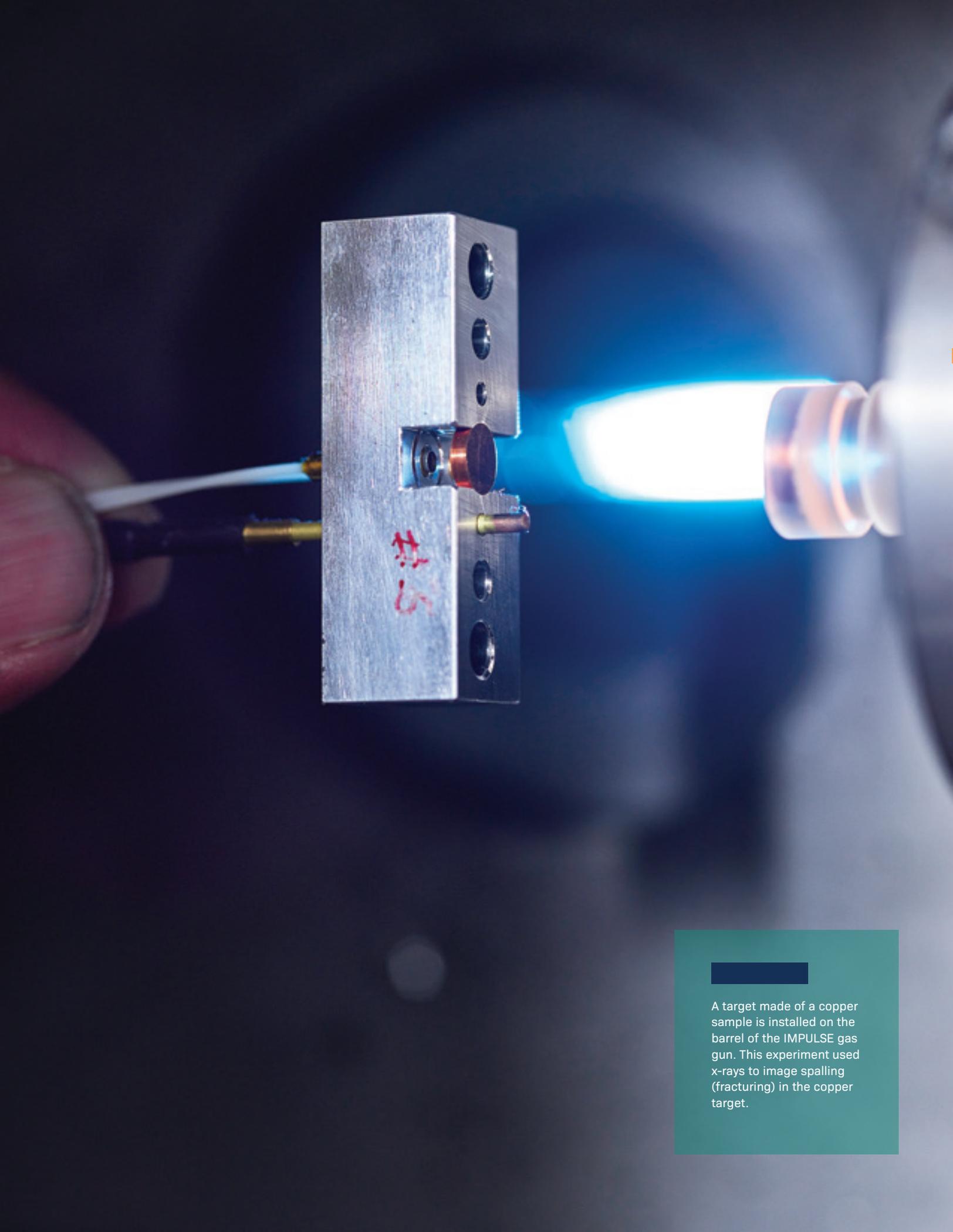


ENLIGHTEN

Advances in Mesoscale Dynamic Materials
Research & Development Through X-ray Light Sources



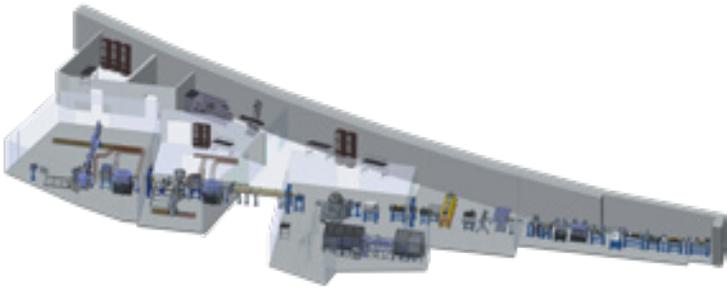
A target made of a copper sample is installed on the barrel of the IMPULSE gas gun. This experiment used x-rays to image spalling (fracturing) in the copper target.

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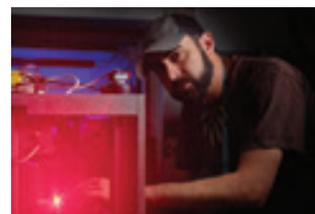
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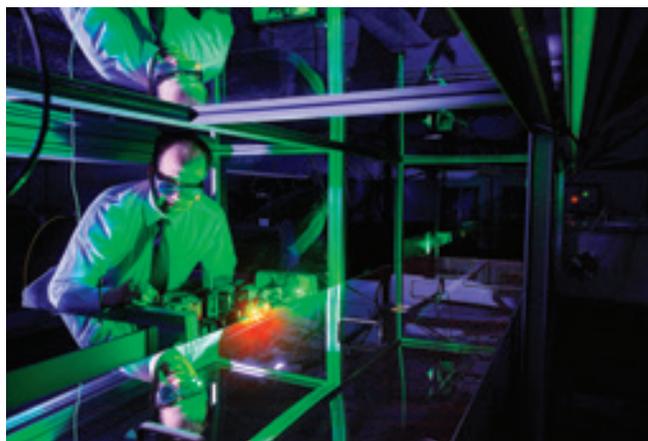
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Dana Dattelbaum inspects a liquid cell containing an electromagnetic gauge membrane for use in shock initiation experiments on liquid explosives.

INTRODUCTION

*“In the right light, at the right time, everything is extraordinary.”
– Aaron Rose*

DANA DATTELBAUM

The nuclear stockpile presents numerous challenging materials problems. Along the weapons lifecycle, from production to disassembly and from storage to delivery, the behavior and evolution of stockpile materials must be well understood. This understanding must include anticipating how material properties change with age, assessing complex interactions of co-located materials, and predicting responses under extreme weapons environments. The end of nuclear testing brought about a new era in science-based stockpile stewardship, and the nation’s predictive capabilities and computing power applied to nuclear weapons assessments have advanced significantly ever since. Yet many longstanding physics questions, including those about the dynamic response of materials in weapons regimes, remain.

High-brilliance, high-repetition-rate x-ray light sources hold promise for interrogating materials dynamics in situ, in real time, and in extreme and transient pressure, temperature, and strain-rate environments. Recent improvements in detector efficiencies and frame rates, dedicated high-pressure/ extreme condition beamlines, and the coupling of x-ray synchrotrons and free-electron lasers with dynamic drive platforms have opened up experimental measurements that were only dreamed of a decade ago. Traditional techniques have frequently encountered limits in these experimental regimes, whether they are spatially averaging, temporally slow, or not able to penetrate into materials of interest.

For the first time, researchers are starting to obtain high-time-resolution details about materials’ phases, states, and their dynamics in extreme conditions. By understanding the fundamental mechanisms of how materials transform, we eventually can be more quantitative in our descriptions of

materials physics, and therefore more predictive and better positioned to design function into future materials.

The data obtained at x-ray light sources is complementary to those attained through experiments at our Laboratory gas and powder gun facilities, including the new Dynamic Equation of State (DEOS) facility, indoor and outdoor firing sites, mechanical and thermal test laboratories, and proton radiography at the Los Alamos Neutron Science Center. In total, the dynamic experimentation capability provides a breadth of responsive and unique tools for addressing stockpile mission needs.

Here, we highlight some of Los Alamos National Laboratory’s early experiments and successes in applying x-ray light sources to materials physics pertinent to defense programs. From measuring residual stress in additively manufactured metals to measuring how detonators function in real time, Los Alamos research has been at the leading edge of applications of x-ray light sources. Many of our research scientists split their time between the Laboratory and light sources around the globe as experimental platforms become more widely used in their research programs. The next generation of staff scientists, our postdocs and students, now have unprecedented access to a diverse set of techniques based on x-rays.

I hope you will enjoy learning more about our people and their research results. What they have achieved to date using x-ray light sources is exciting, and the advancement of diagnostics based on x-rays will most certainly play a key role in the next 20 years of stockpile stewardship.

The Dynamic Compression Sector at the Advanced Photon Source

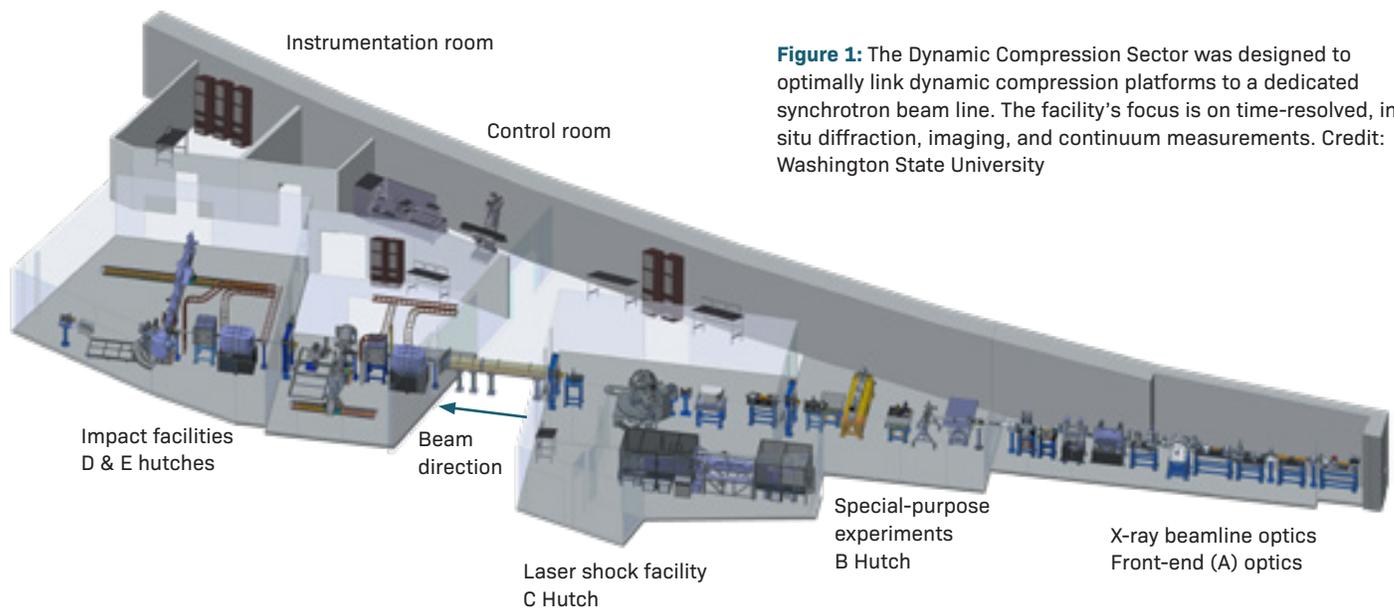


Figure 1: The Dynamic Compression Sector was designed to optimally link dynamic compression platforms to a dedicated synchrotron beam line. The facility’s focus is on time-resolved, in situ diffraction, imaging, and continuum measurements. Credit: Washington State University

A central theme for the National Nuclear Security Administration's Experimental Sciences Programs and for national security interests is the scientific need to examine microscopic, time-dependent changes in materials at extreme conditions. Experiments are needed that can provide information on the growth of new phases, observe defect nucleation and growth, study the compaction process in granular or porous materials, or observe the response of additively manufactured materials. The newly commissioned Dynamic Compression Sector (DCS) at Argonne National Laboratory pairs dynamic compression platforms with a dedicated x-ray beam line at Argonne’s Advanced Photon Source.

DCS provides x-ray diagnostics such as x-ray diffraction, x-ray phase contrast imaging, and small-angle x-ray

scattering to obtain in situ, real-time data that directly accesses the atomistic length scales. Such data will help explain the dynamic processes governing the response of materials at extreme conditions.

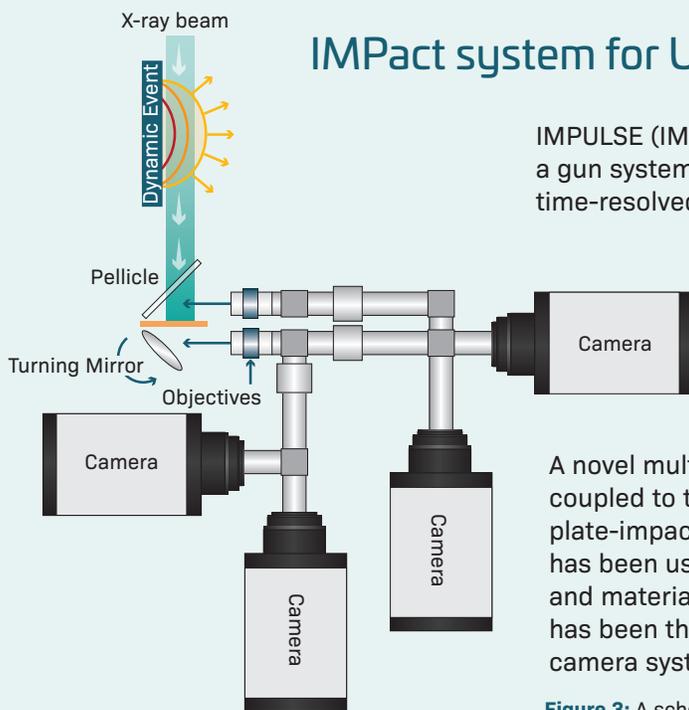
There are several impact facilities with gas and powder guns central to DCS capabilities. These tools are capable of reaching impact velocities up to 5.5 km/s and include a 100-J, 351-nm wavelength laser with temporal pulse-shaping capabilities that will provide peak stresses above 350 GPa. DCS also has an experimental hutch dedicated to more prototypical or special experimental campaigns. This hutch includes detonation vessels, Hopkinson bar, mobile gas guns, and a full suite of traditional shock wave diagnostics.



Figure 2: An exterior view of the DCS and part of the APS synchrotron ring. The DCS sector is shown mid-photo. Credit: DCS

Los Alamos National Laboratory’s proposed experimental capability for Matter-Radiation Interactions in Extremes (MaRIE) will address the aforementioned research needs for materials at extremes while providing high-energy, high-repetition-rate x-rays. The program will couple high-pressure drivers with advanced diagnostics that use x-ray, proton, and electron beams to study material in situ and in real time at the mesoscale. Existing light sources—such as synchrotrons, x-ray free-electron lasers, IMPULSE (see below), and the DCS—are critical for the roadmap to MaRIE. They help researchers develop new diagnostics, design and analyze experiments, and perform exciting new scientific studies on matter at extremes.

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IMPact system for ULtrafast Synchrotron Experiments

IMPULSE (IMPact system for ULtrafast Synchrotron Experiments) is a gun system designed by Los Alamos National Laboratory to make time-resolved, in situ measurements using advanced light sources. It has played a central role in DCS research and capability developments. IMPULSE is stationed at the Advanced Photon Source (APS) at Argonne National Laboratory, where it combines an impact facility with the APS x-ray beam. Its development was partially funded by Mission Support and Test Services.

A novel multi-frame, x-ray phase contrast imaging (mPCI) system coupled to the IMPULSE gun obtained the first “shock movies” at plate-impact experiments at a synchrotron source. The mPCI system has been used to measure shock propagation, localization, failure, and material compaction, and is available for user experiments. It has been the foundation for systems such as the x-ray diffraction camera system used at the DCS.

Figure 3: A schematic of the current mPCI system that uses a dual-scintillator imaging scheme to increase the optical efficiency and to allow for two independent objectives to provide a dual-zoom feature. A mirror and pellicle made of aluminum-coated mylar are used to image both sides of the scintillator.

Matter in Extreme Conditions instrument at the Linac Coherent Light Source

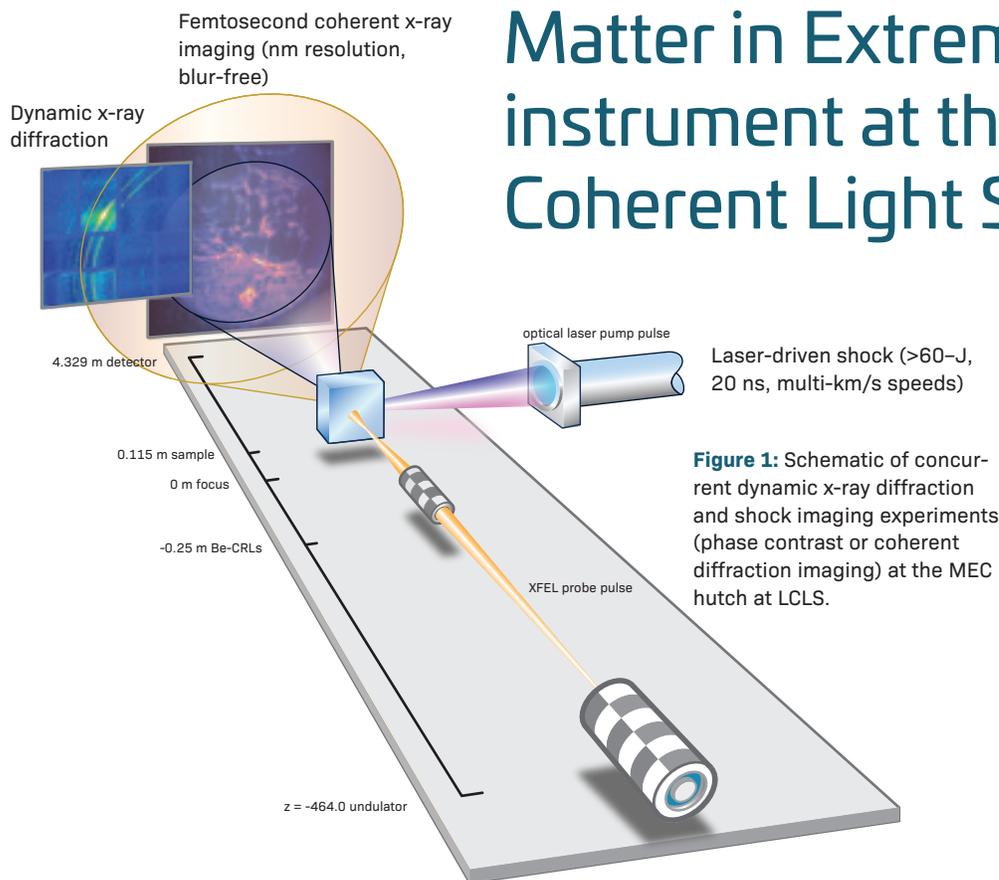


Figure 1: Schematic of concurrent dynamic x-ray diffraction and shock imaging experiments (phase contrast or coherent diffraction imaging) at the MEC hutch at LCLS.

The Matter in Extreme Conditions (MEC) instrumental hutch was established in 2012 and jointly funded by the Department of Energy’s Office of Basic Energy Sciences and Office of Fusion Energy Sciences. With its high peak brightness, short pulse duration, and tunable x-ray photon energy, this beam provides revolutionary capabilities to study the transient behavior of matter in extreme conditions. It is housed at the world’s first hard x-ray free-electron laser—the Linac Coherent Light Source (LCLS) of SLAC National Accelerator Laboratory.

The MEC instrument’s particular strength comes from its combination of the LCLS beam and high-power, optical laser beams. It also offers a suite of dedicated diagnostics tailored for this field of science, including an x-ray Thomson scattering spectrometer, an XUV spectrometer, a Fourier domain interferometer, and a VISAR system.

