dynamic loading at picosecond temporal resolution.

Los Alamos National Laboratory has proposed the MaRIE (Matter-Radiation Interactions in Extremes) capability for characterizing the behavior of interfaces, defects, and microstructure between the spatial scales of atomic and engineering. MaRIE will provide the ability to offer time-dependent control of material processes, structures, and properties during manufacture and production. Experimental characterization will be complemented by capabilities in synthesis and fabrication and will be integrated with advanced theory, modeling, and computational tools.

Below: the imaging figure-of-merit (iFOM), the ratio of the size of the field-of-view over the spatial resolution, defines a band of spatial scales that can be effectively diagnosed at any given size or scale of experiment.



Mechanisms behind silica's transformation to dense glass have high-impact implications

First-ever observation calls for revising traditional shock metamorphism stages

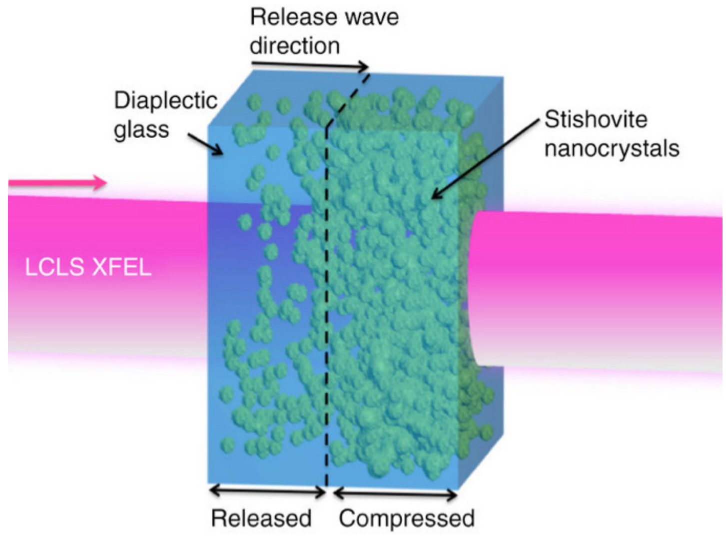
Understanding how rock-forming minerals transform under shock loading is critical for modeling collisions between planetary bodies, determining the meaning of shock features in minerals, and for using these minerals as diagnostic indicators of impact conditions. Historically, understanding shocked materials' formation processes was based only on ex situ and post mortem analyses of recovered samples. As a result, formation mechanisms and origins of commonly observed mesoscale material features, such as shocked glass found at many meteor impact sites, have been controversial and unresolvable. This is in part due to the fact that the mineral's final state depends upon the specific timing and pressure of phase transformations in these extreme conditions.

Using the novel capabilities of the Matter in Extreme Conditions (MEC) end-station at SLAC National Accelerator Laboratory's Linac Coherent Light Source, a Los Alamos-led team observed for the first time how shocked, fused silica crystallizes into dense glass (stishovite) and its conversion to an amorphous phase upon shock release. This work was recently published in *Nature Communications*. Glass fragments recovered after meteor impact suggested permanent densification for many minerals. The information gleaned from these new observations has implications for revising traditional shock metamorphism stages.

The in situ pump-probe x-ray diffraction measurements show this conversion happening in only 2.4 ns from 33.6 GPa, a lower pressure than previously thought to result in shocked glass, and that a thermal instability is the cause of the reversion.

Combining ultrafast light pulses with atomic resolution, next-generation light sources such as the LCLS allow researchers to explore the mesoscale, the "middle" scale where imperfections, defects, and heterogeneities are critical to controlling macroscopic behaviors and properties.

Los Alamos's proposed Matter-Radiation Interactions in Extremes (MaRIE) capability for time-dependent materials science at the mesoscale would provide a unique tool to study materials under extreme conditions and to interrogate complex materials in non-crystalline forms with high spatial and temporal resolution measurements on a single target. MaRIE would allow researchers to visualize the entire transformation process during the passage of a shock event in a single target with even longer timescales and multiple shock driver platforms.



Target schematic for sample during the shock-release process. During the onset of release, newly formed grains of stishovite (green sphere-like features) dissolve over a few nanoseconds, leaving behind diaplectic glass.

Researchers include Arianna E. Gleason (Shock and Detonation Physics [M-9] and SLAC National Accelerator Laboratory); Cindy A. Bolme (M-9); H. J. Lee, B. Nagler, and E. Galtier (SLAC); R. G. Kraus (Lawrence Livermore National Laboratory); Richard Sandberg (Center for Integrated Nanotechnologies, MPA-CINT); W. Yang (Center for High Pressure Science and Technology Advanced Research, Shanghai, and Carnegie Institution of Washington); F. Langenhorst (Friedrich Schiller University Jena, Germany); and Wendy L. Mao (Stanford University and SLAC).

Gleason was supported by the National Science Foundation Geophysics Program and the Los Alamos Laboratory Directed Research and Development Program via a Reines Distinguished Postdoctoral Fellowship. The work supports the Laboratory's Nuclear Deterrence mission and its Materials for the Future science pillar.

Reference: "Time-resolved diffraction of shock-released SiO_2 and diaplectic glass formation." *Nature Communications* **8**, 1481 (2017).

