

Roadmap to MaRIE

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Revolutionizing materials in extremes



From the desk of... **Cris Barnes**

A facility for discovery of next-generation materials

The MaRIE (Matter-Radiation Interactions in Extremes) experimental facility will be used to discover and design the advanced materials needed to meet 21st-century national security and energy security challenges.

Above, MaRIE Capture Manager Cris Barnes is shown with an illustration of Los Alamos National Laboratory's proposed experimental facility in the background.

Welcome to the first of what I hope will become a regular newsletter with science and technology highlights on the roadmap to MaRIE. I began as the "champion" for Matter-Radiation Interactions in Extremes (MaRIE) in June, and immediately recognized the importance of communicating the significant scope of great work already being performed related to the challenges MaRIE is intended to solve.

MaRIE is the experimental facility for control of time-dependent material performance for national security missions. The mission need is to achieve "product-based" certification, providing certifiable, flexible and low-cost solutions to the materials problems in the nuclear deterrent stockpile. The challenge is that interfaces, defects, and microstructure between the scales of atomic structure and engineering continuum are key to determining time-dependent properties, from shock response to manufacturing processes to aging. The capability gap is the ability to see into and through this middle scale or "mesoscale" with coherent, brilliant x-rays of sufficient energy and gigahertz repetition rate. Coupled with synthesis, fabrication, and characterization of samples at the mesoscale and with full integration with advanced theory, modeling, and computation, MaRIE will subject samples to time-dependent extremes and use both imaging and diffractive scattering from multiple probes at multiple spatial and time scales to connect to product performance. Such a facility is needed by nuclear weapons activities; the capability can be applied to broader national missions such as accelerating the qualification and certification of materials to markets using advanced manufacturing.

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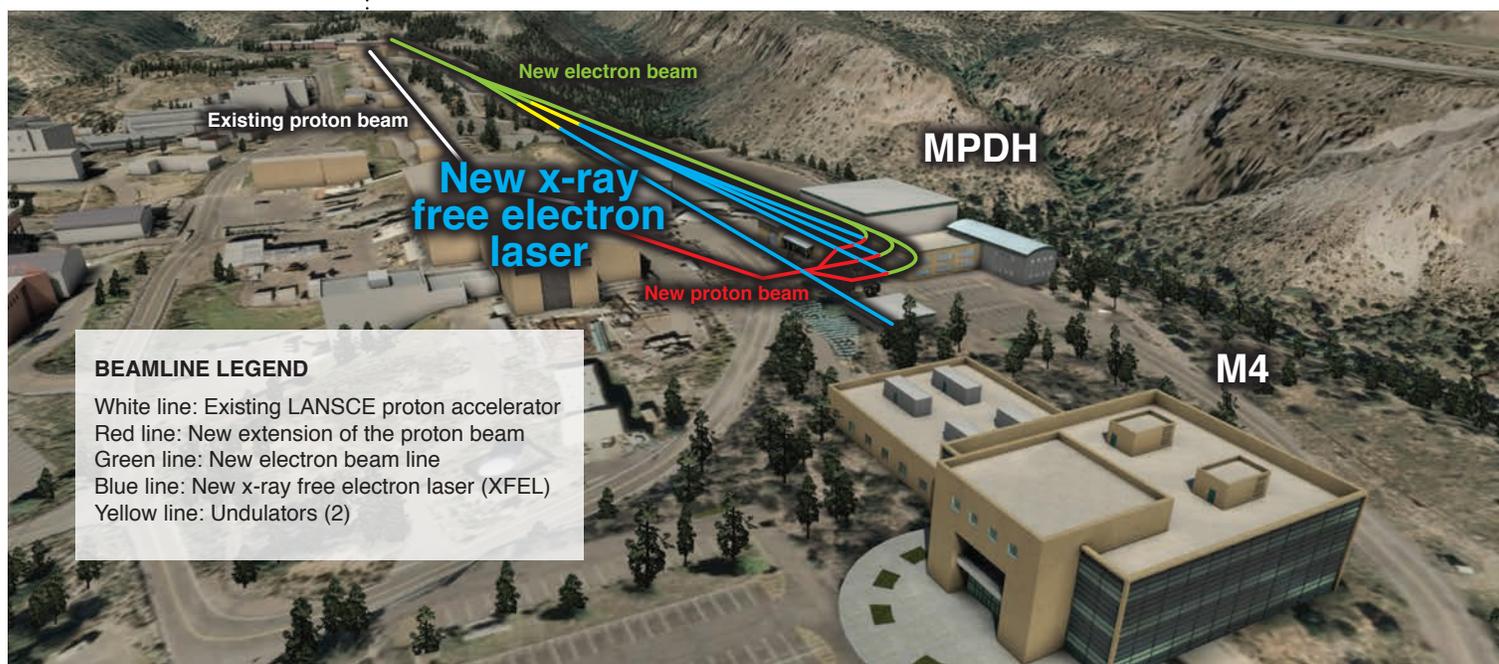
The mesoscale lies between atomic structure and the homogenous continuum of engineering design.