Los Alamos National Laboratory was one of the early adopters of MEC. It has routinely participated in 3–5 experiments per year both through competitive proposals and collaborations with LCLS staff. Through partnerships with MEC, Los Alamos researchers have developed dynamic, time-resolved x-ray diffraction and concurrent phase contrast or coherent diffraction imaging (figure above).

MEC overview

- Tunable (412 keV), ultrafast (few to 200 fs), intense x-ray pulses at 120 Hz
- Highly configurable, large vacuum chamber (2-m diameter)
- 1-J, 40-fs short-pulse laser system
- 60-J, 20-ns long-pulse
- Angle- and energy-resolved x-ray scattering
- SAXS, WAXS
- Phase contrast imaging or coherent diffraction imaging

MEC diagnostics

- Various detector systems (140-k CSPADs, 4x4 CSPAD, others)
- XUV, x-ray emission spectrometers
- X-ray Thomson scattering spectrometer

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High-Pressure Collaborative Access Team at the Advanced Photon Source

A frontier synchrotron facility for advancing compression science and technology

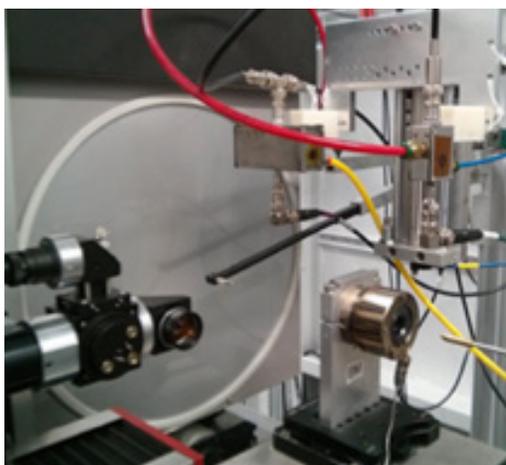


Figure 1: A membrane-based diamond anvil cell in one of the hutches at HPCAT.

High-Pressure Collaborative Access Team (HPCAT) is a research consortium established in 1999 to advance compression science in multidisciplinary fields with synchrotron x-ray radiation. The consortium operates Sector 16 at the Advanced Photon Source (APS) of Argonne National Laboratory.

Using the largest synchrotron facility dedicated to high-pressure research, HPCAT researchers study the movement of atoms at pressures even higher than those found in the Earth's core. The consortium has made numerous

breakthroughs studying high pressures in physics, materials science, chemistry, and Earth and planetary sciences.

The integrated HPCAT facility has four simultaneously operational beamlines (16BM-D, 16BM-B, 16ID-B, and 16ID-D). These beamlines provide users with a variety of techniques: high-pressure x-ray diffraction, x-ray spectroscopy, and x-ray imaging. Other capabilities include diamond anvil cells and Paris-Edinburgh large-volume press platforms.

HPCAT's operation has been supported by the Department of Energy's National Nuclear Security Administration and its Office of Basic Energy Sciences. Instrumentation funding has partially come from the National Science Foundation. As one of HPCAT's core partners, Los Alamos National Laboratory has a dedicated allocation of experimental time for work in support of programs such as Primary Assessment Technologies (Campaign 1), Dynamic Material Properties (Campaign 2), the Global Security program, and the Los Alamos Laboratory Directed Research and Development program.

HPCAT also provides opportunity for collaborations with NNSA laboratories such as Lawrence Livermore National Laboratory and Sandia National Laboratories, the Capital/DOE Alliance Center, faculty and students that are part of NNSA Stewardship Science Academic programs, and many researchers from the global high-pressure community.

16ID-D: Spectroscopy station

- Nuclear forward scattering
- Nuclear resonant inelastic x-ray scattering
- Inelastic x-ray scattering
- X-ray Raman scattering
- X-ray emission spectroscopy
- Resonant x-ray emission spectroscopy

16ID-B: Micro-diffraction station

- Micro-diffraction
- Powder and single-crystal diffraction
- Radial diffraction
- Online laser heating system
- Micro-diffraction with cryostat
- High-resolution diffraction

16BM-B: Micro-diffraction with polychromatic beam

- Laue diffraction
- High-pressure liquids
- Large-volume press

16BM-D: Micro-diffraction and spectroscopy station

- Micro-diffraction
- Anomalous diffraction/scattering
- Powder and single-crystal diffraction
- X-ray absorption spectroscopy

Supporting capabilities

- Laser heating system, online
- Raman system, ruby fluorescence system, cryostats, sample preparation laboratory
- Brillouin system

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The case for the Matter-Radiation Interactions in Extremes project

For more than 20 years, the science and engineering capabilities of the Stockpile Stewardship Program have allowed the United States to sustain a safe, secure, and effective nuclear deterrent. Most of the challenges within the nuclear stockpile relate to its aging materials. The Matter-Radiation Interactions in Extremes (MaRIE) capability will advance the Stockpile Stewardship Program's excellent record by addressing such materials problems.

MaRIE provides control of both performance and production of materials vital to national security missions.

The National Nuclear Security Administration (NNSA) requires the ability to understand and test how a material's structures, defects, and interfaces affect performance in extreme environments such as in nuclear weapons. To do this, MaRIE will be a laser-like, brilliant x-ray source with flexible and fast pulses that see at weapons-relevant time scales and with high enough energy to study critical materials (Fig. 1).

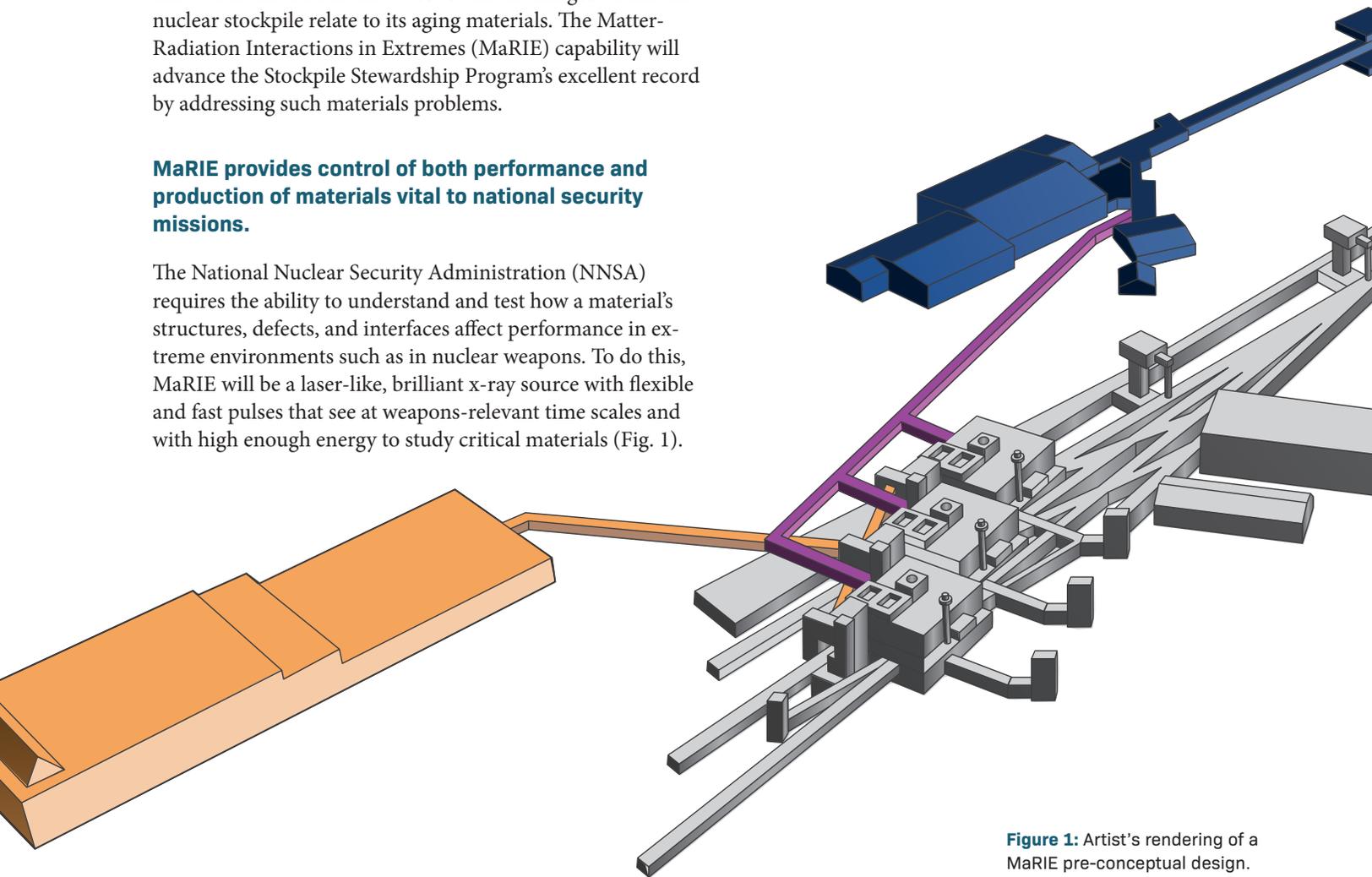
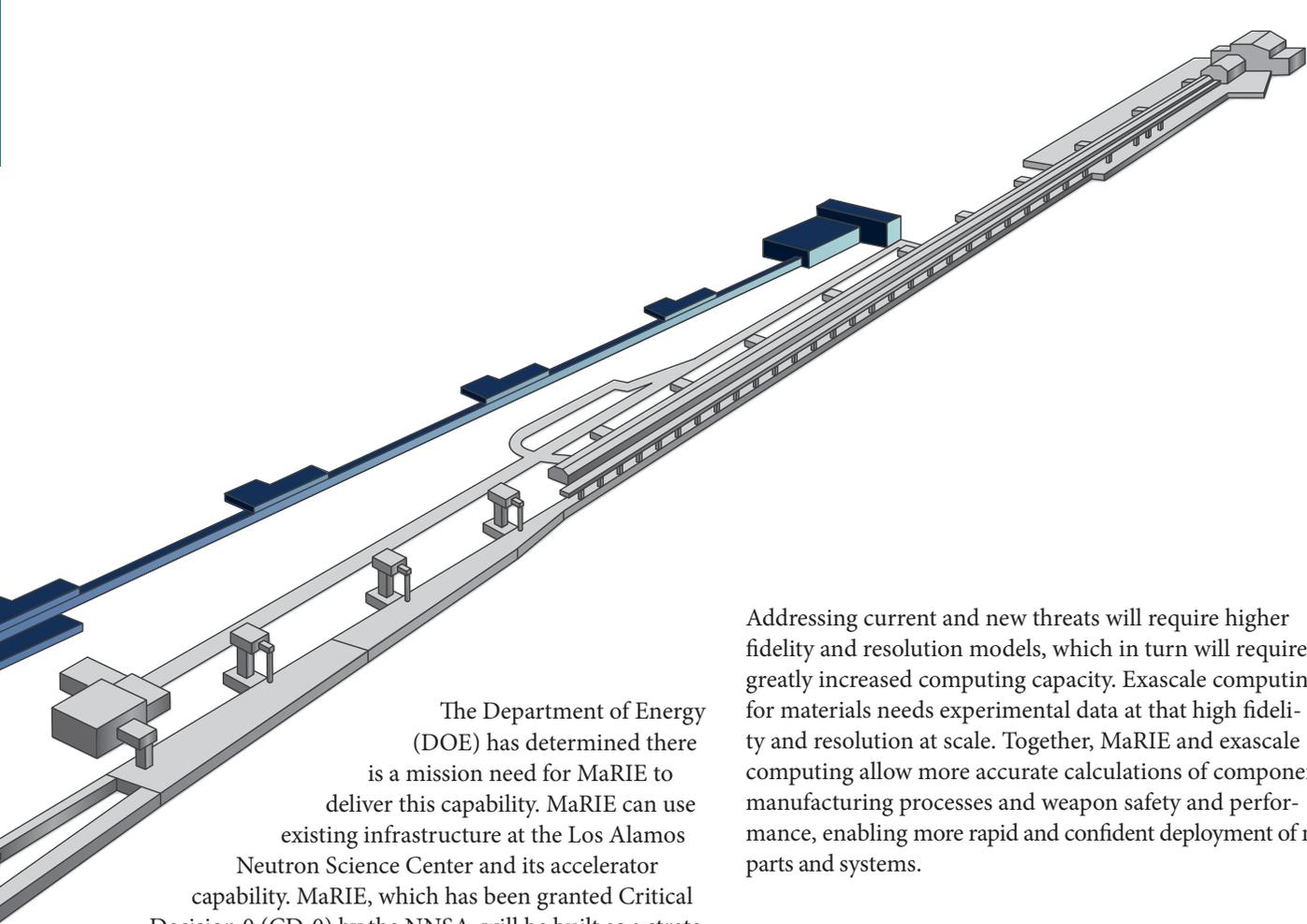


Figure 1: Artist's rendering of a MaRIE pre-conceptual design.



The Department of Energy (DOE) has determined there is a mission need for MaRIE to deliver this capability. MaRIE can use existing infrastructure at the Los Alamos Neutron Science Center and its accelerator capability. MaRIE, which has been granted Critical Decision 0 (CD-0) by the NNSA, will be built as a strategic partnership of DOE national laboratories and university collaborators.

There is an urgent need for accelerated delivery of integrated materials solutions to the nuclear deterrent and other national security missions.

The nation's design labs must annually assess whether the aging stockpile will continue to work as designed. These assessments (performance, reliability, safety, and security) are increasingly reliant on detailed scientific understanding of material properties. MaRIE will provide NNSA with more rigorous science-based approaches to manufacturing and certification supporting a more responsive, agile enterprise for U.S. stockpile needs and meet new security challenges in the nonproliferation and counter proliferation contexts.

The United States must prepare for an uncertain future.

National security in the 21st century requires state-of-the-art computing platforms as well as experimental facilities like MaRIE to generate data to inform models and challenge the computations.

Addressing current and new threats will require higher fidelity and resolution models, which in turn will require greatly increased computing capacity. Exascale computing for materials needs experimental data at that high fidelity and resolution at scale. Together, MaRIE and exascale computing allow more accurate calculations of component manufacturing processes and weapon safety and performance, enabling more rapid and confident deployment of new parts and systems.

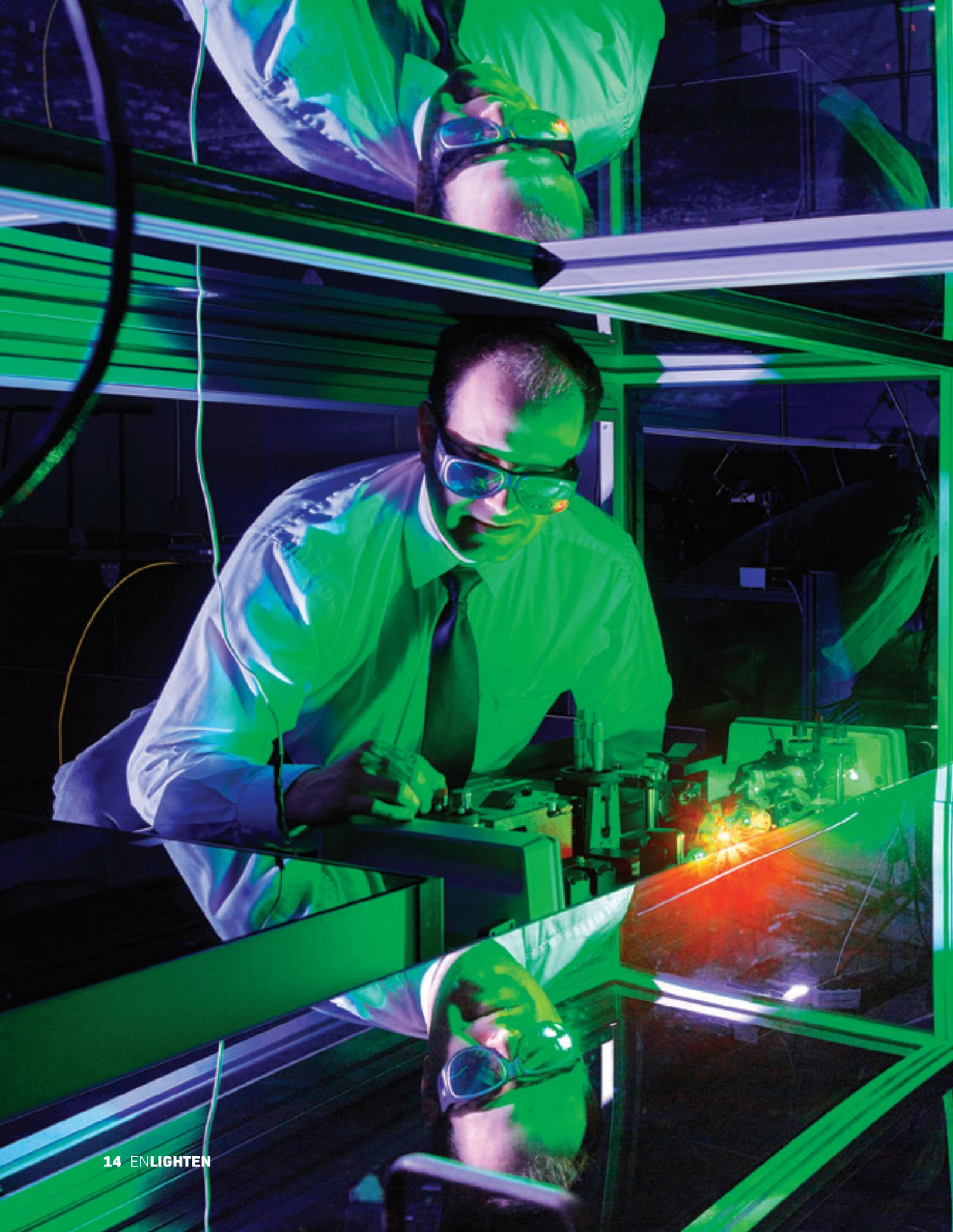
We need to ensure U.S. technological preeminence as a nation.

Basic research provides the greatest potential for fundamentally new ways of creating technological advances with national security and economic implications. Materials innovations have been at the core of the majority of big technological advances since the start of the industrial revolution. MaRIE will provide a comprehensive materials discovery facility with a unique capability to address the control of strategic materials at a middle (mesoscale) of material structure, the scale recognized as a major science grand challenge.

A skilled workforce is crucial for U.S. national security.

MaRIE will transform our ability to compete for intellectual capital and signal to the international community, allies, and adversaries that the nation's best and brightest are prepared to solve any national security challenge.

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OPTICAL RESEARCHER

RICHARD SANDBERG

For more than 10 years, Richard Sandberg has applied coherent diffraction imaging (CDI) to research high-resolution x-ray imaging from coherent sources. He has been a Los Alamos staff member since 2011, working in the Laboratory for Ultrafast Materials and Optical Sciences (LUMOS) at the Center for Integrated Nanotechnologies.

Coherent x-ray sources are undergoing an extraordinary revolution in their brilliance—in some cases they are now a billion times brighter. Our team is trying to harness that unprecedented brilliance to study how materials are damaged and fail in extreme conditions at the mesoscale. We work with tabletop extreme-ultraviolet laser sources, using the synchrotrons and x-ray free-electron lasers located at large facilities to perform coherent diffraction imaging and peer inside these materials.

Richard received his PhD in 2009 from the University of Colorado at Boulder in optics research. His interest in science exploded at an early age.

When I was about 8 years old, I took my weekly Saturday bath and was admonished by my mom to not go back outside and get dirty. I turned on the TV instead and immediately saw an explosion. It happened to be a star exploding in a supernova on Carl Sagan's "Cosmos" series playing on PBS. I was hooked and watched it for nearly two hours. I then tuned into it over the next several weeks. While other kids were saying they wanted to be a firefighter or a baseball player, I was saying I wanted to be a scientist.

In graduate school, Richard and his collaborators demonstrated the world's first application of CDI on a tabletop ultrafast laser system. Now, as a team leader at Los Alamos, Richard performs research that revolves around x-ray CDI and studying materials dynamics with x-ray light sources.