Technical contact: Arianna Gleason

Nanoindentation explains plasticity and shear stress for fragile molecular crystals

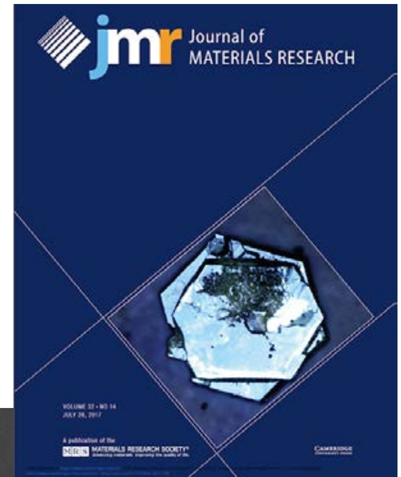
Los Alamos and Purdue University researchers used nanoindentation (indentation hardness tests applied to small volumes) to uncover new insights into the plasticity of organic molecular crystals. Molecular crystals are a broad category of materials that include energetics, foods, nonlinear optics, and pharmaceuticals. Understanding deformation in these crystals could lead to improved energetic materials and pharmaceuticals. The *Journal of Materials Research* featured their study on its cover.

The researchers aimed to quantify the mechanical properties of a selection of pharmaceutical and energetic molecular crystals with minimal processing. The goal was to broadly define the window of plasticity for multiple molecular crystal structures and determine if the onset of plasticity in these materials is particularly sensitive to structure. Demonstrating the utility and accuracy of the nanoindentation technique on materials for which data can be compared to accepted measurements using minimally processed samples provides a method to obtain properties for which no experimental data has previously been available. Their results provide guidance for mechanical models of tableting, machining, and property assessment for molecular crystals.

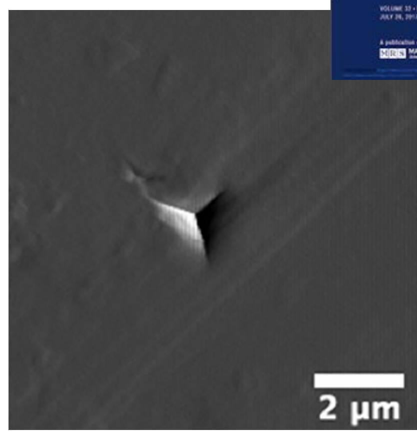
Most molecular crystals have noncubic structures. The formability of powders into tablets is often evaluated using qualitative or semiquantitative mechanical properties such as compactibility and brittleness, which are related to industrial processes like comminution (reduction to minute particles). Understanding these materials' quantifiable mechanical properties is important for engineering molecules for optimal performance, but such measurements are difficult to make for low-symmetry, fragile molecular crystals.

The team used nanoindentation to assess elastic and plastic properties of representative monoclinic, orthorhombic, and triclinic molecular sub-mm crystalline structures. The research determined that the variation in modulus due to in-plane rotational orientation is about equal to the variation of a given crystal at a fixed orientation. The onset of plasticity occurred consistently at shear stresses between 1-5% of the elastic modulus in all three crystal systems, and the hardness-to-modulus ratio suggested that conventional Berkovich tips (a three-sided pyramid that is geometrically self-similar) do not generate fully self-similar plastic zones in these materials.

Plastic deformation in organic crystalline compounds is far-reaching in terms of downstream processing and ultimately performance in energetic and pharmaceutical applications. Mechanical stresses applied during processes (e.g., milling and compaction) can lead to changes in dissolution or thermomechanical behavior. Assessing the properties of small powders of molecular crystals in their as-produced form helps explain ambiguous properties while providing microstructure-based insight to performance differences where defects such as dislocations could be present. Understanding the behaviors of as-produced materials is fundamental to predicting responses of real materials from mesoscale understanding. The mesoscale, or the "middle" length scale, is often critical to controlling the performance of materials. These crystals, in the form tested, are exactly what are formulated into pharmaceutical tablets and plastic-bonded explosives. This fundamental research into the mechanics and fundamental properties of materials can lead to materials with altered properties that respond differently, thereby achieving controlled functionality, a central vision of the Laboratory's Materials Strategy.



Cover of the *Journal of Materials Research,* which features an optical microscopy image of the energetic material TATB after surface layer removal.



Representative AFM gradient residual indent impression of an indent in the energetic material HMX showing no signs of surface cracks.

Reference: "The mechanical properties of as-grown noncubic organic molecular crystals assessed by nanoindentation," *Journal of Materials Research* **14**, 2728 (2017). Authors: Matthew R. Taw, Teresa M. Carvajal, and David F. Bahr (Purdue University); John D. Yeager (High Explosives Science and Technology, M-7), and Daniel E. Hooks (Sigma Division, Sigma-DO).