From the desk of... cont.

We use the metaphor of “roadmap” based on a plan requested in 2009 by the then-Assistant Deputy Administrator for Research Development Testing and Evaluation in NNSA, Chris Deeney. He asked for the vision of where the dynamic materials community was at the present, where it would be in several years with planned investments in facilities such as the Dynamic Materials Sector (DCS) at the Advanced Photon Source (APS) at Argonne National Laboratory, and what needed to be done to prepare the user community for an eventual MaRIE facility. I’m proud to say that we’ve been quite successful at executing that roadmap, with examples of highlights in this very newsletter from DCS@APS, the Materials in Extreme Conditions (MEC) end-station at the Linac Coherent Light Source (LCLS) at the Stanford Linear Accelerator Center, and even dynamic results from the first proton radiography facility in western Europe at the GSI Laboratory in Darmstadt, Germany.

We are doing even more than we planned in this frontier field of material science at the scale midway between atomic structure and the continuum of engineering design, or “mesoscale.” And this includes advances in theory and simulation as well as in experimental measurements. A world-class scientific facility such as MaRIE that can really fill the key existing capability gaps to achieve product-based certification will take a long time, another decade or more. Meanwhile, the MaRIE effort has identified a challenging scientific field of growing importance across the missions of LANL and the entire Department of Energy, and we will be pleased to continue to highlight present ongoing work in this fascinating field.

MaRIE Capture Manager Cris Barnes



As shown in this conceptual illustration, MaRIE 1.0 builds on Los Alamos Neutron Science Center’s powerful 800-MeV proton linear accelerator, with new proton and electron beamlines, the world’s first very hard x-ray free-electron laser, a Multi-Probe Diagnostic Hall (MPDH), and a Making, Measuring, and Modeling Materials Facility (M4).



Comprehensive energetic materials development, characterization, and testing are strengths at Los Alamos National Laboratory. An experimental explosive is shown igniting during small-scale impact testing.

Science and technology on the roadmap to MaRIE

New Explosives Center addresses evolving national security mission needs

Building on more than 70 years of nuclear weapons energetic materials science, technology, and engineering expertise, Los Alamos National Laboratory continues to define the field of energetic materials and their characteristics.

A new Explosives Center brings together a powerful set of capabilities and expertise for experiments supporting LANL mission areas, which require full-spectrum energetic materials capability and prowess. Through formal agreement between weapons and global security, this new center integrates the high explosives capability at LANL that is supported by and exists in many line and program organizations. These capabilities, vital to the core nuclear weapons mission, are also crucial to the evolving global security missions.

One of the Center's immediate goals is to ensure success of the ongoing explosives consolidation and modernization plan, which includes consolidated and modernized firing sites and replacement buildings—an explosives “campus.” This core capability investment also plays a vital role in the development of MaRIE. World-leading explosives materials development and characterization capability is central to the grand challenge of controlling materials (including explosive materials) in dynamic extremes—central to MaRIE's goal of furthering understanding of dynamic materials performance and process-aware manufacturing.