I love using x-rays to do materials studies that have never been done before. Some of the unusual experiments we have tried at different facilities are expanding how we understand and think about studying materials. There have been instances where our data is so far beyond materials models that our theoretical colleagues literally have to create new models to see what we are finding. It is really exciting.

The capabilities at the proposed Matter-Radiation Interactions in Extremes (MaRIE) capability would take us from proof-of-principle experiments to work that tackles the stockpile stewardship missions of the future at Los Alamos. MaRIE's ability to reach harder x-ray energies, its well-matched materials driver systems like high explosives, and its unique time structure will mean we can make mesoscale movies of mission-relevant materials dynamics.

Richard Sandberg aligns an ultrafast laser system for CDI experiments. He and his collaborators develop high-resolution x-ray coherent diffraction imaging at light sources to study materials dynamics at extremes.

Novel technique combines time-resolved spectroscopy with ultrafast laser shocks

X-ray method observes chemical dynamics under extremes

Researchers have used time-resolved optical spectroscopies to study photoinitiated chemistry since the advent of pulsed lasers. Recently, investigators from Los Alamos National Laboratory and SLAC National Accelerator Laboratory paired x-ray absorbance spectroscopy (XAS) with thousands of ultrafast, laser-driven shocks (Fig. 1) to observe chemical dynamics under extreme pressure 300,000 times greater than the atmosphere and temperatures of 2000 K.

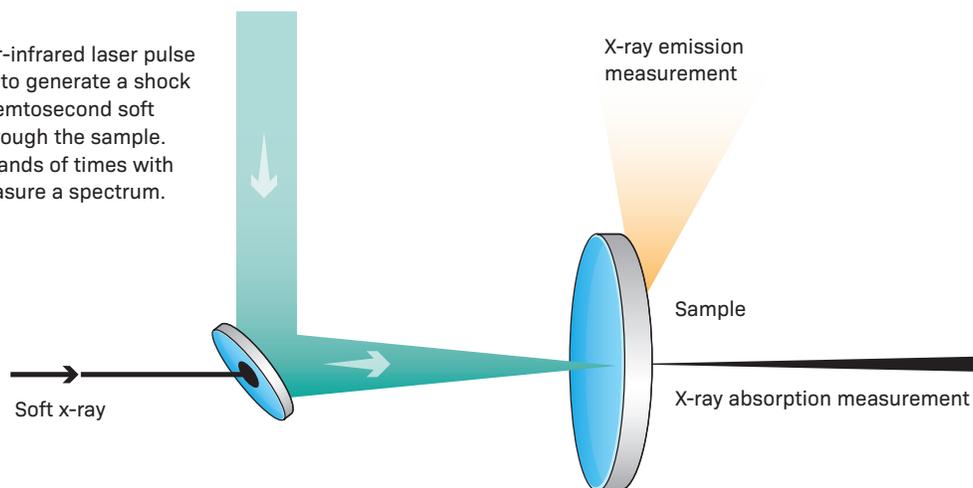
This knowledge can help explain how current explosives work and how to design safer, higher performing explosives

This x-ray technique, which provided time resolution in the soft x-ray regime, could only be performed at the Linac Coherent Light Source. Low-energy

x-rays resonant with the carbon, nitrogen, and oxygen in explosives can only penetrate micrometers of material, meaning that the shock measurements had to be made in less than a nanosecond.

The team focused a 100-ps near-infrared laser pulse onto an aluminum film to generate a shock wave in a thin layer of explosive called PVN. A femtosecond soft x-ray pulse was then transmitted through the sample. This was repeated at different energies and delays. Quantum molecular dynamic simulations were then performed to predict initial chemical products (Fig. 2) and time-dependent density functional theory was used to predict the x-ray absorption spectrum of these products. Analysis is ongoing to compare the shock-induced changes to the predictions (Fig. 3).

Figure 1: Experiment: A 100-ps near-infrared laser pulse was focused onto an aluminum film to generate a shock wave in a thin layer of explosive. A femtosecond soft x-ray pulse was then transmitted through the sample. The experiment was repeated thousands of times with different energies and delays to measure a spectrum.



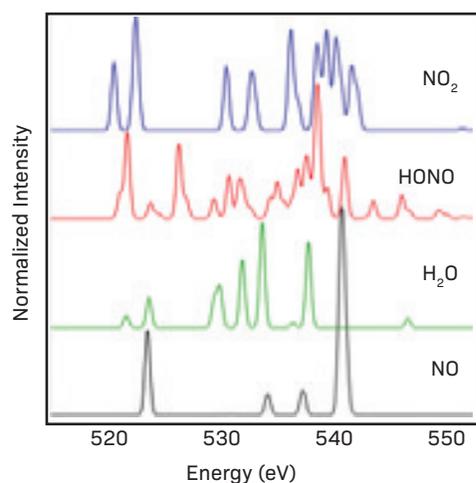


Figure 2: Quantum molecular dynamic simulations of the high-pressure and temperature-shocked material were performed to predict initial chemical products. Time-dependent density functional theory was used to predict the XAS of these products.

These were the first time-resolved XAS studies of shocked high explosives performed at SLAC. These novel experiments are important to understanding the shock-induced chemistry in explosives. The knowledge, in turn, can help explain how current explosives work and how to design safer, higher performing explosives in the future.

An ultrafast, laser-driven shock platform located at Los Alamos was used to perform preliminary experiments and build portable velocimetry diagnostics. The Lab's high-explosive crystal laboratory provided sample preparation expertise and support. A future capability such as low-energy XAS with single-shot-dispersive spectral acquisition and accurate normalization to spectral fluctuations could make this technique orders of magnitude higher in signal-to-noise ratio.

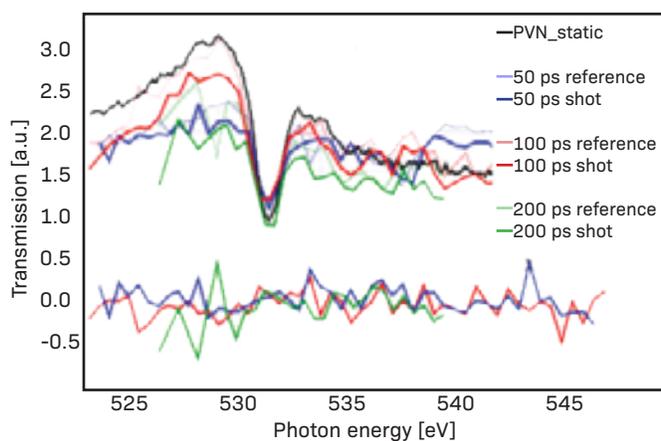


Figure 3: The result was first XAS of shocked high explosives and the first soft x-ray absorption during shock. Analysis is ongoing to compare the shock-induced changes to the predictions.

Publication citation: "Shock-Induced Reaction Observed via Ultrafast Infrared Absorption in Poly(vinyl nitrate) Films," *Journal of Physical Chemistry A* **108**, 9342 (2004)

Source of funding: Los Alamos Laboratory Directed Research and Development program

Researchers: LANL: Shawn McGrane, Cindy Bolme, Katie Brown, Adam Golder, Kyle Ramos, Marc Cawkwell, Ping Yang, Romain Perriot; SLAC: Arianna Gleason, Michael Minitti, Alexander Reid

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New approach improves understanding of explosives' mesoscale, thermomechanical behavior

Even low-velocity impacts to high explosives can cause violent reactions—deformations in the explosive microstructure can result in high local temperature fields that cause chemical reactions. Predicting this response and the resulting material damage is an unsolved technical challenge. In order to understand the dynamic loading behavior of energetic molecular crystals, which are the heart of high explosives, reliable models of the thermomechanical behavior of these constituents must be developed and validated using small-scale experiments.

... the fracture networks in these brittle molecular crystals are not constrained to specific crystallographic planes

resolved, in situ x-ray diffraction and imaging (Fig. 1) during dynamic compression on single-crystal and plastic-bonded formulations of the explosive cyclotrimethylene trinitramine (RDX). Diffraction patterns quantified the average lattice response during elastic-plastic and phase transition. Imaging quantified the response between microstructure and continuum scales and allowed for direct comparison of experiments and simulations.

This research resulted in several discoveries about the behavior of energetic molecular crystals (Fig. 2). For example, velocimetry data from gas-gun-driven plate-impact experiments showed the existence of previously unknown crystallographic planes in RDX that are favorable for accommodating

Using the Advanced Photon Source synchrotron and the Linac Coherent Light Source x-ray free-electron laser, a large research team performed time-

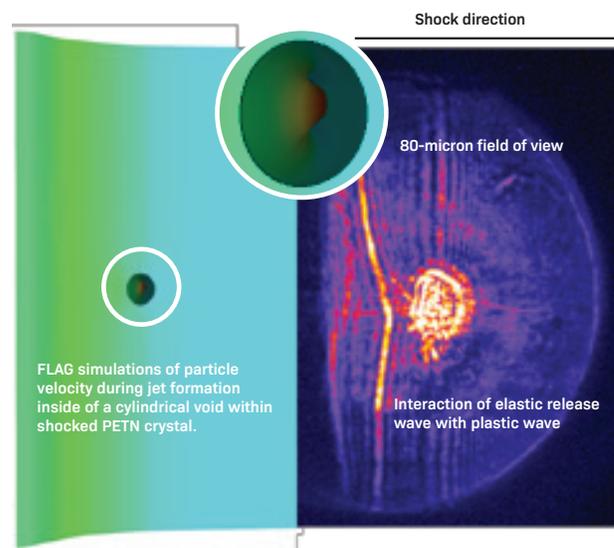


Figure 1: Collapse of a cylindrical pore within a single crystal of the explosive pentaerythritol tetranitrate. The images at left and inset show the particle velocity field predicted from 3D FLAG simulation of the shock-loading experiment. At right is a depiction of the phase contrast imaging generated from in situ x-ray diffraction measurements performed at LCLS during shock compression.

plastic slip during dynamic loading. Another key scientific question has been how fracture networks develop in these brittle molecular crystals. Preliminary analysis of images suggested fracture networks that are not constrained to specific crystallographic planes.

With improved models that show how individual crystals interact in composite explosives, researchers are nearly able to quantify the spatio-temporal evolution of temperature fields and create macroscale reactive burn models that can be applied to assess the safety of explosives. In situ x-ray diagnostics are answering outstanding questions about the effects of anisotropic plasticity, strain rate dependence, and the shock path through the phase diagram.

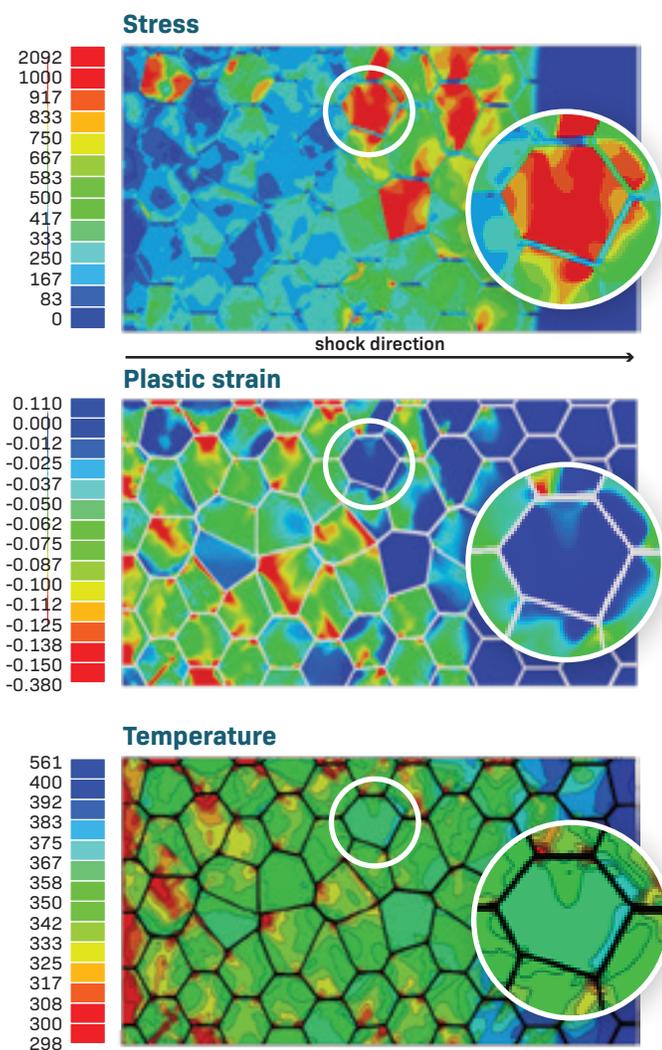


Figure 2: Results from a two-dimensional mesoscale simulation of heterogeneous Estane/RDX polymer-bonded explosive. The anisotropic behavior of individual randomly oriented crystals leads to heterogeneity in the plastic deformation, thus leading to a non-uniform temperature field.

Publication citations: “A dislocation density-based continuum model of the anisotropic shock response of single crystal α -cyclotrimethylene trinitramine,” *Journal of the Mechanics and Physics of Solids* **98**, 63-86 (2017)

“Plasticity in Crystalline Molecular Explosives—A Key to Unraveling ‘Unpredictable’ Responses,” *Propellants, Explosives, Pyrotechnics* **41** (2), 203-204 (2016)

“A single-crystal model for the high-strain rate deformation of cyclotrimethylene trinitramine including phase transformations and plastic slip,” *Journal of Applied Physics* **121** (18), 185902 (2017).

Source of funding: Dynamic Material Properties (Campaign 2), Los Alamos Laboratory Directed Research and Development program

Researchers: LANL: Frank Addressio, Claudine Armenta, John Barber, Cindy Bolme, Katie Brown, Marc Cawkwell, Frank Cherne, Margo Greenfield, Arianna Gleason, Adam Golder, Tate Hamilton, Ernie Hartline, Dan Hooks, Brian Jensen, DJ Luscher, Shawn McGrane, David Montgomery, Chuck Owens, Tim Pierce, Kyle Ramos, Ramon Saavedra, Richard Sandberg, Ken Windler, John Yeager, ARL: Dan Casem, Chris Meredith, Brian Schuster, NSTech: Carl Carlson, Adam Iverson, MIT: Leora Cooper, APS: Alex Diery, Kamel Fezzaa, Thomas Gog, Paulo Rigg, Nick Sinclair, SLAC: Eric Galtier, Eduardo Granados, Phil Heimann, Haeja Lee, Bob Nagler

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MATERIALS SCIENTIST

SARYU FENSIN

Using experiments and simulations, Saryu Fensin examines the relationship between material microstructures and properties in thermodynamic and mechanical extremes. She investigates the pairing of material microstructures and dynamic loading parameters to develop a predictive capability for damage and failure in materials.

Due to the ban on underground testing, it is critical to be able to certify our stockpile with confidence by developing an understanding of how and to what extent material microstructure affects equation of state, damage/spall, strength, and ejecta. This understanding is indispensable to develop accurate models to describe these dynamic properties. However, it's very challenging to "see" inside a material as it is deforming and to know how various microstructural features contribute to these properties. This becomes even more complicated at higher strain rates. I'm hoping to solve this puzzle and develop a predictive capability for material response.

Saryu is passionate about coupling atomistic simulations with experiments to both design and understand the physics behind experimental observations.

"Seeing" inside materials as they are subjected to an external stimulus is the holy grail for material science. Advanced light sources let us perform cutting-edge experiments and shed light on undiscovered phenomena. If I had an even more advanced hard x-ray capability such as MaRIE [Matter-Radiation Interactions in Extremes], I'd love to discover in real time where voids nucleate in metals and to measure their growth rates. I also want to understand the basic mechanisms that contribute and dictate the overall mechanical response of metals.

It's wonderful to interact with world-class scientists at Los Alamos, where you do not have to be an expert in everything because a colleague down the hall probably is. I like being able to perform cutting-edge experiments that aren't possible to pursue elsewhere in the world. I enjoy working in an application-based field. Everyone needs materials!



Saryu Fensin studies a projection of molecular dynamic simulations of tantalum. The various colors indicate local crystalline orientation. These atomistic simulations help guide and understand her experimental work.

Dynamic measurements ‘see’ carbon form during high-explosive detonations

When a high explosive (HE) is detonated, a shock wave drives exothermic chemical reactions that rapidly release large amounts of energy. The reactions generate high pressures and temperatures and create a mixture of gases and, frequently, solid carbon particles. Depending on the pressures and temperatures reached, different sizes, shapes, and compositions of carbon particles can form. Quantitatively understanding how these particles form and evolve during detonation is important for improving computer models of explosive products that, in turn, will result in better predictive capabilities for the U.S. nuclear deterrent.

PBX 9502 is an insensitive high explosive based on triaminotrinitrobenzene (TATB) and used in nuclear weapons to drive the primary to critical mass. The exact time-resolved dynamics of chemical/physical transformations and the resulting energy release during detonation are not fully understood. Using time-resolved small-angle x-ray scattering (TR-SAXS), researchers investigated the dynamics of carbon particle formation during PBX 9502 detonation. SAXS probes nano- to mesoscale structure, between the length scales measured by diffraction and imaging; using this technique at fast time scales resulted in snapshots of mesoscale structure during a dynamic event.

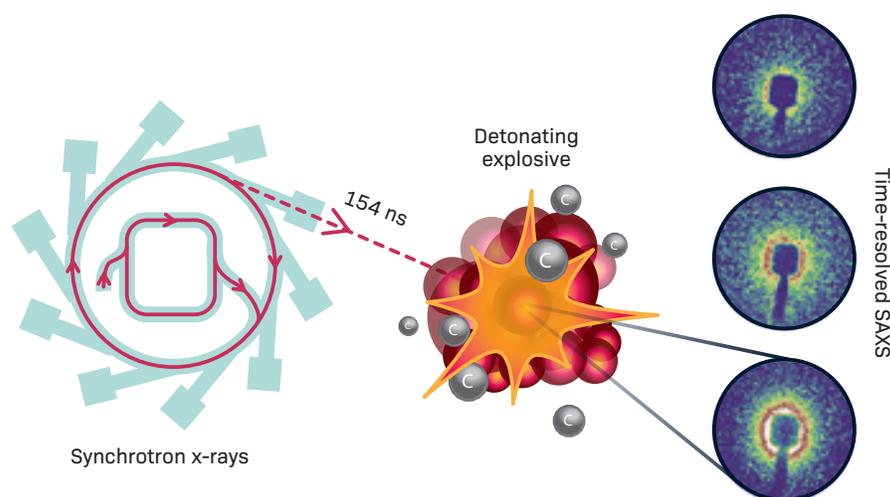


Figure 1: Illustration of the time-resolved SAXS experiment to study carbon products formed in HE detonations.

The experiments were performed at the Advanced Photon Source synchrotron and used instrumentation at the Dynamic Compression Sector to gather four sequential SAXS snapshots during detonation. Measurements showed rapid growth of carbon particles that were an average diameter of ~8.4 nm in the first 200 ns after the detonation front passed. After 200 ns, no further growth was observed. The investigators found good agreement between simulations and measurements that indicated the growth of carbon particles stops abruptly when the temperature of the detonation products dropped below ~2,500 K. This suggests that carbon clustering has a finite activation temperature associated with

the rearrangement of carbon bonds when clusters merge. Based on the scattering contrast obtained from TR-SAXS, the researchers were able to approximate the composition of the carbon particles as a mixture of 20% highly ordered and 80% disordered carbon forms. This knowledge will inform future product equation of state models for solid carbon in PBX 9502 detonation product mixtures.

This was the first time in the U.S. that TR-SAXS was used to observe ultrafast carbon clustering and graphite and nano-diamond production in PBX 9502. The work won the team (Fig. 2) a 2016 Defense Programs Award of Excellence from the National Nuclear Security Administration.

The team plans to study larger HE charges and use gas gun shock-driven platforms to better control shock conditions.