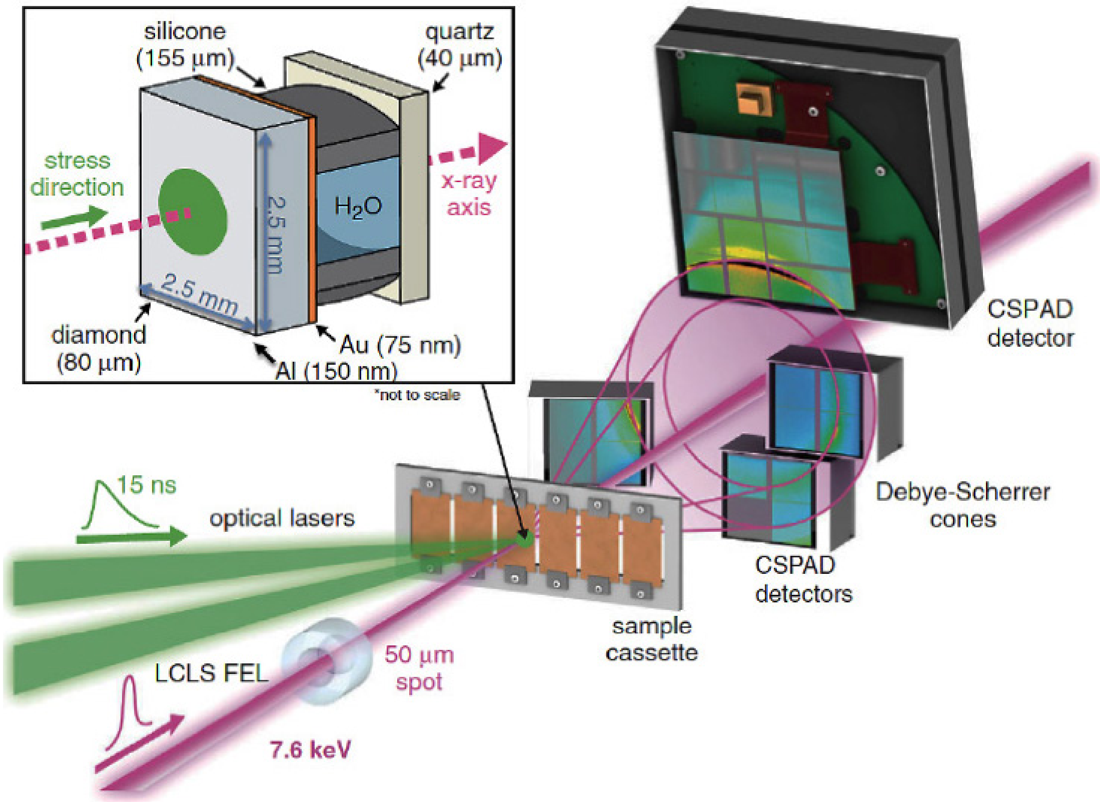
NNSA Campaign 2 (Dana Dattelbaum, LANL program manager) funded the Los Alamos work, which supports the Lab's Nuclear Deterrence and Global Security mission areas and the Materials for the Future science pillar. The explosive crystals used in the study were grown at the Laboratory.

Technical contact: Dan Hooks

Advanced lasers simulate extreme environment of icy satellite impacts

Researchers used the high-brightness, short-pulse Linac Coherent Light Source at the SLAC National Accelerator Laboratory to simulate and image in real time the extreme environment of liquid water shock freezing into ice. *Physical Review Letters* published the research and highlighted it as an "Editor's Suggestion."

Water is one of the most abundant molecules in the Universe. Under the conditions on Earth, ice primarily exists in hexagonal crystal found in glaciers and snowflakes. This form of ice is denoted as ice Ih. The new research revealed the unexpectedly swift transformation of water into high pressure crystalline ice phase VII—a dense ice phase found in the interiors of icy satellites.



Schematic of the Matter in Extreme Conditions target chamber at SLAC. Green beams are the drive laser used to generate the shock wave, while the pink beam (x-rays) probes the changes in the sample's atomic structure. The XRD is recorded downstream of the sample (black arrow). Inset: Schematic of the target package as a cutaway side view.

Although pressure- and temperature-induced phase transitions have been studied for more than a century, little is known about the non-equilibrium processes by which the atoms rearrange. Shock compression, the fastest mechanical loading that can be applied to a material, generates a rapidly propagating high-pressure/temperature condition. In situ x-ray diffraction (XRD) can probe the time-dependent atomic rearrangement that occurs.

The researchers beamed an intense laser at a small target containing a sample of liquid water. The laser instantly vaporized layers of diamond on one side of the target, generating a force that compressed the water to pressures exceeding 50,000 times that of Earth's atmosphere at sea level. As the water compacted, a separate beam from the x-ray free-electron laser arrived in a series of bright pulses only a femtosecond long.

The strobing x-ray laser snapped a set of XRD images revealing the progression of molecular changes while the pressurized water crystallized into ice VII. The phase change took just 6 nanoseconds and revealed a fundamental disorder-to-order transition. The water molecules initially crystallized into needle shapes and not spheres as theory

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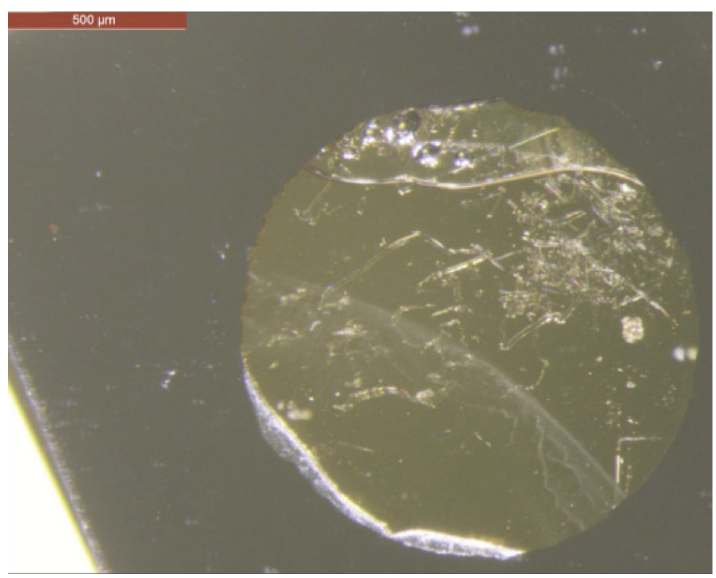


A circular water layer sandwiched between a diamond platelet coated with gold and a quartz platelet. The water layer transforms into ice VII after being blasted by an intense green laser.