From bench-top to large-scale open-air experimentation, Laboratory researchers use a broad suite of diagnostic,

modeling, and simulation capabilities to evaluate nuclear weapon response and performance, as well as a range of scenarios with broad applications, including homemade explosives assessment, lethality, vulnerability, disablement and defeat, aging and surveillance, shock/detonation wave physics, and blast effects. Los Alamos's expertise plays a critical role in effectively assisting the nation's nuclear weapons experts, intelligence analysts, homeland security assets, emergency response teams, and military ground forces in detection, disablement, and defeat of a wide variety of energetic materials threats.

Laboratory capabilities include

- Open-air and confined firing with many types of diagnostics
- Gas and powder guns
- Flash x-rays, high-speed cameras, interferometric techniques, magnetic gauging, pyrometry and many more diagnostics
- Research- and pilot-plant scale formulation, powder production, pressing, crystallization
- Production facility for war reserve detonators, detonator R&D
- Synthetic and analytical chemistry
- Mechanical properties testing
- Thermal response
- Microstructural characterization
- Shock and nonshock initiation
- Dual-Axis Radiographic Hydrodynamic Test Facility
- Proton Radiography Facility
- Lujan Neutron Scattering Center
- Center for Integrated Nanotechnologies
- Materials Science Laboratory
- National High Magnetic Field Laboratory

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New Explosives Center cont.

Daniel Hooks (Weapon Engineering & Experiments, ADW) is center director and Becky Olinger (Emerging Threats, GS-ET) is associate center director. The Explosives Center, established by ADW and Global Security (PADGS), coordinates activities managed and funded by programs and line organizations across the Laboratory.

Technical contact: Daniel Hooks

Flight dynamics of slapper initiators on nanosecond timescales

Los Alamos National Laboratory researchers in collaboration with National Security Technologies (NSTech) and Argonne National Laboratory (ANL) have successfully imaged, for the first time, the operation of copper slapper initiators that are used to initiate high explosive detonators. These data will aid in model development and calibration in order to provide a robust predictive capability for stockpile stewardship and as a design tool in future Life Extension Programs. The experiments are also relevant for MaRIE, combining a unique hard-x-ray free-electron laser with the Los Alamos Neutron Science Center's powerful 800-MeV proton accelerator to learn to control materials performance at the middle or mesoscale of interfaces and microstructures.

The initiation system consists of a copper bridge fixed to a parylene flyer. The copper bridge functions when a capacitor is discharged causing current to flow through the narrow bridge. As this happens, a plasma forms due to the high current densities and ohmic heating, which launches the parylene flyer that impacts a high explosive pellet producing detonation. Unlike traditional measurements, x-ray phase

contrast imaging can see "inside" the process, providing unique information with nanosecond time resolution and micrometer spatial resolution. The team performed experiments on the IMPULSE system at the Advanced Photon Source to obtain high resolution, in situ images of this process in real-time. The figure shows experimental data. From these images, researchers can examine the formation of the plasma instabilities and their interaction with the flyer, determine the flyer velocity, and obtain crucial information on the spatial distribution of mass and density gradients in the plasma and flyer.

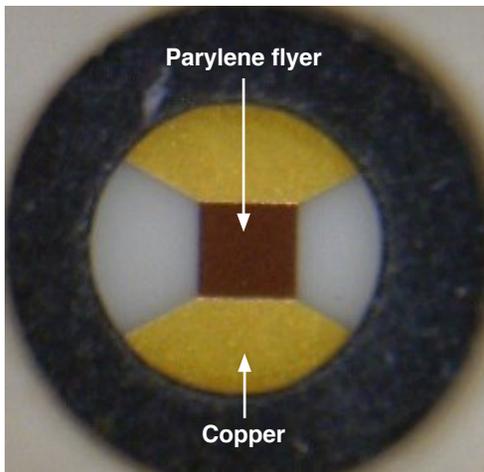
This work is an example of science on the roadmap to MaRIE, Los Alamos's proposed experimental facility for control of time-dependent material properties at these scales. Using MaRIE's advanced capabilities, similar studies could be performed that will also be able to resolve the polycrystalline behavior and hot-spot initiation of the plastic-bonded explosive material itself.