Quantitatively understanding how these particles form and evolve during detonation will result in better prediction for the U.S. nuclear deterrent

formation during detonation using higher flux. This would provide access to earlier times and faster time scales and would extend the suite of x-ray probes to determine chemistry via diffraction and spectroscopy.

Future light source advances could also allow scientists to perform dynamic experiments on carbon



Figure 2: From left to right: Dana M. Dattelbaum, Kirill A. Velizhanin, Erik B. Watkins, Bryan S. Ringstrand, Millicent A. Firestone, Rachel C. Huber, and Rick Gustavsen.

Publication citation: “Evolution of carbon clusters in the detonation products of the triamino-trinitro-benzene (TATB) based explosive PBX 9502,” *Journal of Physical Chemistry C* **121**, 41, 23129-23140 (2017)

Source of funding: Dynamic Material Properties (Campaign 2)

Researchers: LANL: Erik Watkins, Kirill Velizhanin, Dana Dattelbaum, Rick Gustavsen, Rachel Huber, Millie Firestone, Tariq Aslam, Dave Podlesak, Bryan Ringstrand; LLNL: Trevor Willey, Michael Bagge-Hansen, Ralph Hodgkin, Lisa Lauderbach; WSU: Nick Sinclair

Contacts: Erik Watkins (ebw@lanl.gov) and Kirill Velizhanin (kirill@lanl.gov)

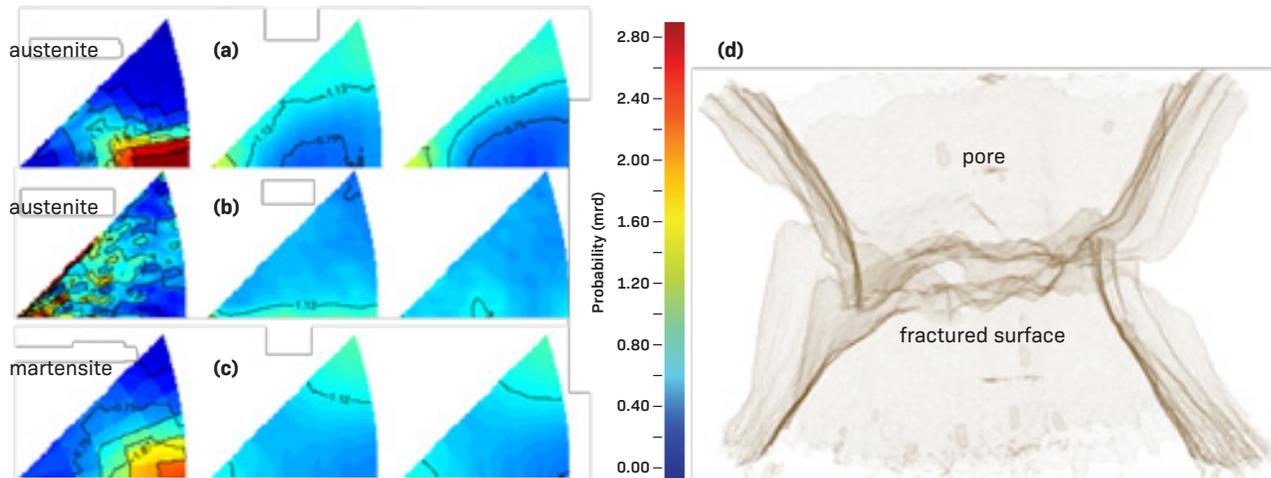
In situ measurements monitor microstructure evolution in AM stainless steel

Metal additive manufacturing (AM) is an innovative fabrication technology that can build engineering components and fabricate other geometries that are too complex for conventional processing methods. One AM process utilizes a heat source to melt a metal wire or powder feedstock, building a component layer by layer. Because deposited materials melt and re-solidify often during fabrication, AM can build microstructures that have inconsistencies such as local heterogeneity, internal stresses, and residual porosity—all of which could result in significantly variable material properties compared with traditionally fabricated materials. The scientific community lacks a physics-based understanding of the process-structure-property-performance

(PSPP) relationship of metal AM components. Nondestructive diagnostics are crucial for establishing the PSPP relationship in AM materials/components. Therefore, in situ

Figure 1. (a)-(c): Inverse pole figures showing texture evolution in the AM 304L steel during uniaxial deformation monitored as a function of the imposed load, where the stress-induced phase transformation was observed, past the elastic-plastic transition. The initial microstructure of the austenite phase shown in **(a)** transformed into a two-phase microstructure consisting of the austenite and the martensite phases shown in **(b)** and **(c)**.

(d) Tomographic density map of the tensile specimen after failure. With increasing strain, process-induced residual porosity grew while new pores nucleated. The pores eventually combined, leading to a ductile failure.



microstructure characterization is critical for developing mesoscale understanding to support the stockpile stewardship mission at Los Alamos.

The Cornell High Energy Synchrotron Source (CHESS) at Cornell University provides the required photon flux and state-of-the-art detector technology to enable in situ measurements of AM structure under various thermomechanical conditions.

Recently, a team of Los Alamos researchers performed in situ experiments at CHESS to capture microstructure evolution during uniaxial tensile loading of AM 304L stainless steel. A tensile specimen extracted from the as-built AM material was subjected to uniaxial tensile deformation. In situ, high-energy x-rays recorded x-ray powder diffraction and micro-computed tomography data during quasi-static loading. The investigators successfully tracked texture, lattice strain, phase, and porosity evolution at 21 different loading stages as the material underwent tensile deformation. Figure 1(a)-(c) shows the initial state and the intermediate deformed state textures while Figure 1(d) shows a volumetric density map in the final state. Individual pores and overall porosity were tracked throughout deformation. The resulting data on texture evolution and void growth rate provide important information for validating predictive strength and ductility models for metal AM.

Preliminary results from these experiments provide specific information for one specimen, but monitoring non-destructive microstructure during deformation with high-energy x-rays will have a long-term impact on understanding the PSPP relationship, which is crucial for qualifying the metal additive manufacturing process. Next-generation detector technology and future facilities such as the Advanced Photon Source Upgrade (APS-U) project and the proposed MARIE capability will further capture mesoscale behavior in bulk metallic materials during dynamic conditions at spatio-temporal length scales that go beyond what is possible at existing light sources.

The team successfully tracked texture, lattice strain, phase, and porosity evolution at 21 different loading stages as the material underwent tensile deformation

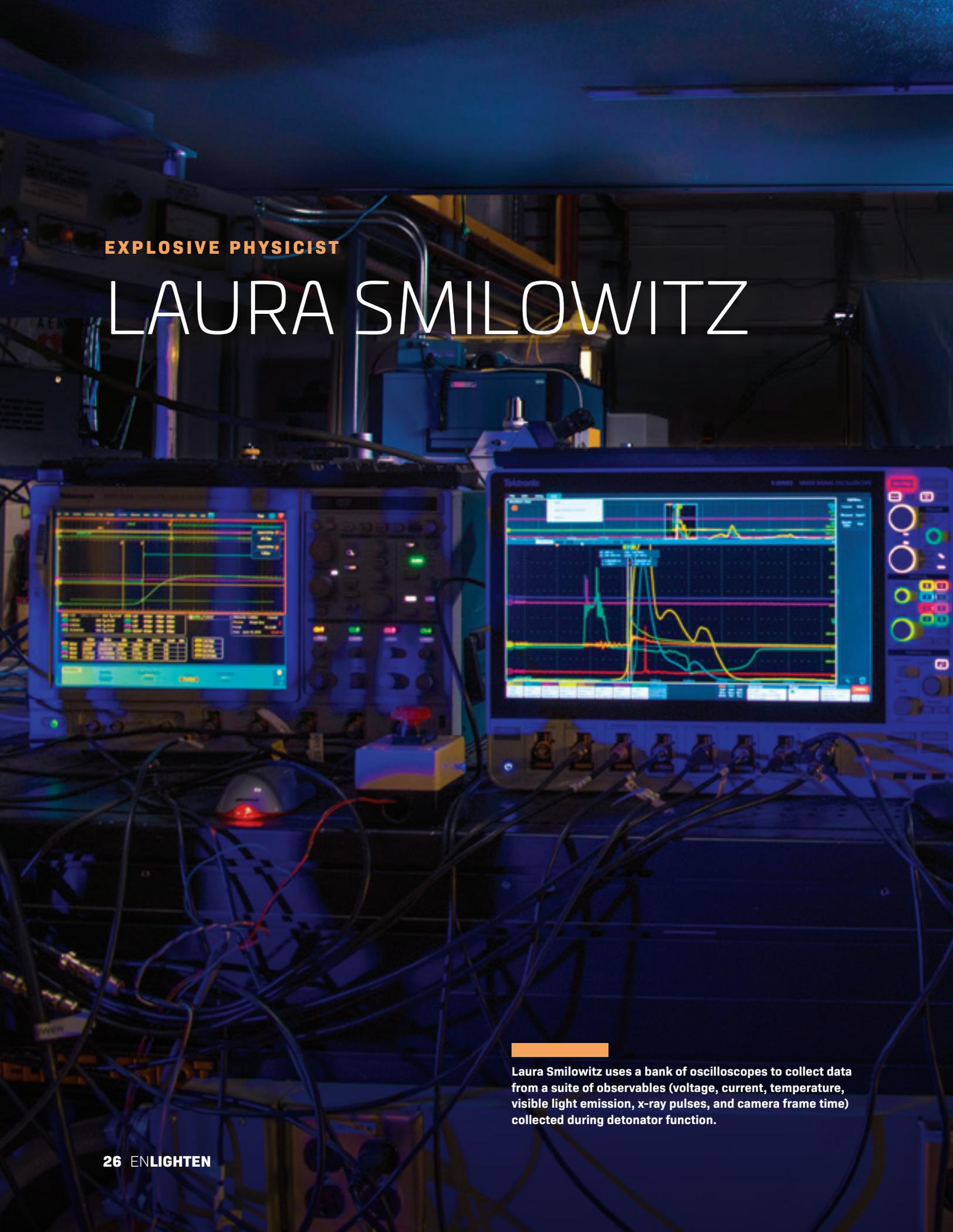
Source of funding: Dynamic Material Properties (Campaign 2)

Researchers: LANL: Reeju Pokharel, Bjørn Clausen, Eloisa Zepeda-Alarcon, Don Brown, and Rusty Gray; **Cornell High Energy Synchrotron Source:** Darren Pagan

Contact: Reeju Pokharel (reeju@lanl.gov)

EXPLOSIVE PHYSICIST

LAURA SMILOWITZ



Laura Smilowitz uses a bank of oscilloscopes to collect data from a suite of observables (voltage, current, temperature, visible light emission, x-ray pulses, and camera frame time) collected during detonator function.



Laura Smilowitz has been at Los Alamos for 20 years, cultivating experience in medical physics, explosives response, and conducting polymers. She studies the thermal response of explosives, following their evolution from slow decomposition that takes many hours until the direct thermal initiation of a detonation—a process that takes less than a microsecond.

A thermal explosion can evolve for days, with the final ignition event consuming the material and releasing its chemical energy within microseconds to nanoseconds. This gives the challenge of assessing such explosions a huge temporal dynamic range—greater than 11 orders of magnitude. Secondary high explosives are also heterogeneous, opaque, often encased in metal, and they take place at extreme temperatures, pressures, and rates. Predicting the thermal response of energetic materials is an extraordinary technical hurdle that could answer problems that directly impact global security and science-based stockpile stewardship missions at Los Alamos.

The goal of Laura's work is to create predictive models for the reaction violence of a thermal explosion. Such models have a direct impact on national security, providing guidance on the potential outcome of an accident involving explosives. Laura's current focus is developing and applying tabletop x-ray imaging techniques to observe density evolution in explosions. She is looking forward to mission-focused discoveries that x-ray capabilities will bring.

New x-ray capabilities are allowing us to directly see what is happening in explosions and detonations. These are things that have absolutely never been seen before and are dramatically improving our understanding of explosive behavior. We are working to understand questions we considered impossible to answer only a few decades ago. Our understanding and the tools are both evolving rapidly and I'm excited to see how far they can take us toward solving decades-old questions predicting the reaction violence of a thermal explosion.

Probing mesoscale features to improve predictions of stress in AM materials

Residual stress determination could help validate AM computational models

Additive manufacturing (AM) shows great promise for producing low-cost, metallic industrial components. One of the main AM processes for producing metals is selective laser melting (SLM), which uses a high-power-density laser to selectively melt and fuse metallic particles together. This process causes rapid solidification and a large thermal gradient, which can form residual stresses that may cause cracks and result in the structure failing. Until now, there has been limited understanding of the process-structure-property-performance relationship of AM components. This limitation has an impact on the usage of AM metallic components and prevents process models from predicting AM structures' final behavior.

Lawrence Livermore National Laboratory (LLNL) has adapted a predictive computational code called Diablo for residual stresses in AM structures. To provide valuable experimental validation data for this code, researchers from Los Alamos and the National Institute of Standards and Technology

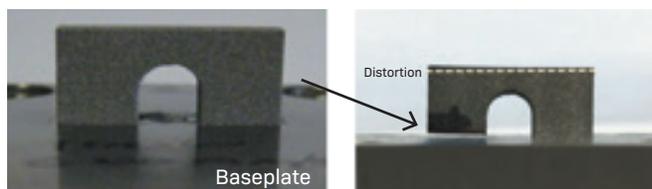


Figure 1: Ti-6Al-4V bridge-shaped specimens were built using SLM to perform a residual stress investigation on AM metallic components. Photo: LLNL

(NIST) performed a residual stress investigation on AM metallic components. The researchers built Ti-6Al-4V bridge-shaped specimens via SLM (Fig. 1) using four different scan strategies: continuous scan aligned with x-axis, continuous scan at 45° to x-axis, island scan aligned with x-axis, and island scan at 45° to x-axis. A 90°-rotation in scan orientation was performed after each layer for all four cases. The team made energy-dispersive diffraction measurements on all four Ti-6Al-4V components at the Cornell High Energy Synchrotron Source (CHESS) A2 instrument. Using x-ray diffraction, the researchers also measured lattice parameter and determined the elastic strains present in these bridges while still attached to the base plate and after one leg had been cut off the base plate (Fig. 2).

The figure shows the strain on a cross-section of one of the bridge-shaped samples before and after cutting of one of the two legs.

Relaxation in the cut leg is apparent. Unexpectedly, the diffraction results showed higher strains

in the bridges built using the island scan strategies, especially near the edges of the parts. The thermomechanical simulations of these bridge builds exhibited good qualitative agreement with experimental results, although current modeling technique did not capture the effects of varying scan strategy.

Until now, there has been limited understanding of the PSPP relationship of AM components

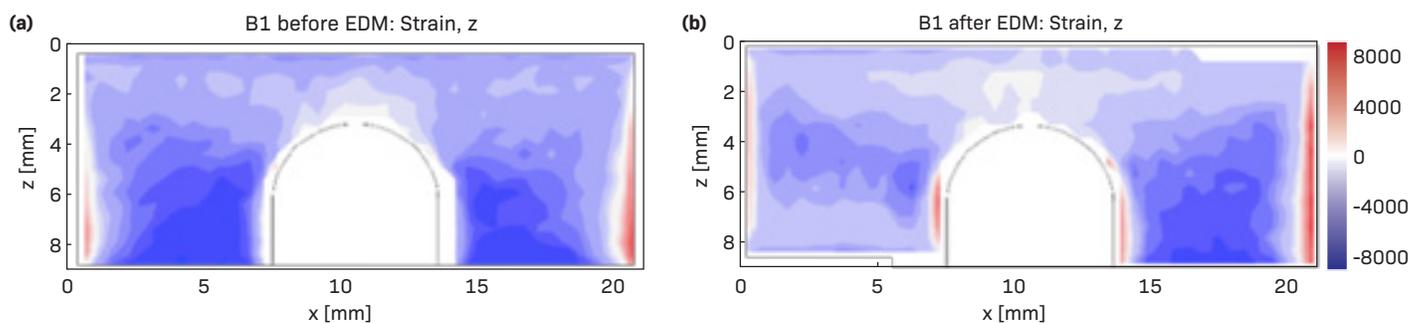


Figure 2: Contour plots of the calculated strain ($\times 10^6$) in z direction, which corresponds to the building direction of the additively manufactured Ti-6Al-4V sample. In (a) the sample is still attached on the baseplate and in (b) the left leg of the “bridge” is detached from the baseplate.

Being able to validate the computational models allows for process optimization and establishes limits for off-normal processes. These are necessary for qualification of AM components in high-value, safety-critical applications, such as in the aerospace industry.

High-energy x-ray light sources such as CHESS provide a novel method to probe the mesoscale, the “middle” scale where imperfections, defects, and heterogeneities are critical to controlling a material’s macroscopic behaviors and properties. The experiment is an example of science that could be furthered with MaRIE, Los Alamos National Laboratory’s proposed Matter-Radiation Interactions in Extremes capability for in situ, time-dependent materials science at the mesoscale. MaRIE would allow researchers to observe—in real time—how residual stresses develop as a part is built, enabling new processes to achieve tailored mechanical properties.



Source of funding: Primary Assessment Technologies (Campaign 1)

Researchers: LANL: Maria Strantza, Bjorn Clausen, and Don Brown; NIST: Lyle Levine and Thien Phan; LLNL: Wayne King, Neil Hodge, Rishi Ganeriwal

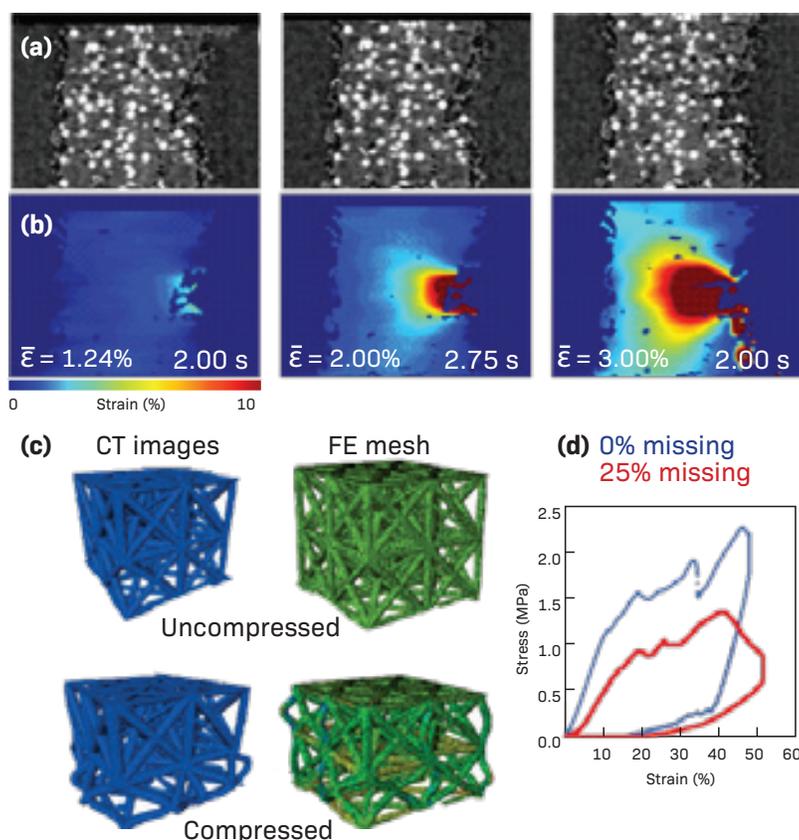
Contact: Maria Strantza (maria.strantza@lanl.gov)

In situ 3D imaging shows how hyperelastic materials deform and fail

Synchrotron experiments that quickly rotate a material during radiographic imaging have proven to be a useful technique to show changing 3D micro-structure without pausing an experiment. The method can explain how hyperelastic materials deform and fail during loading—information that is critical to performance for many modern material systems. For example, fast 3D-imaging rates are needed to see how damage progresses in materials that are crushed.