Advanced lasers cont.

had predicted. These are the first femtosecond-long XRD observations of the shock freezing of water.

The findings may help refine thermodynamic models for solid-liquid phase transitions. These results could lead to a greater understanding of important problems in shock physics and materials science and potentially refine planetary models providing insight for the impact history of the solar system. The new experimental approach advances the study of phase transition kinetics, enabling the design of new materials with improved functionality.

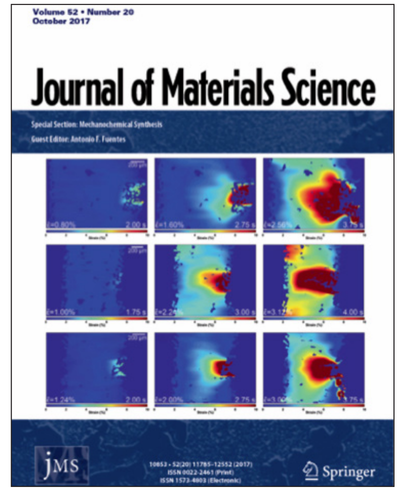
In situ XRD, such as available at the Linac Coherent Light Source and planned at the center of MaRIE (Matter-Radiation Interactions in Extremes), LANL's proposed experimental capability for time-dependent materials science at the mesoscale, provides a unique tool to study materials under extreme conditions. MaRIE would take this research further by allowing structural determination of non-crystalline materials and by performing the time-dependent measurements on a single shock event. Additional dynamic drivers could enable longer time measurements of the crystallization dynamics near the phase boundaries.

Reference: "Compression freezing kinetics of water to ice VII," *Physical Review Letters* **119**, 025701 (2017). Authors: Arianna Gleason (Shock and Detonation Physics [M-9] and SLAC National Accelerator Laboratory), Cindy Bolme (M-9), E. Galtier, H. J. Lee, and E. Granados (SLAC National Accelerator Laboratory); D. H. Dolan, C. T. Seagle, and T. Ao (Sandia National Laboratories); S. Ali, A. Lazicki, D. Swift, and P. Celliers (Lawrence Livermore National Laboratory); and W. L. Mao (SLAC National Accelerator Laboratory and Stanford University).

The Laboratory Directed Research and Development Program sponsored the Los Alamos work, and a Reines Distinguished Postdoctoral Fellowship funded Gleason. The research supports the Lab's Nuclear Deterrence mission area and the Materials for the Future science pillar by demonstrating a strategy and methodology to extract phase transition kinetics using time-resolved x-ray diffraction data. Learning to manipulate those transitions might open the way to engineer materials with exotic new properties for useful applications.

Technical contact: Arianna Gleason

New technique breaks materials while collecting 3D x-ray images



The cover of the *Journal of Materials Science* highlighted the in situ x-ray tomographic imaging technique.

Engineered Materials (MST-7) researchers and colleagues developed a novel in situ x-ray tomographic imaging technique to collect high-rate, three-dimensional (3D) images while breaking materials. The team used the x-ray beamline at Argonne National Laboratory's Advanced Photon Source to collect 20 full 3D x-ray images within 5 seconds. This new technique could enhance scientists' understanding of materials' deformation and failure. The *Journal of Materials Science* featured the work on its cover.

A collaboration between Los Alamos, Arizona State University, and Argonne investigated how advanced materials respond to uniaxial mechanical loading. The team used x-ray computed microtomography and digital volume correlation to examine tensile behavior of an additively manufactured polymer matrix composite. The researchers tested a 3D-printed tensile dog bone made of a polymer-glass composite. The specimen was clamped within a mechanical load cell and pulled apart while the force response was measured. Simultaneously, the dog bone was rotated at 2 Hz within the synchrotron beam while researchers took thousands of x-ray radiographs. The investigators reconstructed the radiographs to create a series of 3D images. Linking 3D images and load response allowed visualization of each of the processes that govern failure, including crack formation and propagation and the elastic response of the material.

The researchers also investigated the role of print direction and recycled material upon the mechanical properties. The study revealed significant variations on both strength and ductility with respect to print direction and the recycled material content in the printed parts. The addition of recycled source material with a thermal history reduced the tensile strength of the additively manufactured composite for all directions. The effect was drastic on the strength in the layering direction.