The team includes Nate Sanchez, Mike Martinez, Gary Liechty, and Steve Clarke (Detonator Technology, W-6); Brian Jensen (Shock and Detonation Physics, WX-9); Adam Iverson (INSTech); and Jason Young (NSTech).

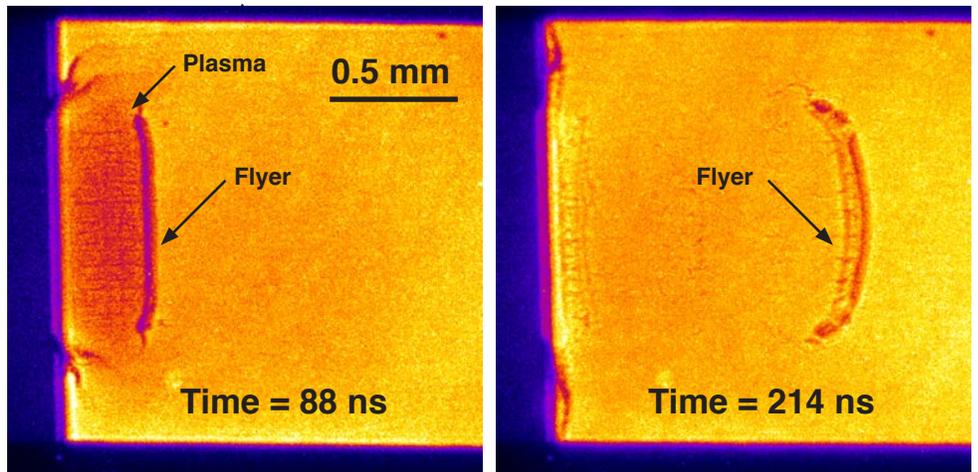
The Joint Department of Defense (DoD)/Department of Energy (DOE) Munitions Technology Development Program (JMP), MaRIE concept, and NNSA Campaign 2 funded different aspects of the work, which supports the Laboratory's Nuclear Deterrence mission area and the Materials for the Future and Nuclear and Particle Futures science pillars.

Technical contact: Brian Jensen

Photo of slapper system



X-ray phase contrast images



Left: Photo of a slapper initiator showing the parylene bridge at the center and the copper bridge. Right: Two images using x-ray phase contrast imaging on IMPULSE show the evolution of the plasma and flyer dynamics.

Proton microscope: The next step towards charged particle microscopy at MaRIE

An international collaboration including Los Alamos scientists has invented a proton microscope, which captured images of objects and structures down to a size of 30 micrometers (one thousandth of an inch) in a series of first experiments.

Protons, like neutrons, are the building blocks of atomic nuclei. Similar to x-rays, they can be used to radiograph objects. However, protons can penetrate hot dense matter that cannot be examined with light or x-rays. The technology, known as proton radiography, was invented at Los Alamos National Laboratory in the 1990s, and has been adopted around the world. The team is pushing the technology by testing higher energies with increased magnification to improve the capabilities of charged particle radiography. The new proton radiography system will be used at the Facility for Antiproton and Ion Research (FAIR), an accelerator under construction in Germany. The combination of proton microscope imaging lenses and increased proton energy, available at GSI—a ring accelerator in Germany—make this capability unique.

In their first experiments, researchers used a proton beam accelerated to an energy of 4.5 GeV (more than 98 percent of the speed of light) by the GSI accelerator facility. A special setup of four quadrupole magnets served as optics to magnify objects with the beam. The GSI facility, called the Proton Microscope for FAIR (PRIOR), achieved resolutions comparable to existing facilities in the United States or Russia. Scientists plan to improve image resolution down to a value of 10 micrometers in experiments this year. Another goal is to record image sequences of moving objects.