Using the high-brightness synchrotron at the Advanced Photon Source (APS) at Argonne National Laboratory, investigators collected 600 x-ray radiographs of a

Figure 1: (a) Successive 3D images of the tension testing of a 3D printed composite material (glass microballoon/Nylon) (b) the stress field of the materials response, (c) compression testing of a 3D printed microlattice and the corresponding finite element model of the deformation. Stress-strain (d) curves of the lattice as ligaments are removed.



sample as it was rotated 180°. The resulting 3D movies revealed deformation of the material at strain rates of $\sim 0.4 \text{ s}^{-1}$. Figure 1 (a) shows a 3D-printed composite material stretched to the point of breakage, causing crack initiation and growth perpendicular to the pull direction. The data indicate that the composite material delaminates at the glass microbeads/nylon plastic interface. The 3D imaging shown in (c) shows additively manufactured microlattice structures being compressed, which is a perfect starting point for finite element modeling.

Three-dimensional x-ray tomographic imaging can provide morphological information on the feature's structure and distribution, but the method does not have a high enough flux to image rapid deformation. The APS experiments show the bending, buckling, and fracture failure of materials in real time without pausing the experiment. Future experiments will include a novel load cell that allows researchers to collect 3D data at greater than 100 Hz, therefore deforming 10^2 s^{-1} strain rates. At this rate, real-world loading conditions will be more realistically investigated.

The APS experiments show the bending, buckling, and fracture failure of materials in real time without pausing the experiment

Publication citations: "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** (20):12185-12206 (2017)

"In situ X-ray synchrotron tomographic imaging during the compression of hyper-elastic polymeric materials," *Journal of Material Science* **51** (1):171-187 (2016)

Source of funding: Engineering Program, Enhanced Surveillance (Campaign 8), Institute for Materials Science, and Dynamic Material Properties (Campaign 2)

Researchers: **LANL:** Brian M. Patterson, James C.E. Mertens, Matthew Herman, Robin Pacheco, Trevor Shear, Lindsey Kuettner, Kevin Henderson; **ASU:** Jason Williams, Nikhilesh Chawla; **ANL:** Sun Tao, Kamel Fezzaa, Xianghui Xiao

Contact: Brian M. Patterson (bpatterson@lanl.gov)

PHYSICIST

ERIK WATKINS

Using dynamic x-ray scattering techniques, Erik Watkins works to understand materials' structural changes and chemical evolution at the meso-scale. He primarily examines carbon in detonating high explosives and shock-compressed materials.

I love inventing new and creative ways to look at tough scientific questions. Dynamic x-ray scattering experiments can assess material changes at extreme pressures, temperatures, and time scales. The kick I get out of this research stems from times when I glimpse something unexpected that no one has seen before. Sometimes this comes as instant gratification, when I see a strange signature or pattern develop as data is collected. Other times it comes during laborious data analysis, when we change our approach or perspective and a new story emerges.

Erik received a bachelor's degree from Hampshire College and went on to study bio-membranes and polymer thin films as a researcher at the Los Alamos Neutron Science Center.



Hampshire did not have grades or majors, so my undergraduate trajectory was like a random walk taking me from history into philosophy, psychology, neuroscience, and computer science before finally arriving at physics. Physics particularly appealed to me because it asks questions about the fundamental nature of the world in ways that are testable.

After college, I spent months driving around the 48 contiguous states, living out of the back of my car until I'd picked my favorite place—northern New Mexico. I spent a few months landscaping and doing night-shift factory work in Albuquerque before an opportunity to work at Los Alamos came up. The Lab saw in me an applicant with experience in physics and in driving forklifts—an interesting combination of skills for a neutron scattering facility where heavy shielding blocks must occasionally be moved. I took the job and am still grateful to have found an area with great natural beauty, a rural lifestyle, and cutting-edge research facilities.

After four years, Erik left Los Alamos to pursue his PhD at the University of California, Davis, and then to work as an instrument scientist at the Institut Laue-Langevin in France. A few years later, he returned to Los Alamos. Though his nomad days are largely over, he's still driven by a desire to explore.

Understanding structure at the mesoscale often results in important impacts on macroscopic materials properties, but this “middle” length scale can be difficult to measure. Dynamic x-ray scattering techniques such as small-angle x-ray scattering (SAXS) bridge the gap between the length scales, allowing us to explore the mesoscale. SAXS tells us about the shape and size distributions of particles or voids within materials. This knowledge provides insight into dynamic events that are critical to Los Alamos missions, such as probing carbon clustering in byproducts of high explosives, defects in material failure, and free-surface instabilities.

Erik Watkins aligns thin film samples on the Asterix neutron reflectometer at the Los Alamos Neutron Science Center to study the mesoscale structure of interfaces.

Dynamic localization in lattice structures

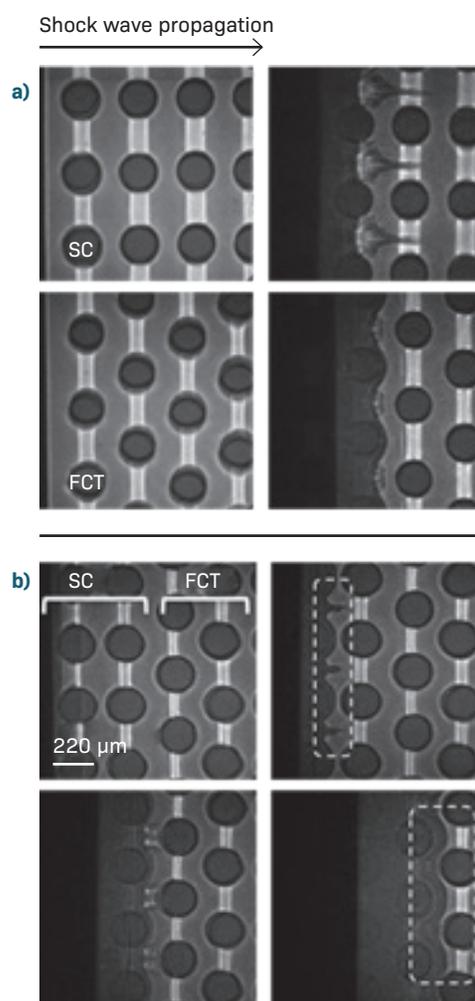
In studies that relied on the IMPact system for ULtrafast Synchrotron Experiments (IMPULSE) capability at Argonne National Laboratory, a team demonstrated the first direct measurement of shock wave modulation via microstructure control in microlattice polymer and energetic foams.

Better knowledge of matter at extreme conditions enables researchers to understand deformation mechanisms of materials that are important for aerospace and military applications. By tailoring the properties and mechanical function of these materials, engineers can develop novel materials with specific function and predictive performance.

Additive manufacturing (AM) techniques such as direct-ink write methods or stereolithography, structural hierarchy in materials can be the tuning feature that controls function and properties. However, these advances have been almost entirely related to tailorable mechanical response—very few studies have assessed the performance of these materials under high-strain-rate deformation at extreme conditions.

The study was enabled by recent advances that combined dynamic loading platforms with advanced light sources and in situ diagnostic techniques; one example is the multi-frame x-ray

Figure 1: (a) Dynamic phase-contrast imaging of shock wave propagation in simple cubic (top) and face centered tetragonal (bottom) elastomer foam architectures. Structural organization dictates how the shock wave couples to the foam. (b) Graded “flow” was demonstrated over <1 mm of propagation distance as the wave propagated from simple cubic to face-centered tetragonal structures.



phase contrast imaging system developed by Los Alamos that is located at the Dynamic Compression Sector at Argonne. Diagnostic advances are still needed to better understand discrete behavior at the sub-micron level. Although the phenomenon observed here was the first of its kind, advances in diagnostics are needed to push the envelope toward understanding discrete behavior at the sub-micron level. An increased field of view for imaging diagnostics would also allow interrogation of components that are more relevant to real world applications, such as armor or structural components in space-reentry vehicles.

Advances in diagnostics are needed to push the envelope toward understanding discrete behavior at the sub-micron level

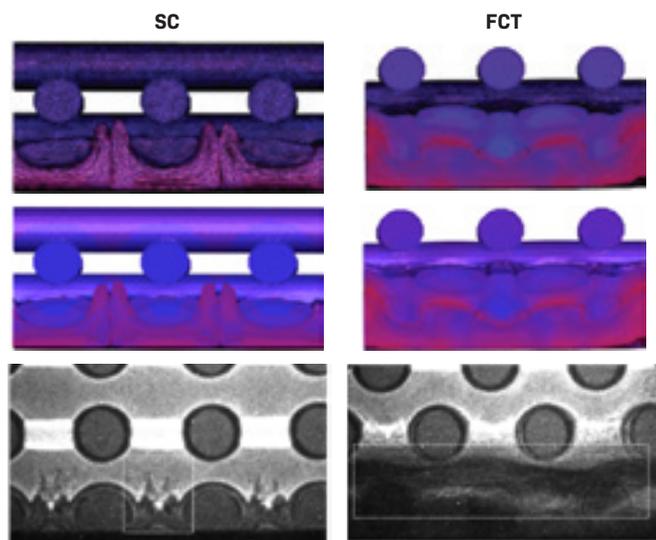


Figure 2: Shock wave experiments were modeled using the Finite Element code ABAQUS.

Publication citations: “Controlling Shockwave Dynamics Using Architecture in Periodic Porous Materials,” *Journal of Applied Physics* **21**, 135102 (2017)

“Characterizing the Dynamic Behavior of Additive Manufactured Mesoscale Energetic Materials,” Joint Army-Navy-NASA-Air Force Propulsion Meeting Proceedings (2017)

Source of funding: Los Alamos Laboratory Directed Research and Development program and Dynamic Material Properties (Campaign 2)

Researchers: LANL: Bradford E. Clements, David S. Montgomery, Alexander Mueller, B. Branch, A.M. Schmalzer, B.C. Clements, A. Ionita, B.M. Patterson, P.R. Bowden, B.J. Jensen, B.C. Tappan, D.M. Dattelbaum, A.H. Mueller

Contact: Brittany Branch (bbranch@lanl.gov)

Visualization of real-time phase transformation points to miscalculation in meteor sizes

Scientists have long known that meteor impacts can change silicates into an amorphous phase known as diaplectic (shocked) glass. The question is how this shocked glass forms—does the rock become molten first or can glass result from the compression release process? New findings indicate that a shocked glass can form on release without melting.

Previously, scientists have tried to estimate the amount of pressure needed to cause this transformation by examining debris from meteor impacts and by squeezing mineral samples in the lab, but they were unable to observe the process as it unfolded. This study shows the first-ever shock-release amorphization of a silicate step-by-step using femtosecond x-ray diffraction (XRD) (Fig. 1).

Using in situ XRD and an intense laser beam that created a shock wave, the team showed that a miscalculation has led

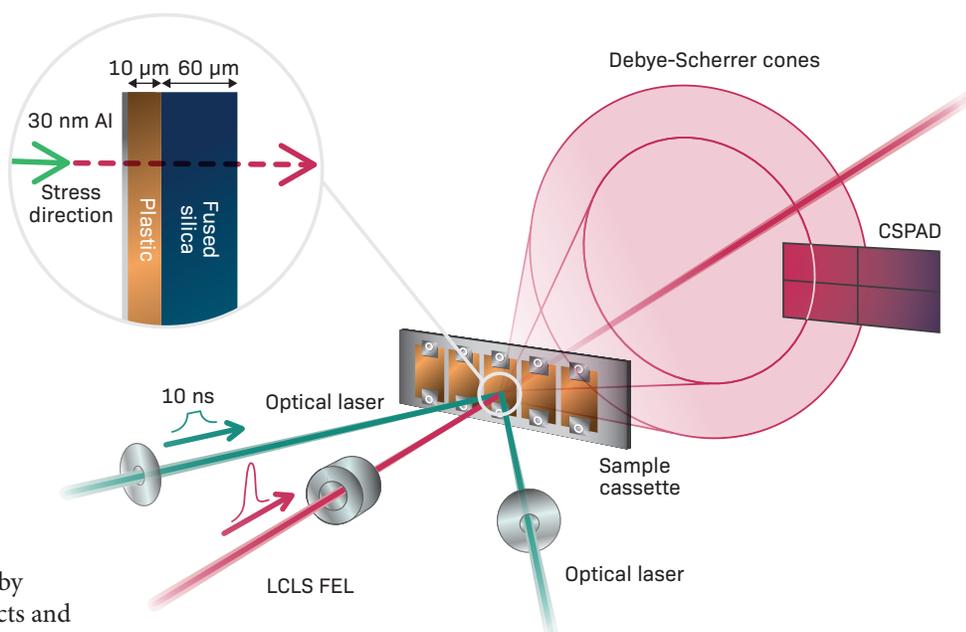


Figure 1: The lattice response of the sample was captured in a Debye-Scherrer geometry. Inset: example of XRD resulting from azimuthal integration of Cornell SLAC Pixel Array Detector data for a suite of time delays under shock compression. A schematic of the target is shown on the right side for each time delay (orange is plastic, blue is fused silica). A dashed line indicates the approximate location of the shock front; arrow is the shock propagation direction.

to inflated assumptions of impactor size; the peak pressure needed to form shocked glass is actually 25% lower than previously thought.

This demonstration of high-pressure metastability was mapped with ultrafast XRD. Continued dynamic materials studies will take this research even further by allowing structural determination of non-crystalline materials and by performing the time-dependent measurements on a single shock event. Future work includes developing new techniques in coherent x-ray imaging to examine extreme chemistry in nano- to microscale 3D structures, temperature diagnostics, and x-ray spectroscopy techniques.

The Matter in Extreme Conditions (MEC) instrument used to conduct this study combines SLAC's Linac Coherent Light Source with high-power optical laser beams and a suite of dedicated diagnostics tailored for warm-dense-matter physics, high-pressure studies, shock physics, and high-energy-density physics. Los Alamos-based XRD analysis tools and sample characterization tools were used on this and other MEC campaigns, and LANL researchers are collaborating on numerous experiments at SLAC.

The peak pressure needed to form shocked glass is 25% lower than previously thought



Publication citations: "Ultrafast visualization of crystallization and grain growth in shock-compressed SiO₂," *Nature Communications* **6**, 8191 (2015)

"Time-resolved diffraction of shock-released SiO₂ and dielectric glass formation," *Nature Communications* **8**, 1481 (2017)

Source of funding: Dynamic Material Properties (Campaign 2) and a Reines Postdoctoral Fellowship, which is supported by Los Alamos Laboratory Directed Research and Development program

Researchers: LANL: A. Gleason, C. Bolme, R. Sandberg

Contacts: Arianna Gleason (ariannag@stanford.edu) and Cindy Bolme (cbolme@lanl.gov)



PHYSICIST

NENAD VELISAVLJEVIC



Nenad Velisavljevic began experimenting in high-pressure materials research as an undergraduate student. This path transitioned seamlessly into his current focus: x-ray synchrotron sources. Nenad has spent much of his career doing experiments at the (now-closed) National Synchrotron Light Source at Brookhaven National Laboratory, Cornell High Energy Synchrotron Source, and the newly opened High Pressure Collaborative Access Team (HPCAT) sector at the Advanced Photon Source.

I study material properties at extreme pressure-temperature conditions. Materials put through these conditions behave unusually: they might turn transparent or become extremely hard, like graphite does when it becomes a diamond. I'm focused on understanding how the material properties change and at what pressure and temperature the changes occur, and so on. I also develop new or advanced experimental capabilities that help researchers learn about material behavior at these extreme conditions.

There is a certain element of inspiration and motivation that comes with being a part of the Los Alamos story. Realizing that the work we do directly impacts our nation—from shaping policy to addressing interesting key problems—gives you a bigger sense of the responsibility. With that recognition comes even more motivation to overcome challenges and produce scientific and engineering achievements.

Nenad's work, interesting in a fundamental sense, has important implications for Los Alamos and its core mission of certifying the nuclear stockpile.

In a global sense, varying pressure-temperature also explains some of the fundamental physics that help engineer or manufacture materials with improved/advanced properties. Studying and understanding material properties at extreme conditions helps answer a broad range of technical questions about weapons and other systems of interest to the Laboratory. In short, through fundamental research we can address specific mission-related challenges.

Nenad Velisavljevic uses a gas loading system to prepare diamond anvil cells for high-pressure material measurements.

Probing the atomic structure of metals shocked to high pressures using x-ray diffraction

Understanding the dynamic response of materials at extreme conditions is important to understanding parts of fundamental condensed-matter physics, flow behavior, and planetary and geological sciences. These types of material response studies have relied on continuum diagnostics such as gauges and velocimetry for more than 50 years, but recently, new synchrotron-enabled techniques such as x-ray diffraction (XRD) and x-ray phase contrast imaging (PCI) have provided unique opportunities for studying materials at extremes at the microscopic scale. These dynamic experiments can help locate phase boundaries, obtain

New synchrotron-enabled techniques provide unique opportunities for studying materials at microscopic extremes

equation-of-state information on the pure phases, and understand microstructural evolution during dynamic loading.

Using dynamic XRD at the new Dynamic Compression Sector (DCS) at Argonne National Laboratory, researchers shocked both iron and cerium to high pressures in well-defined plate impact experiments, detailed below.

CERIUM

This element exhibits a rich phase diagram that includes four solid phases at zero pressure, additional solid phases at higher pressures, and an anomalous melt boundary. The well-known isostructural phase transition that occurs in cerium at low pressures was especially interesting to this study. This phase boundary ends at a unique solid-solid critical point above which the volume change is continuous. Below the critical point, crossing this phase boundary leads to a large volume collapse that results in a low-pressure melt transition that

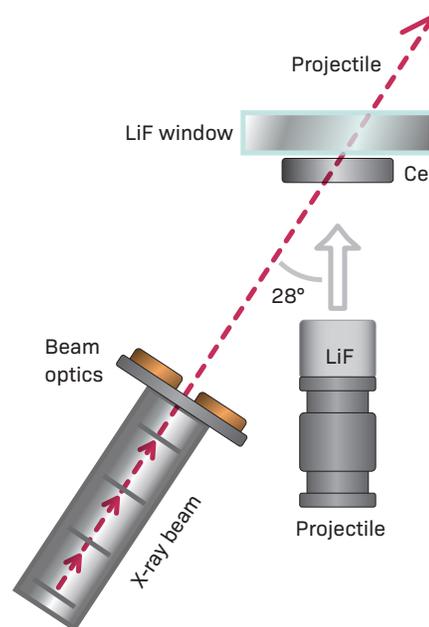


Figure 1: Experiment configuration for dynamic XRD experiments. A projectile with a lithium fluoride (LiF) impactor impacts a cerium sample backed by a LiF window. Impact generates a shock wave that compresses the cerium to high pressure. By changing the projectile velocity, the stress is varied to systematically step through the melt transition.

puts cerium in a liquid state. This study used dynamic XRD (Fig. 1) to study the melt transition at the microstructural level to determine the stress level at which cerium melts.

The data showed a complete melt transition near 16 GPa, which provides information essential to further develop and validate existing multiphase equations of state that describe the dynamic response of cerium. The data also provided an important verification for indirect methods of examining melt, such as sound speed and pyrometry measurements.

IRON

Iron's high-pressure response has been studied for decades because this element is so abundant in the earth's core (and therefore is geophysically significant). Although prior experiments have shown that a well-known polymorphic transition occurs in iron at 13 GPa, there is a lack of data describing this transition at the microscopic level for dynamic loading conditions. These experiments sought to determine what shock-stress level caused the iron sample to fully transform to the epsilon phase when shocked above 13 GPa.

The team used dynamic x-ray diffraction to perform shock wave experiments that showed the evolution of iron's microstructure as it was shocked from the low-pressure alpha phase to the high-pressure epsilon phase. The resulting data were well correlated to data from previous interface velocimetry measurements. They first showed clear

diffraction peaks consistent with the alpha phase at low pressures, then a mixed phase region, and lastly a complete transition to a hexagonal close-packed phase for longitudinal stresses of more than 18 GPa for peak stress values near 17 GPa (Fig. 2). The results may provide insight into the atomic mechanisms that govern shock-induced phase transitions in metals.