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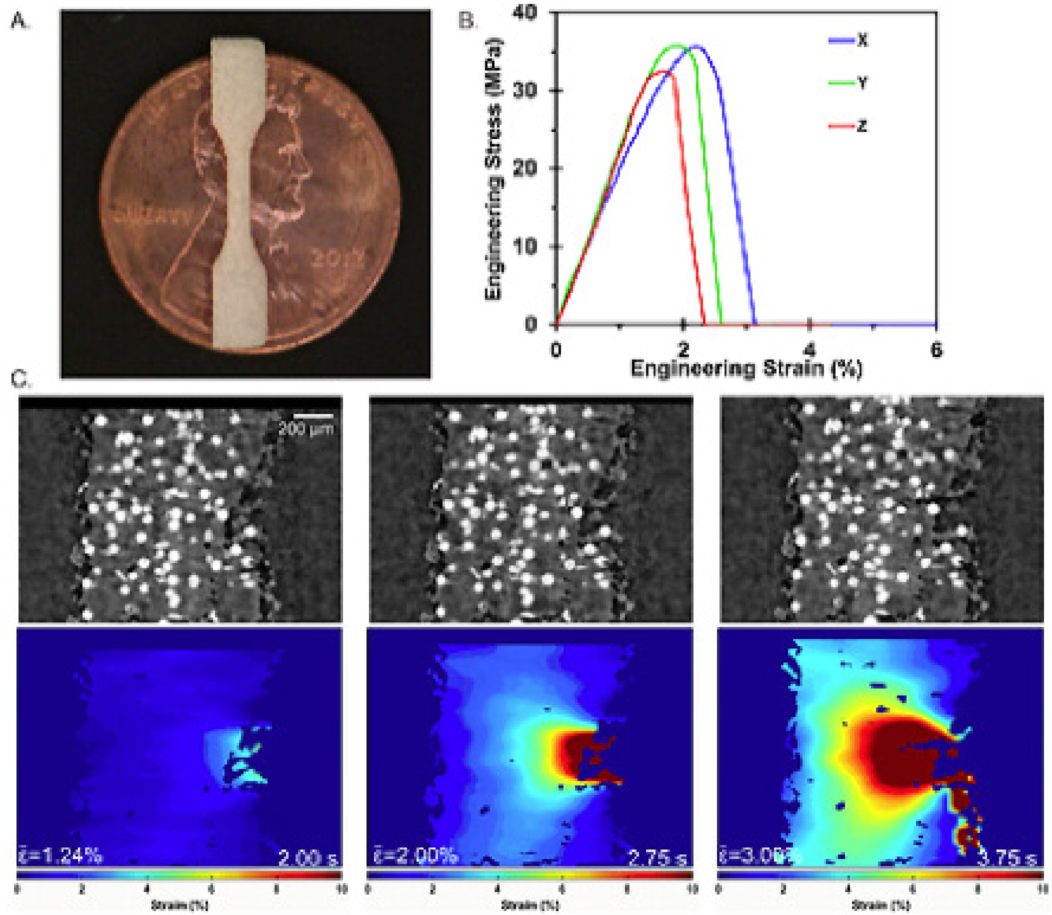
New technique cont.



A) Photograph of the 3D-printed tensile specimen (dog bone),
B) Stress-strain curve during the tension experiment, and
C) 3D-reconstructed slices and digital volume correction strain maps through a specimen as it is pulled apart. The crack propagation is visible midway down the slices.

Because the 3D imaging takes place while the material is being loaded, this method could provide insight into deformation and failure in materials. This multi-institutional collaboration has increased the imaging rate beyond the demonstrated 4-14 Hz in the publication. Future work will seek to increase the 3D imaging to 100 Hz, creating images critical to material model development and validation.

MaRIE, the Lab's proposed experimental capability for studying matter-radiation interactions in extremes, could enable researchers to take this research further. The combination of MaRIE's unique hard x-ray free-electron laser and in situ characterization tools could enable measurements that are dynamic, in situ, and multi-modal. Such measurements are critical to observe the sequential phenomena of composite mesoscale materials and could reveal properties that matter at the "middle" length scale that may be essential to controlling the performance of materials.

Reference: "Analysis of thermal history effects on mechanical anisotropy of 3D-printed polymer matrix composites via in situ x-ray tomography," *Journal of Materials Science* **52**, 12185 (2017). Authors: James C.E. Mertens (formerly MST-7, now at Intel); Brian M. Patterson, Kevin Henderson, and Nik Cordes (MST-7); Robin Pacheco (Sigma Division, Sigma-DO); Xianghui Xiao (Argonne National Laboratory); and Jason J. Williams and Nikhilesh Chawla (Arizona State University).

The NNSA Enhanced Surveillance Campaign (Tom Zocco, Los Alamos program manager), the Engineering Campaign (Antranik Siranosian, Los Alamos program manager), Directed Stockpile Work (Jennifer Young, Los Alamos program manager), and Technology Maturation (Ryan Maupin, Los Alamos program manager) funded the technology development. The work supports the Lab's Nuclear Deterrence mission and its Materials of the Future and Science of Signatures science pillars.

Technical contact: Brian M. Patterson

Spotlight on people

Brian Jensen: Expanding the impact of dynamic materials research

Strengthening shock physics research by connecting the dynamic materials community

Brian Jensen is an energetic advocate for the ability of high-energy x-rays to better understand materials at extremes. As Los Alamos National Laboratory's point-of-contact for the Dynamic Compression Sector (DCS) at Argonne National Laboratory, he coordinates the Lab's dynamic compression activities at Argonne, conducts research in shock physics and other mission-relevant programs, and promotes opportunities for dynamic materials research using DCS. A team leader in Shock and Detonation Physics (M-9), Jensen has been lending his expertise in high pressure and shock physics to DCS users since 2010.

A newly developed National Nuclear Security Administration (NNSA)-funded capability operated by Washington State University, DCS combines impact and laser-shock facilities, x-ray detectors and diagnostics, and traditional optical diagnostics with a dedicated x-ray beam line at Argonne to produce in situ, time-resolved measurements of materials under dynamic compression. The DCS user program offers capabilities that include two single-stage gun systems, a two-stage gun system with impact velocities exceeding 6 km/s, a 100-J laser drive system, advanced x-ray diagnostics, and a standard suite of shock physics diagnostics.

Using the capabilities at DCS, the Mechanisms of Initiation team, which includes Jensen, received a Laboratory 2016 Small Team Distinguished Performance Award for discoveries in the complex physics of bridge burst and flyer performance, which have resulted in innovative detonator designs. That same year, the team received an NNSA Defense Programs Award of Excellence for development of the multi-frame x-ray phase contrast imaging (MPCI) detector system, which provided the first shock-movies of materials at extremes using x-ray PCI.