The Multi-Probe Diagnostic Hall (MPDH) at MaRIE will bring together three probes (x-rays, electrons, and protons) simultaneously to diagnose dynamic systems. The combined information from the three probes will provide information that would be difficult to collect through many experiments

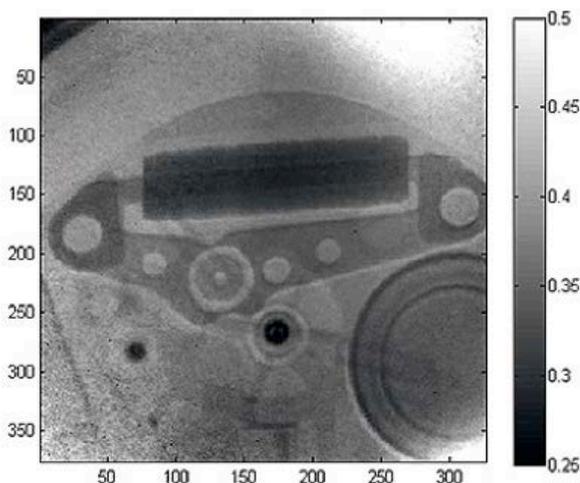
with a single probe. In this facility 800-MeV protons and 12-GeV electrons will be used as direct radiographic probes to study material behavior under extreme conditions. The development of the proton microscope system at PRIOR was a key step for extending charged particle radiography to the charged particle microscopy that is required to meet the measurement requirements of the experiments planned at the MPDH and MaRIE.

In the next two years, the Los Alamos team plans to extend charged particle radiography to the use of electrons for imaging applications at the MaRIE facility. They will demonstrate the first measurements of this type with electrons provided by the SLAC accelerator. The Lab's research at PRIOR and the SLAC National Accelerator Laboratory will provide the experience base required in proton and electron radiography to design and learn how to optimally combine these probes with x-rays at the Multi-Probe Diagnostic Hall.

Los Alamos participants include members of the proton radiography team: Alexander Saunders and Fesseha Mariam (Subatomic Physics, P-25), Christopher Danly, Carl Wilde, and Frank Merrill (Neutron Science & Technology, P-23). Collaborators are researchers from GSI Helmholtzzentrum für Schwerionenforschung GmbH (Helmholtz Centre for Heavy Ion Research) and the Technical University Darmstadt, both Germany; and the Institute for Theoretical and Experimental Physics, Russia.

The NNSA Advanced Radiography Science Campaign 3 and the MaRIE project funded the LANL imaging work. The research supports the Lab's Nuclear Deterrence mission area and the Science of Signatures and Nuclear and Particle Futures science pillars through the development of dynamic imaging systems.

Technical contact: Frank Merrill



A wristwatch was one of the first items imaged by the new proton radiography system. At far left, the inner workings of the mechanism are visible.

First measurements: Structure of titanium under dynamic loading conditions

Recent pioneering dynamic measurements of titanium's structure under pressure are helping Los Alamos researchers to develop models that provide a better understanding of this sturdy, corrosion-resistant metal. Using the latest tools in dynamic compression science to validate the new models, the research will reveal hidden details about titanium (Ti) and aid development of advanced strength models important for stockpile stewardship.

Dynamic experiments such as these described above reveal the structure of a material under dynamic pressures. As such, this is a first step toward understanding the meso-scale mechanisms responsible for material properties under extreme loading conditions—an understanding required to physically represent these processes in next-generation strength and damage models. The experiments performed here have been done on relatively thin foil type samples with a single x-ray diffraction probe. Future facilities like MaRIE will take this type of work even further by allowing multi-granular samples rather than thin foils to be examined in extreme dynamic loading conditions and to perform this examination with additional multiple probes such as electrons and protons, simultaneously.