Publication citations: "Dynamic x-ray diffraction to study the shock-induced α - ϵ phase transition in iron," AIP Conference Proceedings **1979**, 040001 (2018)

Source of funding: Dynamic Material Properties (Campaign 2)

Researchers: LANL: B.J. Jensen, B. Branch

Contact: Brian Jensen (bjensen@lanl.gov)

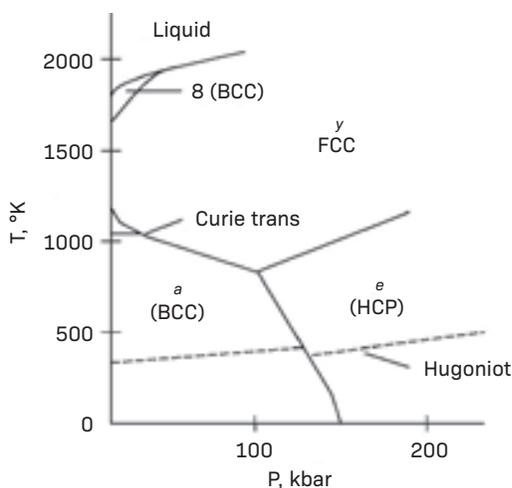
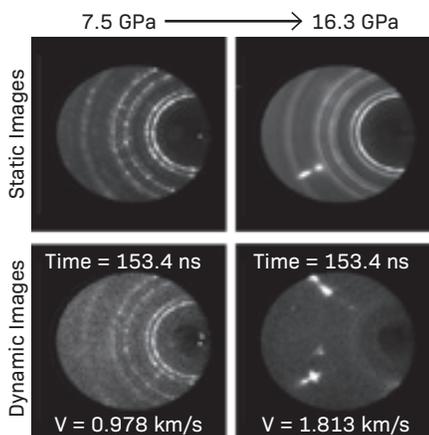


Figure 2: (far left) Example XRD data for two experiments at impact stresses of 7.5 and 16.3 GPa. Static images taken prior to impact are shown in the top row for the two impact stresses. Dynamic Laue images taken during shock loading showing the loss of x-ray intensity as the impact stress is increased. The loss of intensity and diffraction rings in the image are a signature of the melt transition of cerium.

Figure 3: (left) Using dynamic x-ray diffraction, the team performed shock wave experiments showing the evolution of iron's microstructure as it was shocked from the low-pressure alpha phase to the high-pressure epsilon phase.

Dynamic compression at light sources unlocks key information about phase transitions in metals

The ability to predict the performance of a material in extreme environments depends on understanding how that material behaves under stresses. Phase transformations (how one phase changes to another and at what rate) have been a large uncertainty in the effort to understand stressed materials. However, new light source facilities are enabling researchers to directly observe phase transitions during shock loading for the first time. This capability reveals key details about the kinetics (or rates) and pathways of phase transitions.

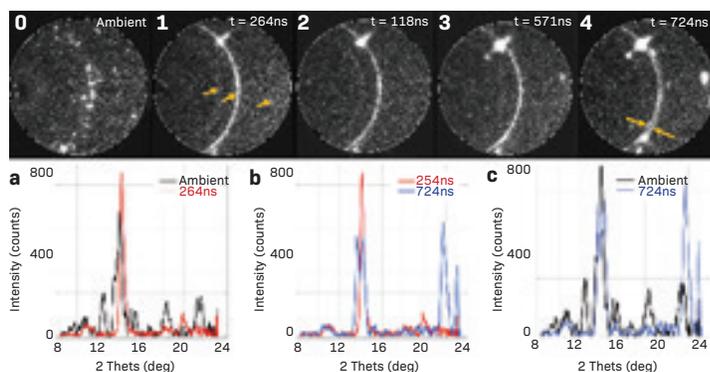
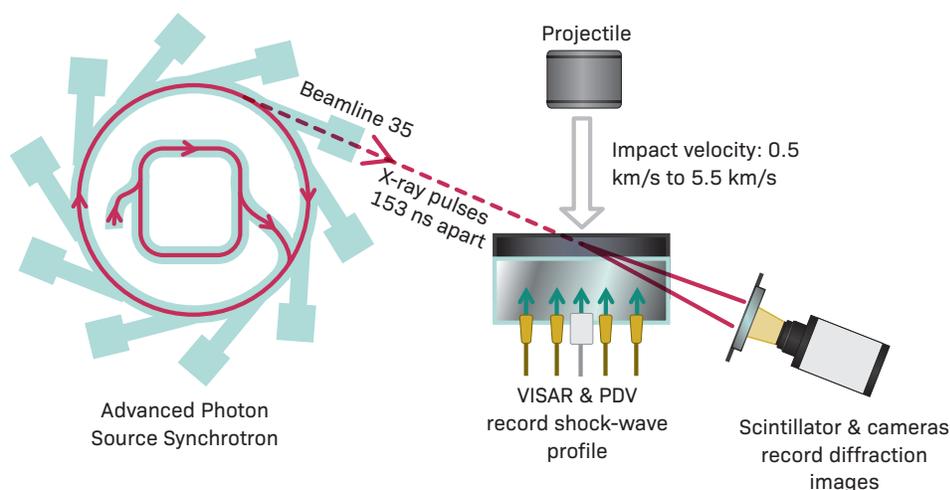


Figure 1: (above) A schematic of the experiments performed at the Dynamic Compression Sector. The projectile is launched at high velocity into the target. X-ray pulses spaced to every 153 ns from the synchrotron pass through the sample. Diffraction patterns are captured by a high-speed camera setup.

Figure 2: (left) Diffraction patterns of ambient and shocked Ti, showing new omega ring formation after loading (yellow arrows in Frame 1). At late time (Frame 4), strong ring bifurcates into distinct alpha and omega peaks. Line profiles show the evolution of the integrated intensity of the rings over time.

A time-resolved look at the evolution of the microstructure during shock-loading would not have been possible without in situ techniques at light sources

In a study that used the Impact Facilities of the Dynamic Compression Sector at the Advanced Photon Source, Los Alamos and Washington State University researchers were able to watch the microstructure of titanium as it changed during shock loading. Previous studies have shown that the presence of omega phase modifies the strength and ductility of titanium, but the details of this progression were largely unknown.

The team collected transmission Laue diffraction patterns for thin foils of titanium that were shocked above the phase-transition stress. The resulting data showed that the element's microstructure was rapidly refined immediately after impact. It also showed that titanium did not undergo a full transformation to omega phase at these conditions, and, unlike similar metals, did not revert from omega to alpha on unloading. Additionally, the kinetic transition from alpha to omega was somewhat sluggish. A time-resolved look at the evolution of the microstructure during shock loading would not have been possible without in situ techniques at light sources.

Publication citation(s): "In-situ Experiments to Capture the Evolution of Microstructure During Phase Transformation of Titanium Under Dynamic Loading," *European Physical Journal Web of Conferences*, 12th International DYMAT Conference in Arcachon, France, Sept 9-14, accepted (2018)

"Shock and Microstructural Characterization of the α - ω Phase Transition in Titanium Crystals," *Journal of Dynamic Behavior of Materials* **3**, 526-533 (2017)

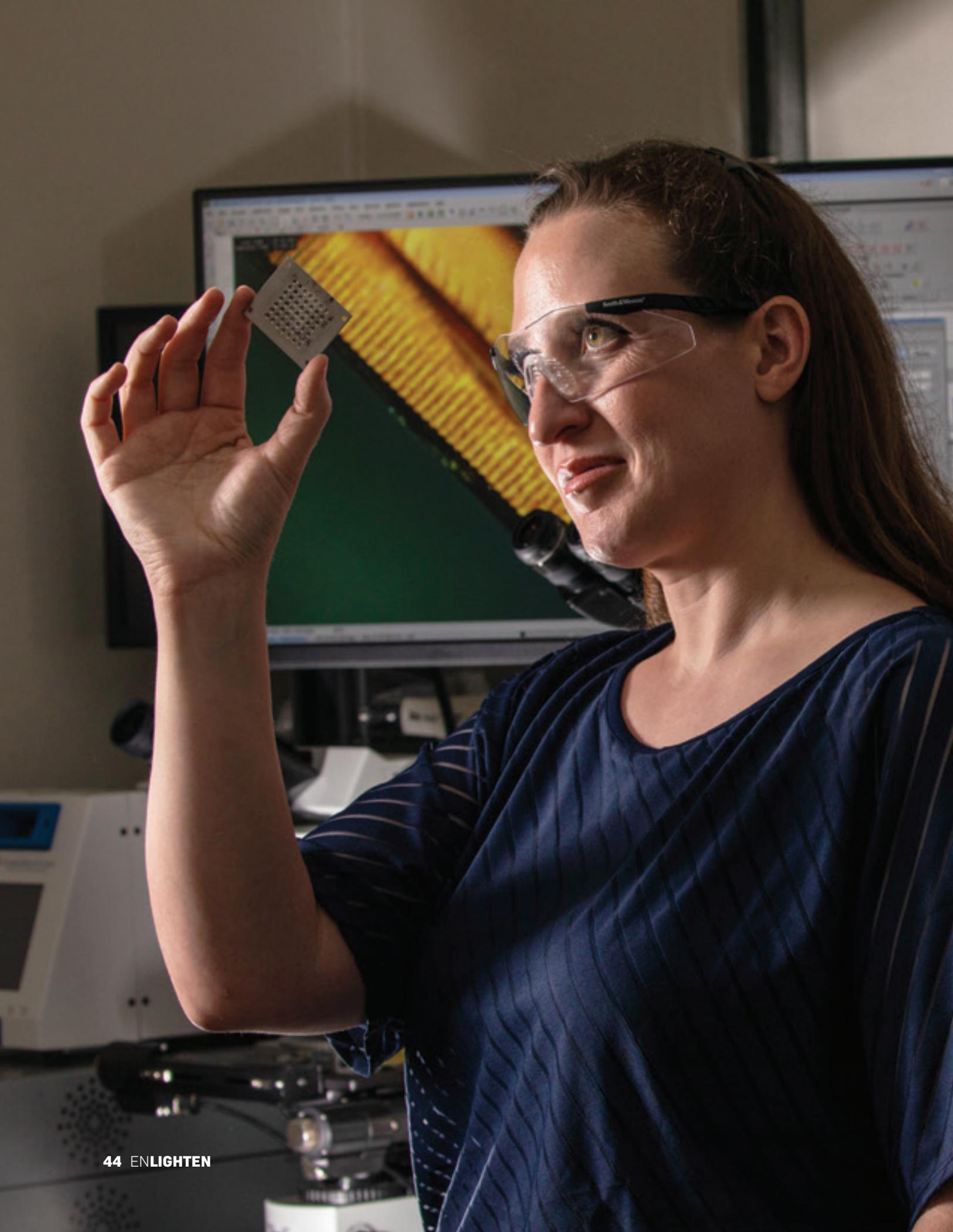
"The alpha-omega phase transition in shock-loaded titanium," *Journal of Applied Physics* **122**, 045902 (2017)

Source of funding: Dynamic Material Properties (Campaign 2)

Researchers: LANL: Ben Morrow, David Jones, Ellen Cerrera;

Washington State University DCS: Paulo Rigg

Contact: Ben Morrow (morrow@lanl.gov)



SHOCK PHYSICIST

CINDY BOLME

Cindy Bolme develops ultrafast time-resolved diagnostics for shock and detonation physics. She came to Los Alamos as a research scientist after receiving her PhD in physical chemistry from the Massachusetts Institute of Technology in 2008.

My team develops predictive computational capabilities and designs materials for specific functionalities. The materials we use for the Los Alamos mission were developed through trial and error, which gives us an empirical understanding of how they will behave. I'm working to gain new information through experiments that explain the mechanisms of dynamic materials response. Most of my research and development is focused on creating new diagnostics to explain how materials respond to compression and developing models that better represent the material's behavior.

Most of Cindy's dynamic compression work takes place at the Linac Coherent Light Source and the Advanced Photon Source. As Los Alamos National Laboratory's point of contact for materials experiments at international x-ray free-electron laser facilities, she collaborates with researchers to help advance their studies with brilliant x-ray beams.

New x-ray facilities have given us the ability to perform unprecedented experiments. We are now able to measure important fundamental processes that are occurring; for example, we can measure the timescale during which the atoms or molecules of a material will rearrange, melt, or crystallize. These measurements are important for understanding the material response since the response is governed by the material structure.

The future MaRIE [Matter-Radiation Interactions in Extremes] capability would allow a whole new class of experiments that also include measurements in different orientations and with different types of probes. It would also let us measure material dynamics in a single experiment—at current x-ray free-electron lasers, we have to repeat the same experiment many times while changing the time delay between the shock wave and x-rays. MaRIE would show us how unique features or experimental conditions influence material response.

Cindy Bolme inspects targets for laser shock experiments that will be performed on an x-ray free-electron laser.

Using x-rays to study detonator initiator systems

Explosive bridge wires (EBW) and explosive foil initiators (EFI) are key to initiating explosives in weapons systems.

In spite of their wide application, understanding exactly how these two components operate has been a longstanding engineering challenge. Current detonator models can capture performance characteristics but lack details of the initiation process; because of this, models assume point-detonation and neglect the early-time physics entirely. Several questions about the initiation process remain, and this research sets out to understand two of them: (1) Is the mechanism for EBWs' performance a compaction-to-detonation process, a result of thermal initiation, or a combination of both? (2) What are the plasma densities and how do they evolve, leading to the flyer/bridge response observed during launch?

Experiments at the Advanced Photon Source have used Los Alamos National Laboratory's multi-frame x-ray phase contrast imaging (mPCI) system to study the response of EFIs and EBWs for years. These experiments take advantage of the penetrating and imaging power of the x-ray beam, the spatial resolution of 1–3 μm , and the 80-ps width x-ray bunch that

Applying the mPCI system to EFIs and EBWs will help pin down critical parameters and inform future designs

provides data precisely resolved in time. Some of these experiments are shown above (Fig. 1).

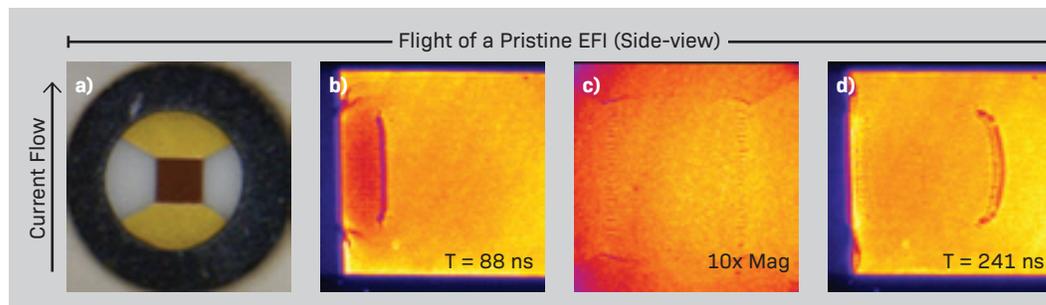


Figure 1: (above) Using mPCI to study the response of EFIs. (a) Photo of an EFI the parylene flyer (brown) is held between the two copper cathodes (gold). (b,d) Images of the EFI flyer in-flight viewed from the side. (c) Early time image looking through the flyer as the current flows through, initiating the launch. Effects of a cylindrical defect (hole) are shown in (e and g) and a gouge in the flyer is shown in the square in (f). Radiation effects at 4800 Gy are shown in (h).

The possibility of reconstructing high-velocity flyer morphology is an exciting opportunity to provide the high-fidelity data needed for model validation. To this end, a team of researchers from Los Alamos and Lawrence Livermore National Laboratory has attempted a 3D tomographic reconstruction of an EFI flyer in flight. A series of experiments provided images of EFIs in action while rotating the orientation of a flyer in the beam. Algorithms of computed tomographic reconstructions generated a 3D image of the flyer at two different times from initiation (Fig. 2).

Applying the mPCI system to EFIs and EBWs will help explain their performance, pin down critical parameters, validate current magnetohydrodynamic models and stockpile systems, address life-extension programs, and inform future designs. Efforts are underway to further develop the mPCI system to enable density retrieval for multiple-constituent materials, making it possible to study the plasma behind the flyer.

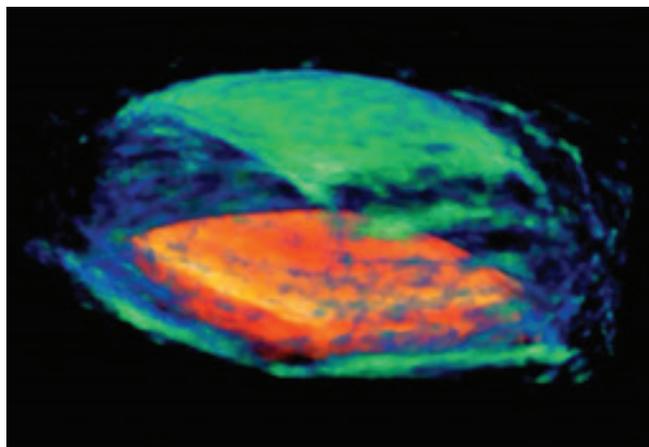
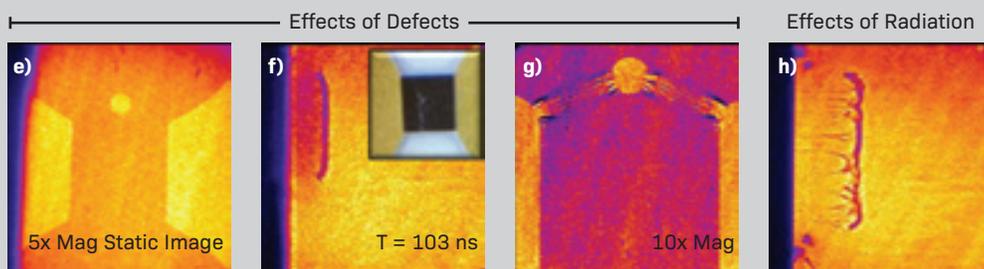


Figure 2: (left) 3D reconstruction of an EFI in flight at two flight distances (or times from initiation). The orange color portion indicates the early time image and the green colors indicate the later time.

Publication citations: “X-ray Imaging and 3D Reconstruction of In-Flight Exploding Foil Initiator Flyers,” *Journal of Applied Physics* **119**, 235901 (2016)

“The Effect of Surface Heterogeneities in Exploding Metallic Foils,” AIP Conference Proceedings **1979**, 180007 (2018)

“Shock Waves Generated by Exploding Bridge Wires in Condensed Media,” submitted to the 2017 GSCCM Shock Compression Conference of Condensed Matter, Missouri (2017)

“Dynamic Exploding Foil Initiator Imaging at the Advanced Photon Source,” AIP Conference Proceedings **1979**, 160023 (2018).

Source of funding: W88 Refresh, B61 LEP, Joint Technology Demonstrator, Dynamic Material Properties (Campaign 2), Joint Munitions Program

Researchers: LANL: N. Sanchez, B.J. Jensen; LLNL: T. Willey, K. Champley, R. Hodgkin, L. Lauderbach, M. Bagge-Hansen, C. May, T. van Buren; **Atomic Weapons Establishment:** W. Neal; **Mission Support and Test Services:** A.J. Iverson, C.A. Carlson

Contacts: Nate Sanchez (nsanchez@lanl.gov) and Brian Jensen (bjensen@lanl.gov)

These experiments are an example of science on the road-map to MaRIE, LANL’s proposed experimental capability for studying Matter-Radiation Interactions in Extremes. This capability’s combination of hard x-rays from an x-ray free-electron laser and diagnostics such as PCI and coherent diffractive imaging will provide improved timing and spatial resolution along with the increased x-ray intensities and energies needed to image complete systems.

Radiographs show ‘lost time’ of detonator function

Despite their widespread use and reliability, the mechanism of exploding bridge wire (EBW) detonator function is still controversial. After realizing that secondary high explosives are organic crystals with the same range of density as addressed by medical x-ray radiography, Los Alamos National Laboratory investigators combined a tabletop-scale x-ray apparatus with a suite of diagnostics to make direct observations on the mechanism of detonator function.