As part of the DCS user program, researchers are invited to propose experiments using Los Alamos's Collaborative Access Team (CAT) beam time. Additional capabilities provided to CAT members include a Kolsky bar, a small explosive vessel, and the IMPULSE (Impact System for Ultrafast Synchrotron Experiments) mobile gas gun. In 2011, Jensen led the development of IMPULSE, an award-winning, NNSA-funded platform for making imaging measurements with small quantities of explosives. Through a grassroots interest in IMPULSE's capabilities, Jensen, who earned his PhD in physics from Washington State University, built a network of dynamic materials researchers that use IMPULSE and Los Alamos's novel MPCI system to image material response and study a wide range of phenomena: jet formation in metals, crack nucleation and propagation, damage and spall, and compaction of granular materials.

Jensen's collaborations with this community and his ongoing work to develop DCS's user base have informed his efforts to help shape MaRIE, the Laboratory's proposed capability to observe materials under extreme conditions at the mesoscale. Recently, Jensen collaborated with postdoctoral researcher Anbirban Mandal (M-9) to develop a novel experiment configuration consisting of a cylindrical powder cell that dynamically compresses granular materials—a tool that may influence MaRIE's design for similar experiments. The pair is testing the configuration under high pressure using lunar and martian soil simulants, nickel, and aluminum.

Jensen already has plans for taking advantage of MaRIE's capabilities. "I'm excited at the possibilities of using x-ray diagnostics such as those proposed by MaRIE to be able to shock a polycrystalline metal and to 'watch' the microstructure evolve in real time as it compresses, fails, and transforms from one phase to another," he said.

Technical contact: Brian Jensen

Carlsten, Sheffield, Nguyen win Free-Electron Laser Prize

At an international science conference held in Santa Fe, New Mexico, Los Alamos scientists Bruce Carlsten (Engineering Sciences ADE), Richard Sheffield (Experimental Physical Sciences, ADEPS), and Dinh Nguyen (Accelerators and Electrodynamics, AOT-AE) received the 2017 Free-Electron Laser (FEL) Prize. The honor is an international recognition of key technologies that originally developed at Los Alamos in the 1980s and 1990s, such as the radio frequency photoinjector and high-brightness electron beams. These innovations also have enabled the x-ray free-electron laser facilities currently in use worldwide. FELs involve techniques and materials central to the Lab's mission. Notably, this advanced light source technology is central to the Laboratory's proposed future flagship experimental science capability, MaRIE.

Dynamic materials science community offers recommendations for MaRIE instrumentation and R&D

The MaRIE Extreme Environments and Driver Technologies Workshop brought together experts in the dynamic materials community.

More than 60 experts in dynamic materials science from around the world gathered in August to discuss the science requirements and resulting technologies needed for the proposed Matter-Radiation Interactions in Extremes (MaRIE) project.

MaRIE fulfills a National Nuclear Security Administration (NNSA) national security mission need for the ability to understand and test how materials' structures, defects, and interfaces determine performance of materials in extreme environments. MaRIE Extreme Environments and Driver Technologies Workshop participants considered the technologies, examined possible design issues, and identified critical research and development efforts needed to drive materials samples into the relevant extreme conditions, and thus ensure project success. The end result of the workshop will be a milestone report that recommends a path forward both for the facility's design and for investments at present facilities.

MaRIE will simultaneously characterize materials' microstructure and response at the mesoscale, filling a gap between the integral scale addressed by hydrotest facilities such as the Los Alamos Dual-Axis Radiographic Hydrodynamic Test Facility and the Nevada National Security Site's U1A complex, and facilities for materials phenomena at small scale such as Lawrence Livermore National Laboratory's National Ignition Facility and Sandia National Laboratories' Z Pulsed Power Facility. Many of the remaining uncertainties in our assessment of materials arise from uncertainties in properties governed at this mesoscale.

Workshop sessions were devoted to discussing current and planned capabilities at existing facilities and additional challenges for the MaRIE capability such as those related to higher-energy-density materials, plasmas, and hydrodynamic flow. The event featured two sets of breakout sessions. One focused on MaRIE scientific requirements for studies of metal alloys, high explosives and heterogeneous materials, hydrodynamics and turbulent flow, and high-energy-density physics. The second set of breakouts helped define the technical functional requirements and possible design requirements for MaRIE driver technology, including lasers, pulsed power, and more "classic" technologies such as high explosives and gas and powder gun flyers.

Organizing committee members were Gilbert "Rip" Collins (University of Rochester), John Benage (Sandia National Laboratories), Jon Eggert and Rick Krauss (Lawrence Livermore National Laboratory), and from Los Alamos David Moore (Nuclear Materials Science, MST-16), Cris Barnes (MaRIE), Lucy Maestas (Associate Directorate for Experimental Physical Sciences, ADEPS), and Peggy Vigil (Government Affairs and Protocol, GAP).

The event, held at Buffalo Thunder Resort in Santa Fe, New Mexico, was attended by representatives from international research institutions, NNSA, Department of Energy national laboratories, academia, and military research facilities.

Technical contact: Cris Barnes

Confronting the challenge of keeping pace with big data from next-gen light sources

Participants in the recent workshop on computational workflows for x-ray science. Photo credit: Dawn Harmer (SLAC)

The advent of new light sources with advanced computing capabilities has resulted in an overwhelming amount of data that must be analyzed to take advantage of the sophistication of these tools and to enable scientific discovery.