For this study, Los Alamos scientists and collaborators performed x-ray diffraction on shocked Ti using the Matter in Extremes Hutch at SLAC National Accelerator Laboratory's

Linac Coherent Light Source in California and using IMPULSE at the Advanced Photon Source Dynamic Compression Sector in Illinois. A new capability developed by Los Alamos and Argonne national laboratories, IMPULSE is a mobile gas gun capability for plate impact testing with x-ray diffraction diagnostics.

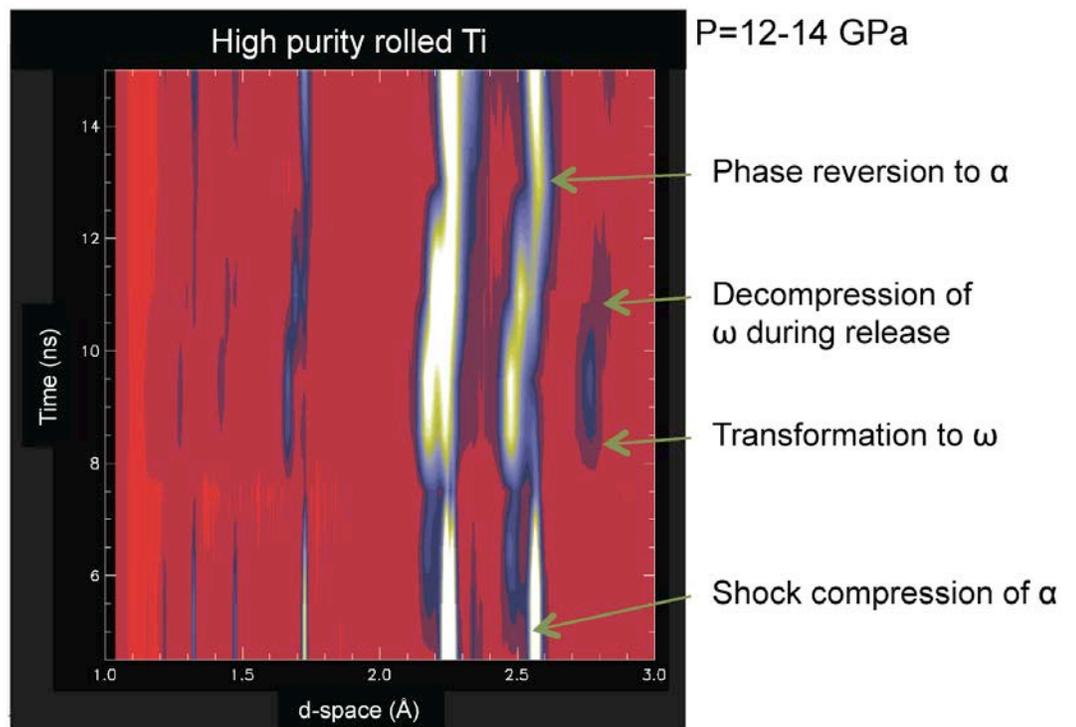
The researchers examined phase transitions and validated molecular dynamics simulation pathways under a range of dynamic loading conditions. They used Laue x-ray diffraction data for shocked Ti to determine the atomic structure at pressure in three regions: low pressure, mixed solid-solid, and high pressure phase. They also examined twinning, reversion, and detwinning.

Experimentalists include Don Brown, Ben Morrow, Ellen Cerreta (Materials Science in Radiation & Dynamics Extremes, MST-8) and Cindy Bolme, Paulo Rigg, and Brian Jensen (Shock and Detonation Physics, WX-9), as well as collaborators from Lawrence Livermore National Laboratory and Washington State University. Theorists include Turab Lookman (Physics of Condensed Matter & Complex Systems, T-4) and Francis Addessio and Curt Bronkhorst (both Fluid Dynamics & Solid Mechanics, T-3).

Los Alamos LDRD and Science Campaign 2 (LANL Program Manager Rick Martineau) funded the work, which supports the Lab's Stockpile Stewardship mission and Materials for the Future science pillar.