The researchers found they could directly observe several features within the detonator in what was previously called “lost time” during function. During this time in the detonation kernel area, there was a continuous rise in temperature caused by the bridge wire bursting prior to detonation’s onset. The data showed a density wave that traveled at 3 km/s

launched when the bridge wire burst and a simultaneous temperature ramp during the lost time. Once the temperature was high enough, kinetics of the explosive PETN took over to show onset of a detonation wave (Fig. 1). This is the first direct observation of what happens in the lost

This modeling work provides the first-ever direct link between a thermal input and a detonation output

time and creates the detonation kernel of an EBW detonator. The modeling work that has resulted from these observations has provided the first-ever direct link between a thermal input and a detonation output.

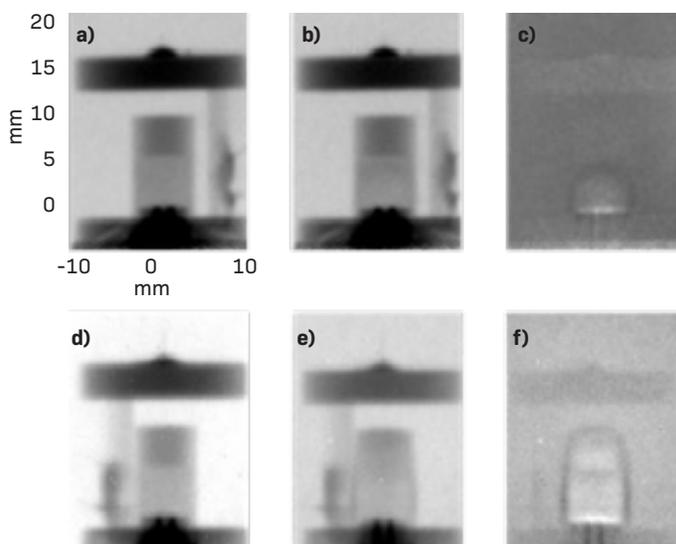


Figure 1: (a, d) is a static x-ray transmission image through an RP-80 detonator. (b, e) is the 50-ns x-ray transmission image collected during detonator function. (c, f) is the ratio showing change in detonator density during function. The top frames (a, b, c) were taken earlier in function time than the bottom frames (d, e, f).

The study was done using simultaneous x-ray transmission, temperature, and visible light emission to separate out the density wave from the detonation wave and view the onset of detonation after a temperature ramp. This approach allowed the researchers to propose a new explanation of detonator function and to directly observe the transition from a



Figure 2: (right) The Lab-scale Asynchronous Radiographic System, a small-scale radiography device for continuous high-speed x-ray imaging of spontaneous dynamic events such as explosions, reaction-front propagation, and material failure.

thermal input to a detonation output. Early demonstration work utilizing the Proton Radiography Facility at Los Alamos guided the design of the tabletop x-ray imaging tool. The apparatus was designed using off-the-shelf x-ray sources from medical and nondestructive testing industries, paired with state-of-the-art scintillator and imaging techniques. This Lab-scale Asynchronous Radiography Setup (Fig. 2) was used in the diagnostics suite, as were ultrafast framing cameras and optical pyrometry techniques available at Los Alamos. Modeling of the detonator function was done using the Henson-Smilowitz kinetics and a method of characteristics-based wave coalescence.

This research area would benefit from pressure measurements and spatially resolved temperature measurements, such as those proposed for the MaRIE, or Matter-Radiation Interactions in Extremes, capability. The researchers would also like to apply x-ray diffraction to the initiation volume in the detonator to directly measure the material phase during initiation in the detonator kernel. As a result of this work, the team is scheduled to return to Proton Radiography Facility and will propose experiments at the Advanced Photon Source synchrotron, both informed by these lab-scale results.



Publication citation: “Experimental Observations of Detonator Function,” Proceedings of APS SCCM, Missouri (2017)

Source of funding: DOE/DoD Joint Munitions Program, DOE’s Nuclear Safety Research and Development program, Engineering Campaign 6

Researchers: LANL: Laura Smilowitz, Bryan Henson, Dennis Remelius, Natalya Suvorova, Dave Oswald, and Pam Bowlan

Contact: Laura Smilowitz (smilo@lanl.gov)

MATERIALS CHEMIST

MILLCENT FIRESTONE



Millie Firestone identifies and advances opportunities that bridge basic nanoscience with Los Alamos National Laboratory's materials mission. She is a materials chemist focused on synthesizing structured soft matter and characterizing it with neutron and x-ray scattering techniques.

I always tell people I was born to do this. I have an innate passion for chemistry and physics that I've turned into a career focused on the exploration, discovery, and synthesis of novel nanomaterials.

Millie, who received her PhD in chemistry from Northwestern University in Illinois, has worked at the University of Illinois, Urbana-Champaign, and she led a DOE Basic Energy Sciences Materials Sciences and Engineering program in biomolecular materials at Argonne National Laboratory. In 2013, she joined the Center for Integrated Nanotechnologies (CINT) at Los Alamos to lead its Soft, Biological, and Composite Materials Thrust.

My background in organic chemistry and nanoscience lets me evaluate post-detonation products in a nontraditional manner, providing a different interpretation of work historically carried out at Los Alamos. In turn, the resources and scope of the research done at Los Alamos have given new perspective to my work: I have the unique opportunity to use a nanoscientist's tools to explore the potential of nanoscale carbons that are only produced under extreme synthetic conditions. By characterizing these byproducts, I can assess their potential as new materials.

Millie has a sharp interest in panoramic materials and composites—an interest she hopes to advance using Matter-Radiation Interactions in Extremes (MaRIE), the Lab's proposed capability for time dependent, in situ materials science at the mesoscale.

This light source would integrate spectroscopy with x-ray scattering for single-shot, multi-length scale characterization. This and many other proposed features would enable MaRIE to probe materials during real-time synthesis and production, such as in additive manufacturing and under extreme conditions. For example, it may be possible to simultaneously collect information on local metal coordination environments while probing molecular, nano-, and mesostructure. I'm very excited to tailor light source capabilities to be useful in nontraditional reaction environments, such as the conditions one finds in mission-related challenges.

Millie Firestone uses a CINT x-ray scattering capability to evaluate materials nanostructure before further characterization at outside facilities.

Data methods enhance ultrafast x-ray imaging

Traditional x-ray crystallography is an extremely powerful technique for understanding periodic structures, but nature is full of nonperiodic “minority” structures with impurities and defects that can dominate material properties and functions. These structures are critical to validating the modeling and code used for many Los Alamos National Laboratory and National Nuclear Security Administration missions. Developing materials that do not exist in nature is also key to Los Alamos missions.

Los Alamos researchers and collaborators developed a new framework that may demonstrate ultrafast x-ray imaging at an accelerated pace

at Los Alamos, experiments at the Advanced Photon Source (APS), high-performance computing, and theory development, Los Alamos researchers and collaborators developed a new

Efficient hard x-ray imaging at a rate above 100 million frames per second can benefit many applications, but several long-term challenges must be addressed before the technique is ready to work on these applications. Using benchtop experiments

framework that may demonstrate ultrafast x-ray imaging at an accelerated pace. The new path combines hardware development with novel data methods to relax the stringent performance requirements for components used in future ultrafast imaging x-ray cameras. The building blocks of the new approach are already in place, thanks to a series of prototype camera systems that was proposed by a new, multi-institute consortium. These systems will be tested first at the APS facility at Argonne National Laboratory and then verified using a fully integrated ultrafast imaging test.

Until recently, high-speed imaging technology development has been a hardware-centric effort requiring a significant investment, so there are few high-speed imaging systems in the DOE complex. However, data methods such as sparse sensing are revolutionizing imaging, and new developments indicate that combining hardware and data methods could improve high-speed imaging development and result in new applications. For example, this new framework for ultrafast x-ray imaging may have applications in dynamic material evolution under shock wave and other impulse conditions (Fig. 1).

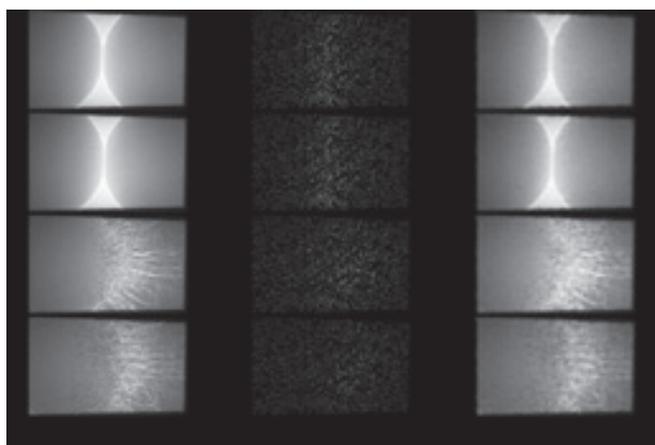


Figure 1: Sparse-sensing data methods can be used to enhance the performance of ultrafast imaging applications. (Left column) Raw images taken using an exiting high-speed camera. (Middle column) Random sampling of the raw imaging with only 10% of the original data. (Right column) Reconstructed images using 10% raw data and sparse imaging codes.

Publication citations: “A compressed sensing x-ray camera with a multilayer architecture,” *Journal of Instrumentation* **13**, C01035 (2018)

“High-sensitivity silicon ultraviolet p+-i-n avalanche photodiode using ultra-shallow boron gradient doping,” *Applied Physics Letters* **111**, 081109 (2017)

“Ultrafast inorganic scintillators for GHz hard X-ray imaging,” in preparation (2018)

Source of funding: Dynamic Material Properties (Campaign 2), MaRIE, and NNSA Stewardship Science Academic Programs

Researchers: LANL: Oleksandr Iaroshenko, Shengtai Li, Pinghan Chu, G. T. Kenyon, Zhehui (Jeph) Wang; **Argonne National Laboratory:** Niranjana Parab; **Purdue University:** Wayne Chen; **Fermi National Accelerator Laboratory:** Ted Liu and Ron Lipton; **University of Wisconsin, Madison:** Zhenyang Xia, Zongfu Yu, Zhenqiang (Jack) Ma; **California Institute of Technology:** Liyuan Zhang and Renyuan Zhu; **University of Nevada, Las Vegas:** Ke-Xun (Kevin) Sun

Contact: Zhehui (Jeph) Wang (zwang@lanl.gov)

3D x-ray diffraction imaging of defects in metals

Defects are generated in materials that are subjected to varying loading conditions. These defects influence and can even dictate a range of properties, from mechanical strength to failure, battery performance, radiation resistance, and crystal growth and dissolution. Researchers have long sought to understand not only how these defects are generated but also how they contribute to strain in a material. This information is important for predicting material failure and designing new materials with specific functionality.

Researchers from Los Alamos and Argonne national laboratories are using Bragg coherent x-ray diffraction imaging (BCDI) at Argonne's Advanced Photon Source to measure (1) the strain fields associated with various defects and (2) how the generation and evolution of these defects during loading contributes to the accumulation of strain in the microstructure of metals.

Currently, the conventional means of inferring information about nanoscale strain inside a material are either digital image correlation or digital volumetric correlation. Both techniques measure surface strain and offer x-ray tomography for bulk strain measurements with a greatly reduced spatial resolution, making them unsuitable for direct measurements of spatially resolved distribution of

Researchers have long sought to understand not only how defects are generated but also how they contribute to strain in a material

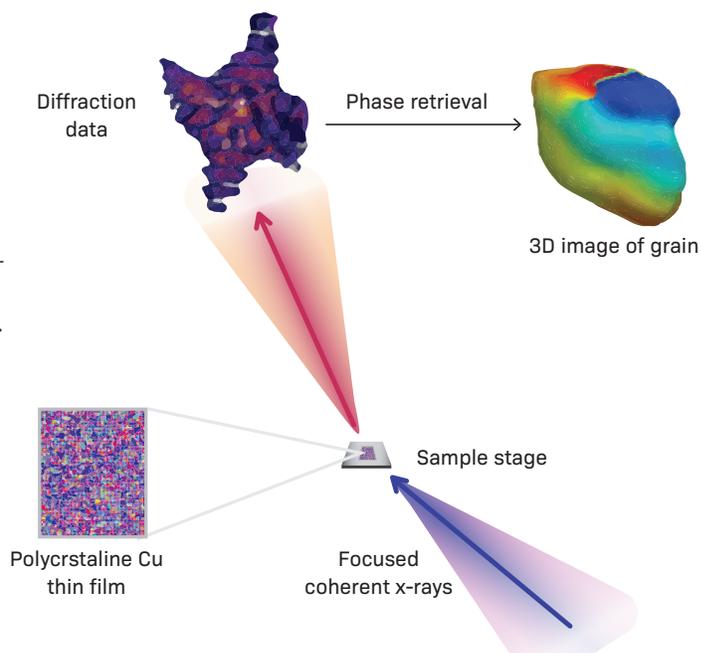


Figure 1: Coherent x-ray diffraction imaging. Focused coherent x-ray pulses are incident on the polycrystalline copper sample. The 3D speckle pattern at the (111) Bragg peak is recorded from two-dimensional diffraction slices obtained by rocking the sample stage through small angles.

two-dimensional lattice defects such as dislocations at the nanoscale. In contrast, BCDI enables quantification of 3D strain fields due to lattice defects such as those generated in an irradiated nanocrystalline material.

As an example, researchers conducted a proof of principle BCDI experiment that measured strain field of a freestanding polycrystalline copper film after tensile loading. By integrating the observed 3D structure into atomistic modeling, they showed that the measured strain field corresponded to a screw dislocation—that is, a specific form of a dislocation in the crystal's lattice structure.

The thin films used in these experiments were manufactured in the Center for Integrated Nanotechnologies, a DOE Office of Science User Facility operated jointly by Los Alamos and Sandia national laboratories. Film characterization was performed in the electron microscopy laboratory at Los Alamos.

The researchers also investigated how strain field varies as a function of helium concentration in metals—this is important for materials subjected to radiation extremes (Fig. 2). This work will be continued by combining BCDI with high-energy-diffraction microscopy to simultaneously obtain information about a material's 3D microstructure and its nanoscale defect distribution and strain information. Currently, the technique is limited by the coherence length, which means data can only be obtained from single grains. As the light sources develop, the experimentalists hope to apply this technique to multiple grains in a microstructure, essentially building a pathway to Matter-Radiation Interactions in Extremes, the Lab's proposed capability for time-dependent, in situ materials science at the mesoscale.

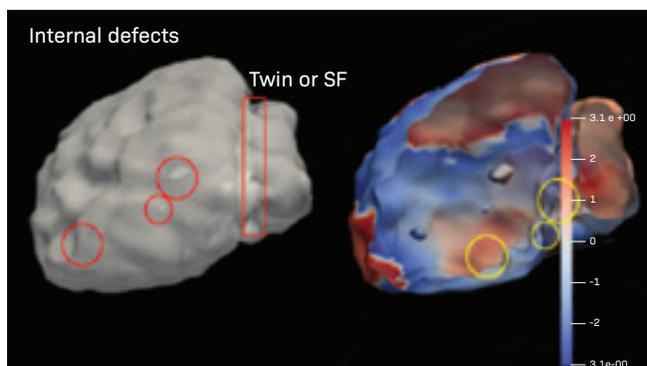


Figure 2: Displacement field with 2000 ppm He⁺ implanted into 33-nm copper nanoparticles obtained from BCDI experiments and reconstructed.

Publication citation(s): “Three-dimensional x-ray diffraction imaging of dislocations in polycrystalline metals under tensile loading” (under review)

Source of funding: Los Alamos Laboratory Directed Research and Development program

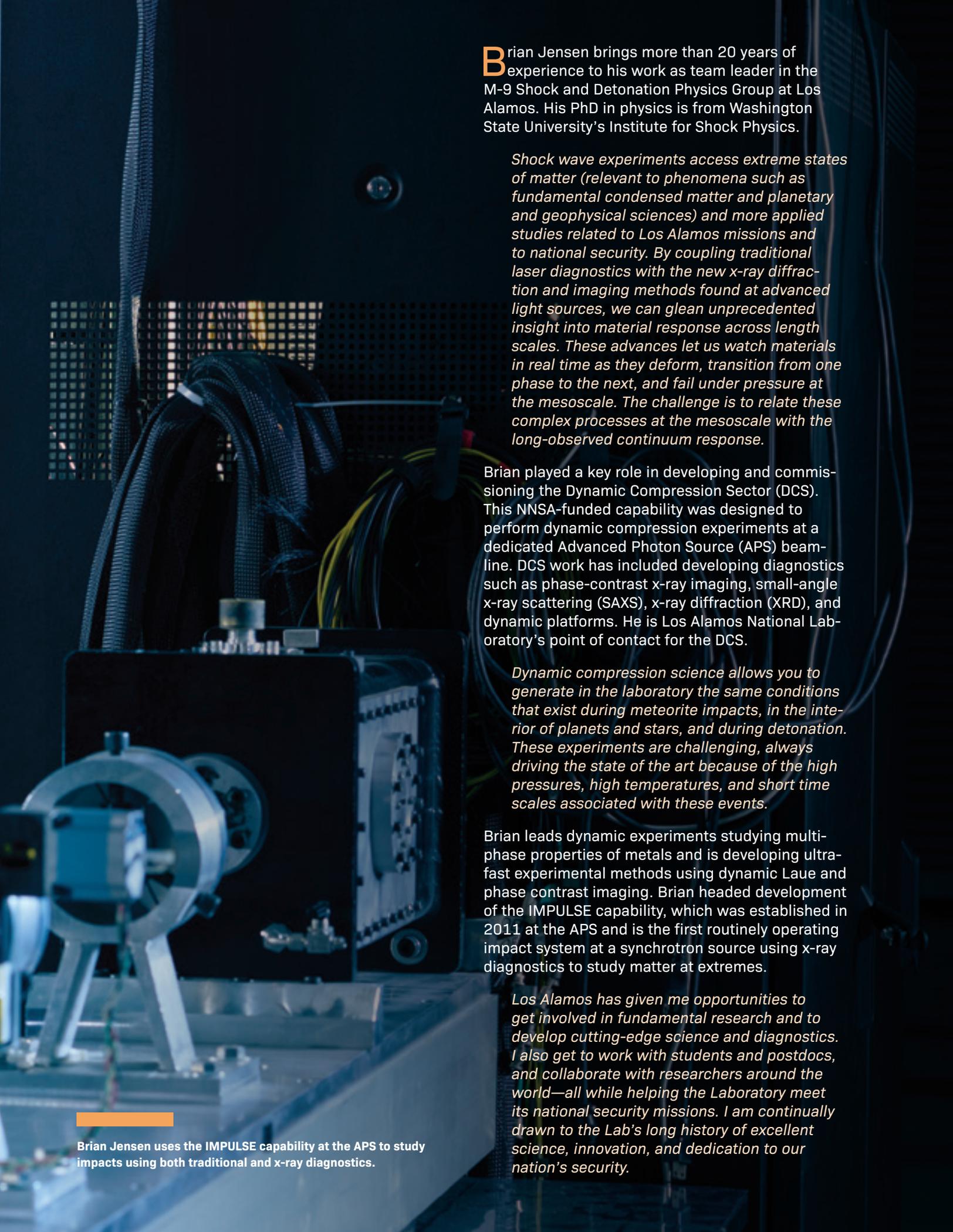
Researchers: ANL: Mathew J. Cherukara, Evan Maxey, Wonsuk Cha, Jorg Maser, Ross J. Harder; LANL: Reeju Pokharel, Timothy S. O’Leary, J. Kevin Baldwin, Saryu J. Fensin, Richard L. Sandberg

Technical contacts: Saryu Fensin (saryuj@lanl.gov), Richard Sandberg (sandberg@lanl.gov), Reeju Pokharel (reeju@lanl.gov)

SHOCK PHYSICIST

BRIAN JENSEN





Brian Jensen brings more than 20 years of experience to his work as team leader in the M-9 Shock and Detonation Physics Group at Los Alamos. His PhD in physics is from Washington State University's Institute for Shock Physics.