To explore ways to accelerate that analysis, Los Alamos researchers recently joined global colleagues in a workshop on computational workflows for x-ray science. Organized by Christine Sweeney (Applied Computer Science, CCS-7), Hari Krishnan (Lawrence Berkeley National Laboratory), James Sethian (University of California, Berkeley), and Chuck Yoon (SLAC National Accelerator Laboratory), the event was one of several parallel workshops held at the Stanford Synchrotron Radiation Lightsource (SSRL) and Linac Coherent Light Source (LCLS) Annual Users Meeting in California.

A beam line workflow combines tasks completed by scientists, beam line instruments, and computers to enable data analysis. This workshop highlighted current novel beam line computational workflows and workflows that are being developed to more efficiently store, process, and interpret the vast amount of data produced at x-ray science user facilities. Techniques discussed included data manipulation, analysis and visualization, computational tools for collaboration between experimenters, and high-performance computing at a user facility or at a computing facility across a network.

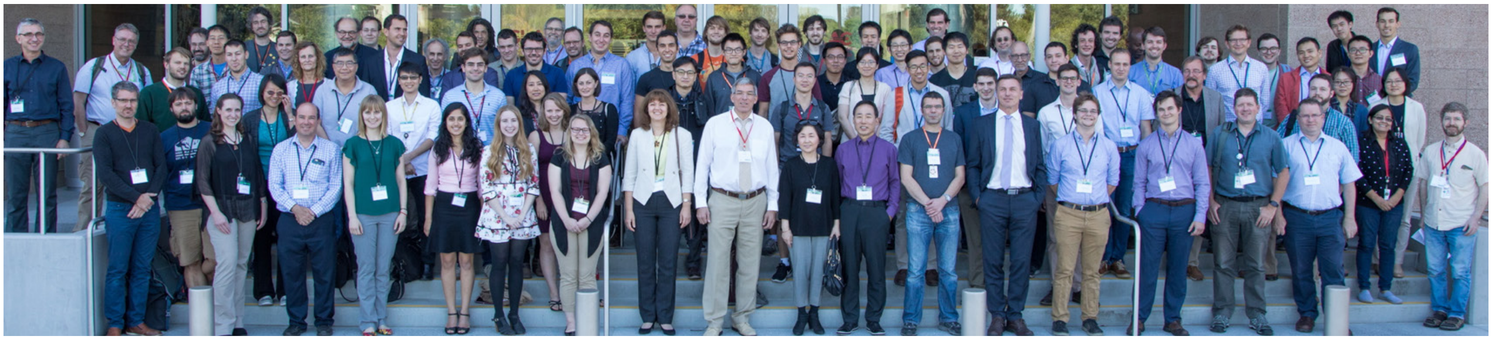
As part of the workshop, Richard Sandberg (Center for Integrated Nanotechnologies, MPA-CINT), the outgoing chair of the LCLS users' executive committee, spoke on "Tools for real-time adaptive acceleration of dynamic compression science at light sources." He and his colleagues propose to accelerate knowledge-discovery from experimental scientific facilities by combining computer and statistical science to produce an adaptive methodology and toolset to analyze data and augment a scientist's decision-making to optimize experiments in real time. Sandberg and his colleagues are developing this capability in dynamic compression experiments from x-ray light sources including LCLS and the Dynamic Compression Sector at Washington State University. When achieved, their approach, which can be applied to multiple scientific domains, will allow researchers to elevate their focus above the mundane tasks required for experiment completion to that of making strategic scientific decisions.

Also speaking were scientists from Lawrence Berkeley National Laboratory, SLAC's LCLS and SSRL, Uppsala University, and Brookhaven National Laboratory.

Light sources such as those at SLAC are enabling materials discoveries with their complex imaging technology and data production. MaRIE, the Laboratory's proposed experimental capability for understanding materials science at the mesoscale, would feature the world's highest energy x-ray free-electron laser with gigahertz repetition ability combined with advanced instrumentation and exascale computing systems capable of 10^{18} calculations per second. Improved computational workflows and data processing will be essential for MaRIE researchers, allowing them to take full advantage of the facility's capabilities and enable scientific discovery.

Technical contact: Christine Sweeney

Workshop explores opportunities for investigating matter in extremes with an ultrafast x-ray laser



Participants from the 5th High-Power Laser Workshop, held recently at SLAC. Photo credit: Dawn Harmer (SLAC)

The 5th High-Power Laser Workshop (HPL-5) was held recently at SLAC National Accelerator Laboratory in California, connecting members of the international high-energy-density physics community with those in SLAC's Linac Coherent Light Source (LCLS) user groups.

Held in conjunction with the general LCLS user meeting, the workshop (conf-slac.stanford.edu/hpl-2017) was organized by Cindy Bolme (Shock and Detonation Physics, M-9) and Siegfried Glenzer and Eric Galtier (both SLAC). The two-day event highlighted opportunities for studying matter in extreme conditions enabled by the combination of high-power laser drivers with the LCLS x-ray beam, in particular the LCLS Materials in Extreme Conditions instrument (MEC). Participants were encouraged to propose future standard configurations for the instrument and to discuss physics proposals and experimental needs for advances in cutting-edge research at MEC. Reports from previous workshops are available in *Synchrotron Radiation News*[1], and the report from this workshop will be available in a future issue.

Bolme, who uses the LCLS MEC for her Los Alamos materials studies, led a workshop discussion on the instrument's long-pulse laser and associated experimental systems. Kyle Ramos (HE Science and Technology, M-7) presented results from a recent experiment that used x-ray diffraction from the ultrafast LCLS x-ray laser to measure deformation and phase transitions in shock-compressed high explosives. LCLS is the only facility in the world where these experiments could be performed because its brilliant x-ray pulses were required to measure the response of the explosives before they were destroyed or chemically reacted. Richard Sandberg (Center for Integrated Nanotechnologies, MPA-CINT), the outgoing LCLS users' executive committee chair and an expert on coherent x-ray diffractive imaging, hosted a user discussion with SLAC x-ray facility directors.