Technical contact: Ellen Cerreta

X-ray diffraction data recorded during the shock compression of high purity Ti show the compression of the α (hcp)-Ti lattice followed by transition to the high pressure ω (hex)-Ti phase. During release, the ω -Ti lattice expands before reverting to the low pressure phase.



Los Alamos showcases accelerator research at conference

Laboratory researchers presented talks relevant to LANL's proposed MaRIE experimental facility and topics related to existing Los Alamos programs at the International Conference on the Application of Accelerators in Research and Industry (CAARI). The conference drew approximately 430 researchers from around the world who use particle accelerators in their research and industrial applications. The Lab's presentations highlighted the latest accelerator technology developments and accelerator-enabled research. The presentations demonstrated the depth and breadth of LANL's accelerator expertise, facilities, and infrastructure. Such capabilities are required by MaRIE, which will have at its core the world's first very-hard (42-keV) and very high repetition rate (few pulses at a GHz) x-ray free electron laser.

Twenty representatives (staff, students, and postdoctoral researchers) from seven Los Alamos technical divisions participated as presenters, topic editors, session chairs, and attendees. LANL, the University of North Texas, and Sandia National Laboratories sponsored the conference. Ion Beam Materials Laboratory Leader Yongqiang Wang (Materials Science in Radiation and Dynamics Extremes, MST-8) co-chaired the conference, and Associate Director for Theory, Simulation, and Computation John Sarrao delivered opening remarks on behalf of the Lab. Bob Garnett (Accelerators and Electrodynamics AOT-AE), Anna Hayes (Nuclear and Particle Physics, Astrophysics and Cosmology, T-2), and Richard Greco (International Threat Reduction, NEN-3) served as topic editors. Steve Wender, Fredrik Tovesson, and Aaron Couture (Neutron & Nuclear Science, LANSCE-NS); Ming Tang (MST-8); Nan Li (Center for Integrated Nanotechnologies, MPA-CINT); Gregg McKinney (Systems Design and Analysis, NEN-5); and Wang served as session chairs.

For learn more about MaRIE, please see marie.lanl.gov, or contact Cris Barnes, capture manager, at cbarnes@lanl.gov.

Roadmap to MaRIE, featuring science and technology highlights related to Los Alamos National Laboratory's proposed experimental facility, is published by the Experimental Physical Sciences Directorate. For information about the publication, please contact adepts-comm@lanl.gov.



Invited talks:

- Bob Garnett (AOT-AE)—accelerators with potential use for homeland security
- Nan Li, Jon Baldwin, and Amit Misra (MPA-CINT); Yun Xu, Jeffery Aguiar, Yongqiang Wang, Anderoglu Osman, and Blas Uberuaga (MST-8)—phase stability and microstructure evolution of a metal-oxide multilayer thin film nanocomposite under ion irradiation
- Rhiannon Meharchand (LANSCE-NS)—Los Alamos Neutron Science Center's nuclear fission research program
- Heather Marie Quinn (Space Data Systems, ISR-3)—how space weather affects electronics and on interactions with neutron radiation in high-performance computing

Invited poster:

Sergey Kurennoy, Bob Garnett, and Lawrence Rybarcyk (AOT-AE)—interrogation of special nuclear materials using neutrons and photons combined.

CAARI is a biennial international conference series and covers such topic areas as accelerator technology, atomic and nuclear physics, ion beam analysis and modification, radiation effects, nanoscience and nanotechnology, teaching with accelerators, accelerator applications in homeland security and medicine, etc.