Shock wave experiments access extreme states of matter (relevant to phenomena such as fundamental condensed matter and planetary and geophysical sciences) and more applied studies related to Los Alamos missions and to national security. By coupling traditional laser diagnostics with the new x-ray diffraction and imaging methods found at advanced light sources, we can glean unprecedented insight into material response across length scales. These advances let us watch materials in real time as they deform, transition from one phase to the next, and fail under pressure at the mesoscale. The challenge is to relate these complex processes at the mesoscale with the long-observed continuum response.

Brian played a key role in developing and commissioning the Dynamic Compression Sector (DCS). This NNSA-funded capability was designed to perform dynamic compression experiments at a dedicated Advanced Photon Source (APS) beamline. DCS work has included developing diagnostics such as phase-contrast x-ray imaging, small-angle x-ray scattering (SAXS), x-ray diffraction (XRD), and dynamic platforms. He is Los Alamos National Laboratory's point of contact for the DCS.

Dynamic compression science allows you to generate in the laboratory the same conditions that exist during meteorite impacts, in the interior of planets and stars, and during detonation. These experiments are challenging, always driving the state of the art because of the high pressures, high temperatures, and short time scales associated with these events.

Brian leads dynamic experiments studying multi-phase properties of metals and is developing ultra-fast experimental methods using dynamic Laue and phase contrast imaging. Brian headed development of the IMPULSE capability, which was established in 2011 at the APS and is the first routinely operating impact system at a synchrotron source using x-ray diagnostics to study matter at extremes.

Los Alamos has given me opportunities to get involved in fundamental research and to develop cutting-edge science and diagnostics. I also get to work with students and postdocs, and collaborate with researchers around the world—all while helping the Laboratory meet its national security missions. I am continually drawn to the Lab's long history of excellent science, innovation, and dedication to our nation's security.

Brian Jensen uses the IMPULSE capability at the APS to study impacts using both traditional and x-ray diagnostics.

RECENT POSTDOCS

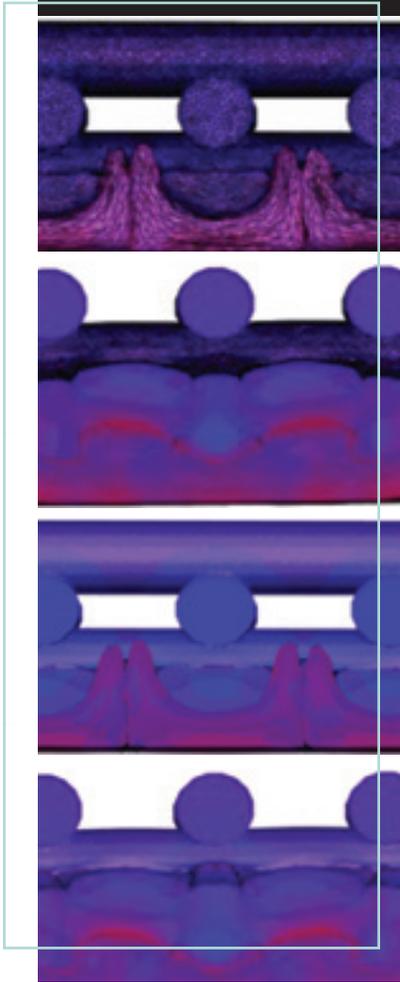


Brittany Branch

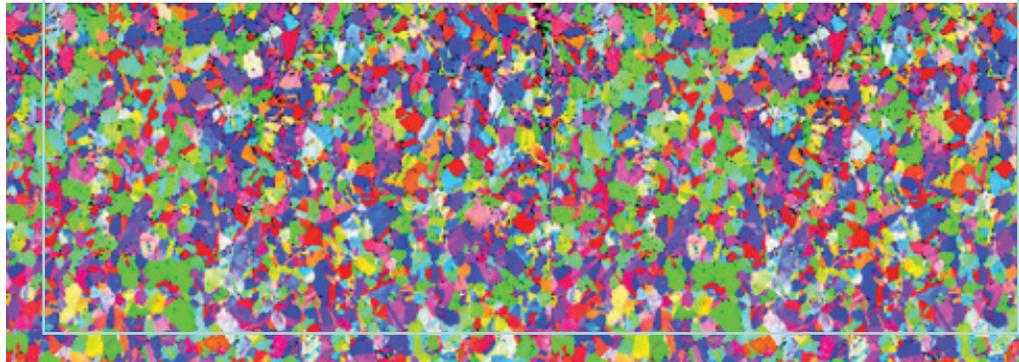
PhD in nanoscience & microsystems engineering
University of New Mexico
Nuclear Materials Science, MST-16
formerly with Shock and Detonation Physics, M-9

Can you describe a usual day at the beam?

I use additive manufacturing (AM) techniques to tailor dynamic material behavior. On a typical day at the beamline, my team and I start with target preparation. We assemble AM material into a holder with specific diagnostics and then place a target onto one end of a gun barrel and a projectile at the other end. Pressure builds up and launches the projectile into the target material, triggering x-ray imaging diagnostics upon impact. On any given day we shoot 10–12 targets and collect and analyze data after each run. The fast-paced nature of these experiments requires a large team of people. Although we are working fast, we have fun and help each other through the long hours. It's exciting to see different shock behavior in real time and to get unexpected results that require the next experiment to be redesigned. At the end of the day, the results keep you coming back for each run cycle.



At the end of the day, the results keep you coming back for each run cycle





Tom Hartsfield

PhD in physics
University of Texas at Austin
Neutron Science and Technology, P-23

What kind of work do you do?

Los Alamos allows scientists to propose their own experiments to probe big science questions in nuclear weapons, materials in extreme conditions, nuclear fusion, and other big science projects in the national interest. I'm an experimental physicist with broad interests, and I consider the Laboratory's deep and varied skills and resources an unparalleled opportunity to design, build, and carry out enormous cross-disciplinary experiments. There is so much capability and expertise here for someone who wants to leverage it. I work to marshal and direct those resources toward the right problems and the right measurements.



With high-brilliance light sources, we can observe processes that were once only described theoretically or inferred with experiments



Rachel Huber

PhD in chemistry
University of California, Los Angeles
Shock and Detonation Physics, M-9

Can you explain the benefits of high-brilliance light?

With high-brilliance light sources, we can observe processes that were once only described theoretically or inferred. For example, my team used the x-ray free-electron laser at the LCLS to understand carbon formation in graphite under extreme conditions. Graphite is most commonly thought of as pencil lead, but it is also a layered, high tensile strength material that reinforces plastics. This material's dynamic behavior has been captured at the Matter in Extreme Conditions beamline [at the LCLS] using laser-driven shocks and at the Dynamic Compression Sector using shocks driven by gas guns. These shock drives captured diffraction that supported diamond formation, which proved bond formation between the layered graphite structures to form tetragonal diamond bonds. This is an example of a long-held assumption about a material's transition that we can finally prove thanks to light sources and their diagnostics.



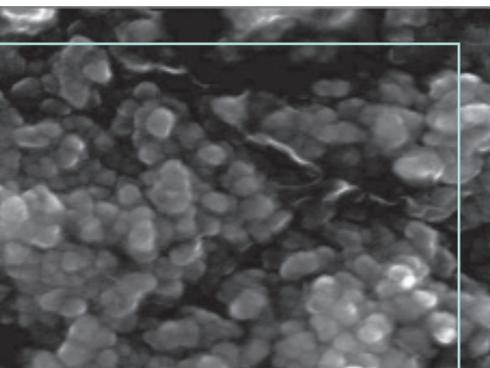


Tom Nizolek

PhD in materials
University of California, Santa Barbara
Materials Science in Radiation and Dynamics Extremes, MST-8

What drew you to the mission of Los Alamos?

The mission of solving national security challenges through scientific excellence makes Los Alamos a fascinating place to work. The Lab researches incredibly complex, wide-ranging problems that require large teams of researchers in areas including nuclear security, intelligence, energy security, and counterterrorism. The result is an environment where (1) the impact and reward of solving a technical problem can be tremendous, and (2) research and discovery in one area may apply to other programs in unexpected or surprising ways. I feel privileged to be part of a team that contributes to the Laboratory's mission by improving our knowledge of material deformation and failure.



Jeffrey S. Pigott

PhD in earth sciences
Ohio State University
Shock and Detonation Physics, M-9

What do you like about your position?

The people, research, history, mission, and location all drew me to Los Alamos. During my initial visit to the Lab, everyone was collegial, welcoming, and (of course) brilliant. The Laboratory and town are steeped in rich, inspiring history; the first time I ever met my mentor was outside of the former house of Hans Bethe, a Manhattan Project scientist and Nobel Prize winner. The opportunity to collaborate and participate in the Lab's cutting-edge research is exciting. Knowing that my research helps protect our country was a driving force in my decision to join Los Alamos.

Knowing that my research helps protect our country was a driving force in my decision to join Los Alamos



Reeju Pokharel

PhD in materials science
Carnegie Mellon University
Materials Science in Radiation and Dynamics Extremes, MST-8

How do you observe change in extremes?

One major challenge of mesoscale science is capturing a 3D view inside of bulk materials at sub-grain resolution throughout different stages of dynamic change. I utilize x-rays, neutrons, and nondestructive techniques to get a detailed, 3D view inside of materials as they change due to processes such as thermal cycling, irradiation, and mechanical deformation. Using experimental data, my team works to develop more accurate, predictive models for various materials in extreme environments. One problem we hope to address is the understanding and control of the material properties of additively manufactured metal components, which have extremely complex microstructure with large local variations. The ability to capture a 3D view inside of a sample and its evolution under extreme conditions provides important fundamental materials understanding that is crucial to developing predictive models.

My team works to develop more accurate, predictive models for materials in extreme environments

Being a national laboratory postdoc

Postdoctoral researchers help national laboratories tackle the many R&D challenges associated with National Nuclear Security Administration-related mission science. At any time, Los Alamos alone has about 400 postdocs working across a diverse set of organizational divisions, scientific disciplines, and national capabilities.

Postdocs working at national laboratories gain unprecedented access to the nation's experimental and computational platforms. Within the Dynamic Materials Properties (Campaign 2) experimental portfolio at Los Alamos, postdocs are leading research using x-rays from light sources at the Advanced Photon Source and the various beamlines and endstations of the Linac Coherent Light Source. In these experiments, postdocs couple static compression, mechanical deformation, and shock wave compression with techniques such as time-resolved x-ray diffraction and different spectroscopies to provide novel information about the evolution of materials under nuclear weapons conditions.

Other postdocs have led research in additive manufacturing, characterized new materials, and synthesized explosives. In many cases, researchers conduct fundamental science with an applied defense focus that is foundational to the missions of our national laboratories.



LANL postdocs in 2018

386 active postdoctoral researchers, **63** of whom are Postdoctoral Fellows



71% work in either physics, chemistry, or engineering

The remaining **29%** research in diverse areas such as earth science, bioscience, mathematics, materials science, and astronomy



39% of those exiting the postdoc program accept a staff position



Contact: Mary Anne With (with@lanl.gov)
lanl.gov/careers/career-options/postdoctoral-research/index.php



EXPLOSIVES EXPERIMENTALIST

JOHN YEAGER



Over his career, John Yeager has studied materials science problems ranging from glass formation and corrosion to fuel cell production. His research at Los Alamos has mainly focused on the performance of plastic-bonded explosives. He uses several characterization techniques across time and length scales to study explosives' properties.

Explosives are tricky to work with, even beyond the obvious safety concerns—they are typically fragile, low-melting-point materials with highly anisotropic properties. I enjoy designing unique experiments that account for these difficult properties to discover new insights.

Despite decades of research on the microstructure of explosives, many fundamental structure-properties relationships are not well understood. Recently, high-fidelity techniques such as synchrotron x-ray phase contrast imaging, neutron diffraction, and computed tomography have been used to examine explosive microstructure at the level of resolution needed to develop and validate new mesoscale models. My role as an experimentalist is to produce samples that are suitable for characterization with these techniques, run experiments, and analyze the resulting data.

John works to establish relationships between a material's microstructure, thermomechanical properties, and explosive performance. Increasingly, these data can be directly incorporated into mesoscale models of explosive behavior in dynamic or extreme environments. His dedication recently earned him the Presidential Early Career Award for Scientists and Engineers, the U.S. government's highest honor for scientists and engineers in the early stages of their research careers.

My "holy grail" of materials science would be measuring everything in situ while using techniques to change the material. I'd love to combine diffraction and imaging with multiple types of particles to study samples with sufficient resolution to directly implement into models.

MaRIE or similar capabilities offer a substantial step forward toward this ultimate goal. With such a capability I could finally directly measure nanoscale and mesoscale structure in explosives while dynamically loading or detonating them. This means we could finally understand and predict general mechanisms that underpin sensitivity, detonation performance, and thermomechanical behavior for all explosives.

John Yeager removes a large single crystal from the solution in which it has been growing for weeks.



THE FUTURE & RECRUITMENT

Laboratory Directed Research and Development

America is facing energy, security, and environmental challenges that, in their scope and complexity, are perhaps unparalleled in the nation's history. The national laboratories are charged with providing scientific breakthroughs needed to develop long-term solutions to those challenges.

In 1992, Congress authorized Los Alamos and the other national laboratories to initiate the Laboratory Directed Research and Development (LDRD) program. The program was set up to foster a research environment that supports scientific innovation and to provide critical financial support for world-class science and engineering.

Investing in science and technology

The LDRD program is a prestigious source of research and development (R&D) funding awarded through a rigorous, highly competitive peer-review process. As the sole source of discretionary R&D funding at Los Alamos National Laboratory, LDRD resources are carefully invested in high-risk, potentially high-payoff activities that build technical capabilities and explore ways to meet future mission needs.

As a result, many of the Laboratory's most exciting innovations—from energy security to large-scale infrastructure modeling, actinide science, and nuclear nonproliferation and detection—can be traced to LDRD investment.

Return on investment

Funded with approximately 6% of the Laboratory's budget, the LDRD program yields an exceptional return on a relatively small investment. The technical output of LDRD researchers,

which includes patent disclosures, peer-reviewed publications, and publications cited by other authors, typically accounts for fully one-quarter of the Laboratory's total.

More importantly, LDRD gives the Laboratory the means to recruit and retain the finest scientific talent. The program traditionally supports more than half of the postdoctoral researchers at the Laboratory and more than half of the conversions from postdoc to regular staff member.

It is the role of the national laboratories, and especially the national security laboratories, to advance the science that will form the foundation of tomorrow's technology. Our robust LDRD program helps Los Alamos sustain the scientific workforce required to meet the nation's long-term national security science needs.

Many research projects that were first supported by LDRD have been taken up by Dynamic Material Properties (Campaign 2), including:

- Bragg coherent diffractive imaging
- Impact response of high-explosive crystals
- X-ray split and delay
- Studying AM response to shocks



Research, Development, Test, and Evaluation

Research, Development, Test, and Evaluation (RDT&E) is an experimental and computational sciences program within the National Nuclear Security Administration's Office of Defense Programs. The RDT&E portfolio focuses on the core research, development, testing, and evaluation needed to develop predictive capabilities for the stockpile. It ranges from computational models and simulations to small-to-large scale dynamic platforms such as dynamic plutonium platforms, the Z Pulsed Power Facility at Sandia National Laboratories, and the National Ignition Facility at Lawrence Livermore National Laboratory.

Many of the experimental facilities in RDT&E validate computer simulations and interrogate materials in extreme, weapons-like conditions. RDT&E also houses the Stockpile Stewardship Academic Alliance Program, which funds university researchers and centers and promotes collaboration between universities and the national laboratories to foster a pipeline of technical staffers.

A hallmark of RDT&E is its balance between forward-looking science and responsiveness to stockpile needs. Future program directions will include developing the Enhanced Capabilities for Subcritical Experiments project at the Nevada National Security Site, backing initiatives from the Nuclear Posture Review, addressing materials aging questions, supporting large-scale computer simulations and computing platforms, and enabling new capabilities such as Matter-Radiation Interactions in Extremes, or MaRIE.



Kathleen Alexander is the assistant deputy administrator for RDT&E. A materials scientist by training, Kathleen's career has included positions at both Los Alamos and Oak Ridge national laboratories.

"When I began studying materials science, I liked the crosscutting nature of the discipline," Kathleen said. "It touched on physics, engineering, and math and had broad applications to real-world problems. Look around you; materials are everywhere."

CONCLUSION

DANA DATTELBAUM

High-brilliance, flexible x-ray light sources are transforming materials research within the National Nuclear Security Administration and laboratories that support its Office of Defense Programs. For the first time, x-ray sources are being paired with extreme condition drivers—such as lasers, guns, explosives, and diamond cells—with pulse characteristics and detector technologies that are better matched to capturing materials evolution in these conditions in situ and with improved spatial and temporal resolution.

The last few years have seen the commissioning of the Matter in Extreme Conditions and Dynamic Compression Sector beamlines at the Linac Coherent Light Source (LCLS) and Advanced Photon Source (APS), respectively, and the construction and first light at the European X-Ray Free-Electron Laser (XFEL). Upgrades to the APS synchrotron and LCLS in the U.S. are also well into the planning stages. This is an exciting time to be in the field, as the coupling of x-ray light sources with static-to-dynamic environments relevant to materials production, dynamics, and aging are maturing rapidly.

This publication highlights just some of the exciting discoveries made over the last three years within our experimental program at Los Alamos. Additional information on these topics is available by reaching out to the technical contacts or through the bibliography. We are also seeking the next generation of technical staff through university collaborations and student and postdoctoral fellow appointments.

The community has come a long way in the last five years, and we continue to tailor our experiments to light source characteristics. We are overcoming challenges in x-ray energies (for penetration), coherence (for imaging and spectroscopy), detector read-out/framing (for time resolution and “movies”), and data acquisition and analysis (for interpretation). These advances are a tiny fraction of those we expect to realize with future capabilities such as the European XFEL, LCLS-II High Energy Upgrade, and eventually Matter-Radiation Interactions in Extremes (MaRIE). These bright light sources indeed have a brilliant future, thanks to the way they continuously evolve to meet national defense challenges and define how materials behave in extreme conditions.

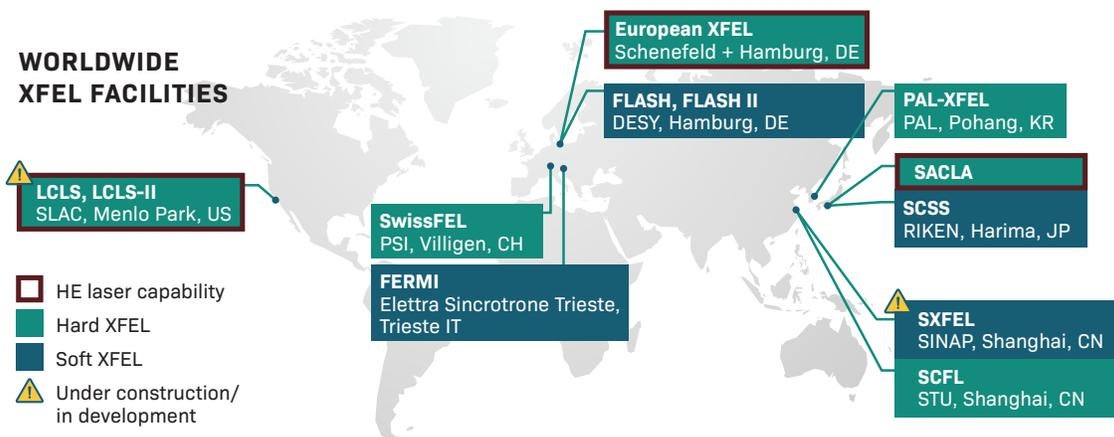


Figure 1: There are a number of recently constructed and developing XFELs across the globe. First light at LCLS-II is expected in the fall of 2020 and the SXFEL (Soft X-ray Free-Electron Laser) may be operational as soon as 2019.



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Stuffed animals sit on a shelf in the control room of the Matter in Extreme Conditions endstation at the Linac Coherent Light Source. Years ago, experimentalists relied on these toys to keep track of a key that enabled the hutch to receive x-rays. Although the hutch now has an updated interlock system, these “key keepers” are still used as mascots for each experiment.

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