Also presenting were researchers from the Department of Energy offices of Basic Energy Sciences and Fusion Energy Science, SLAC, Stanford University, European XFEL, SACLA, Helmholtz-Zentrum Dresden-Rossendorf, University of Edinburgh, Lawrence Livermore National Laboratory, Arizona State University, University of Oxford, Argonne National Laboratory, the Society for Science at User Research Facilities, University of Oklahoma, the Scripps Research Institute, and Hewlett Packard Enterprise.

Femtosecond x-ray free-electron lasers (XFEL), such as those at LCLS, SACLA in Japan, and the European XFEL, are an ideal tool for studying materials in extreme conditions, particularly at the mesoscale. The mesoscale is the spatial scale beyond the atomic, molecular, and nanoscale, where a material's structure strongly influences its macroscopic behaviors and properties. Understanding—and ultimately controlling—mesoscale properties presents tantalizing opportunities for revolutionizing the discovery, design, and application of new materials. However, probing and characterizing materials at the mesoscale is challenging, requiring advanced tools such as these next-generation light sources.

Los Alamos National Laboratory has proposed the development of the first very hard XFEL as part of its MaRIE capability. MaRIE will be used to study the dynamic properties of materials under extreme conditions for national security science missions. As a capability for time-dependent materials science on the mesoscale, MaRIE would fill a National Nuclear Security Administration need for simultaneous characterization of microstructure and response at this scale. More details about how Los Alamos researchers are using LCLS to study mesoscale materials science leading up to MaRIE can be found in journal articles describing experiments led by Arianna Gleason (Shock and Detonation Physics, M-9)[2,3] and experiments on which Los Alamos has collaborated with researchers at Lawrence Livermore National Laboratory, University of Edinburgh, and University of Oxford[4, 5].

Technical contact: Cindy Bolme

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2.“Ultrafast visualization of crystallization and grain growth in shock-compressed SiO_2,” *Nature Communications* **6**, 8191 (2015)
3. “Compression freezing kinetics of water to ice VII,” *Physical Review Letters* **119**, 025701 (2017)
4. “Ultra-fast x-ray diffraction studies of the phase transitions, equation of state and phase diagram of Shock-compressed scandium to 78 GPa,” *Physical Review Letters* **118**, 025501 (2017).
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Materials science university outreach workshop fosters research opportunities

The Materials Science and Technology (MST) Division hosted a two-day University Outreach Workshop on Nuclear Materials in Los Alamos's Materials Science Laboratory. Kimberly A. DeFriend Obrey (Materials Science in Radiation and Dynamics Extremes, MST-8) organized the event, which brought together Laboratory staff and professors from seven universities to discuss research opportunities and collaborations.

The event was the first in a planned series of workshops designed to form collaborations with key professors by offering their students internships at the Lab early in their graduate careers. The workshops also provided an opportunity for professors to conduct research at the Lab as guest scientists or through sabbatical appointments.

MST Division plans to host three more workshops: manufacturing science; damage, shock, and characterization; and polymer science. The Momentum Initiative, which the Associate Directorate for Experimental Physical Sciences (ADEPS) champions, funded the activity. The program sponsors the engagement of scientific communities to enhance the Laboratory's strategic partnerships, especially in the area of mesoscale science.

Presentations by experts in the field highlighted recent research, novel techniques, and unique capabilities. They included the following:

- Mechanical property evaluations on irradiated materials on multiple length scales, Peter Hosemann (University of California, Berkeley)
- Taming the plasma-material interface under reactor-relevant magnetic fusion condition, Jean Paul Allain (University of Illinois at Urbana – Champaign)
- Microstructural evolution in nuclear materials and fuel, Maria Okuniewski (Purdue University)
- Investigating radiation effects in materials by neutron total scattering, Maik Lang (University of Tennessee – Knoxville)
- Development of radiation-tolerant ferritic steels for fast reactor applications, Stu Maloy (MST-8)
- Development of high density fuels for light water reactors, Andy Nelson (Engineered Materials, MST-7)
- Atomistic modeling of nuclear materials–a survey, Blas Uberuaga (MST-8)
- Crystallographic modeling of irradiation growth and thermal creep in zirconium cladding, Carlos Tome (MST-8)
- Neutron scattering applications to nuclear materials, Alice Smith (Nuclear Materials Science, MST-16)
- Computational modeling of long-term kinetic processes in materials with atomistic insights, Donghua Xu (Oregon State University)
- Nuclear materials and fuels research at UF, Assel Aitkaliyeva (University of Florida)
- Multiscale modeling of radiation-induced microstructural evolution and physical property degradation in materials, David Bai (Virginia Tech)

The workshop included tours of the Ion Beam Materials Laboratory and the Electron Microscopy Laboratory in the Lab's Materials Science Complex. Laurent Capolungo (MST-8), Clarissa Yablinsky (MST-16), and Andy Nelson (MST-7) helped identify and engage professors for the event. Esther Palluck (MST-8) prepared visitor agreements, and Megan Espinoza and Angela Martinez (MST-8) managed logistics during the workshop.

Technical contact: Kim Obrey

Nuclear scientist Alice Smith (MST-16) works on the high-pressure/preferred orientation diffractometer (HIPPO) at the Lab's Lujan Center. She discussed neutron scattering applications for nuclear materials at the outreach workshop.