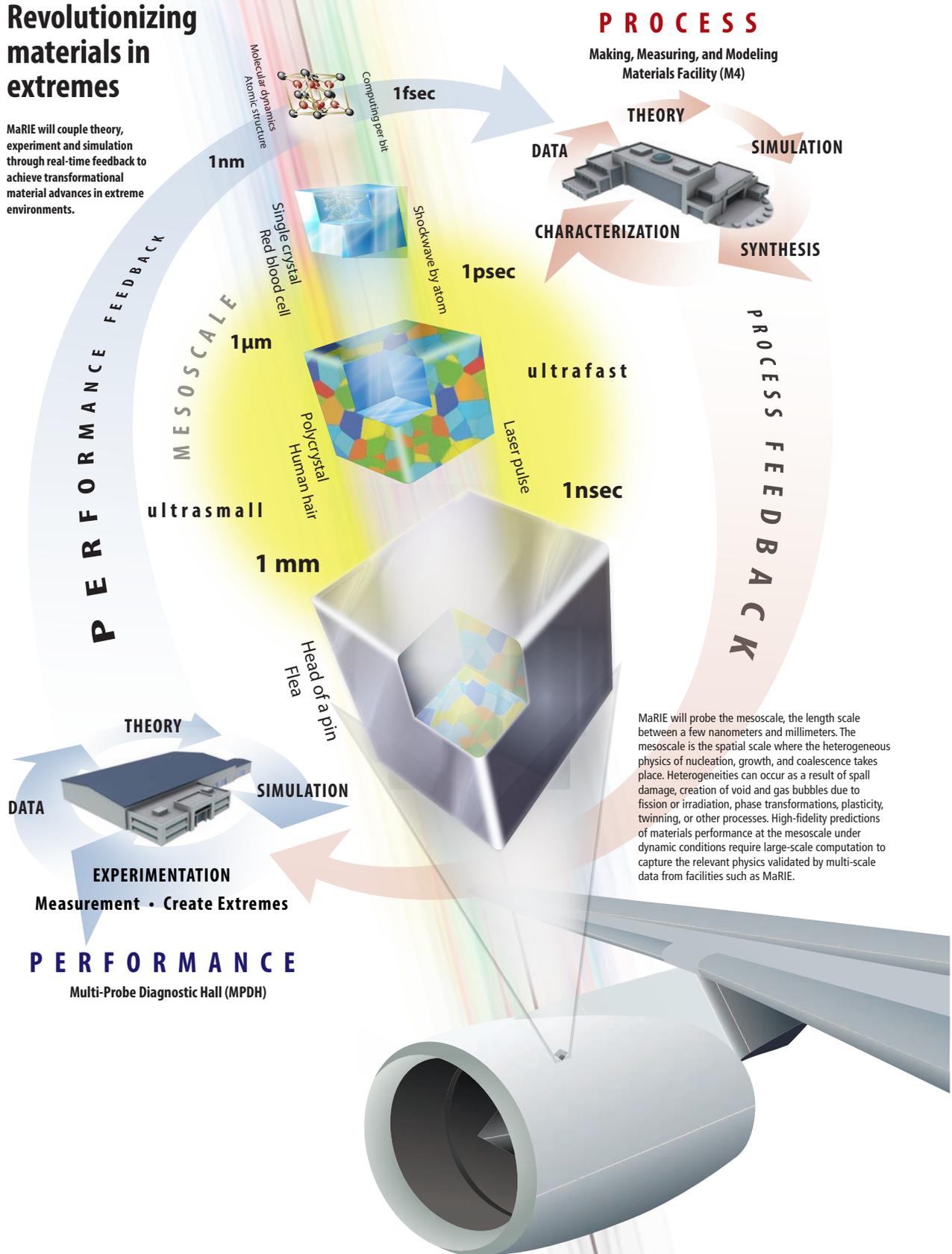
Technical contact: Yongqiang Wang

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Revolutionizing materials in extremes

MaRIE will couple theory, experiment and simulation through real-time feedback to achieve transformational material advances in extreme environments.



MaRIE will probe the mesoscale, the length scale between a few nanometers and millimeters. The mesoscale is the spatial scale where the heterogeneous physics of nucleation, growth, and coalescence takes place. Heterogeneities can occur as a result of spall damage, creation of void and gas bubbles due to fission or irradiation, phase transformations, plasticity, twinning, or other processes. High-fidelity predictions of materials performance at the mesoscale under dynamic conditions require large-scale computation to capture the relevant physics validated by multi-scale data from facilities such as MaRIE.

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