Summer 2017

Mesoscale Connections

Science and technology on the roadmap to MaRIE

INSIDE

Mastering the middle

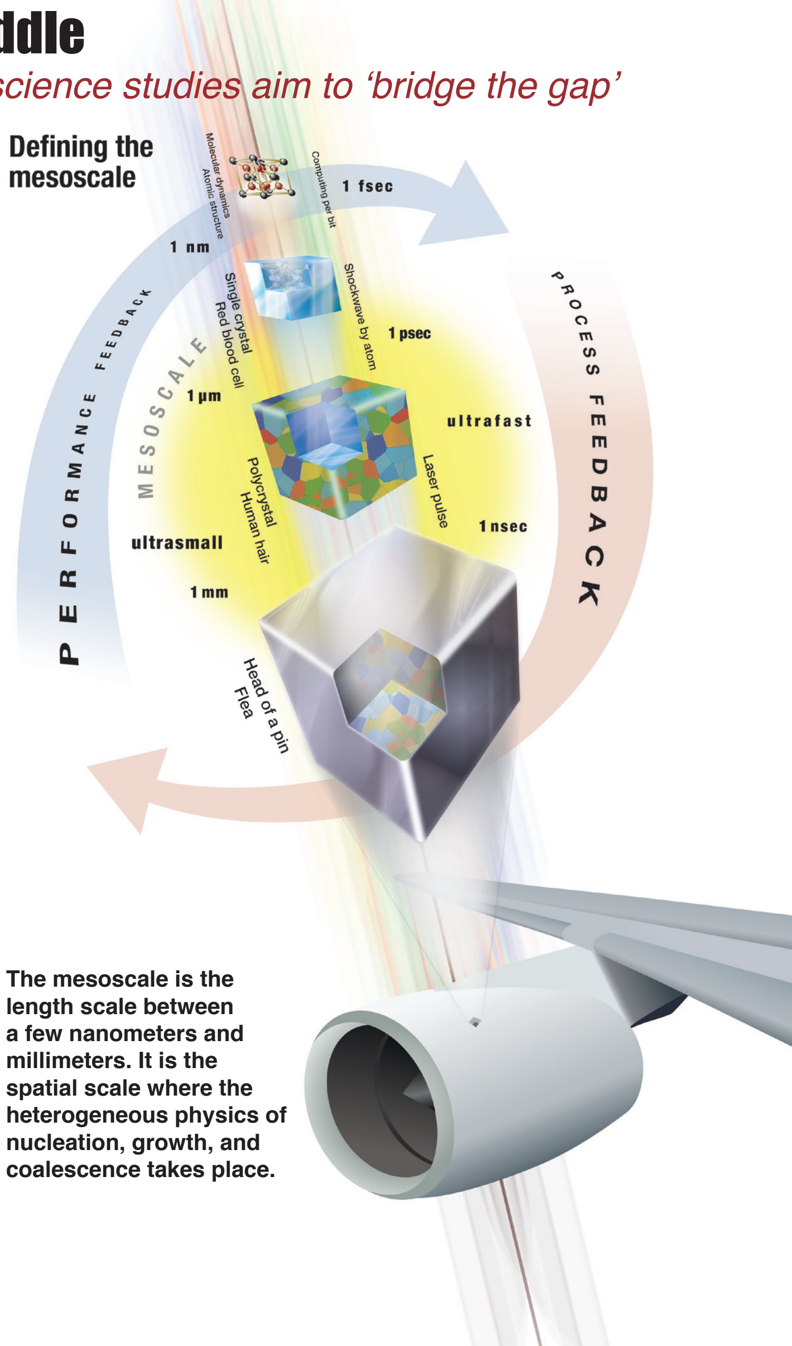
Los Alamos materials science studies aim to 'bridge the gap'

You are reading the first edition of *Mesoscale Connections*.

Our challenge derives from the fact that in metals or explosives grains, interfaces and defects control engineering performance in ways that are neither amenable to continuum codes (which fail to rigorously describe the heterogeneities derived from microstructure) nor computationally tractable to first principles atomistic calculations. This is a region called the mesoscale, which stands at the frontier of our desire to translate fundamental science insights into confidence in aging system performance over the range of extreme conditions relevant in a nuclear weapon.

For dynamic problems, the phenomena of interest can require extremely good temporal resolutions. A shock wave traveling at 1000 m/s (or 1 mm/μs) passes through a grain with a diameter of 1 micron in a nanosecond (10^{-9} sec). Thus, to observe the mesoscale phenomena—such as dislocations or phase transformations—as the shock passes, temporal resolution better than picoseconds (10^{-12} sec) may be needed.

As we anticipate the science challenges over the next decade, experimental insights on material performance at the micron spatial scale with picosecond temporal resolution—at the mesoscale—are a clear challenge. This is a challenge fit for Los Alamos in partnership with our sister labs and academia.



The mesoscale is the length scale between a few nanometers and millimeters. It is the spatial scale where the heterogeneous physics of nucleation, growth, and coalescence takes place.

Mesoscale Connections will draw attention to our progress as we tackle the mesoscale challenge. We hope you like it and encourage suggestions of content you are interested in.

Associate Director Experimental Physical Sciences
Mary Hockaday

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Accelerator Development Project Office created for MaRIE and ECSE

Last year the Office of Defense Programs, with the support from U.S. Department of Energy leadership, including the Deputy Secretary, approved critical decision-0 (CD-0), declaration of the mission need, for two new capabilities: Enhanced Capabilities for Subcritical Experiments (ECSE) and Matter-Radiation Interactions in Extremes (MaRIE). Each concept has been developed as part of a decadal strategy for constructing new flagship experimental science facilities supporting National Nuclear Security Administration missions.

ECSE and MaRIE present key opportunities to meet the objectives of the Stockpile Stewardship Management Plan. Both rely on state-of-the-art development in accelerator technology and, for that reason, a new Accelerator Development Project Office has been set up within the Weapons Program Directorate. The office includes Cris Barnes and Jeff Paisner as project directors for MaRIE and ECSE respectively. As both projects are major scientific facilities and both are in the project definition phase, there is considerable synergy in goals, supporting staff, and technology. A key aspiration of both projects is to use project execution lessons learned from the Department of Energy, Office of Science, including benchmarking and project management methods. For that reason John Tapia serves as the deputy project director for both projects.

Mesoscale Connections
is published by the Experimental Physical Sciences Directorate. Its goal is to promote awareness of mesoscale materials research relevant to the NNSA, advances in mesoscale science capabilities at user facilities, and modeling challenges and needs for big data sets in service of materials co-design.
For information about the publication, please contact adeps-comm@lanl.gov.

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

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

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NNSA National Nuclear Security Administration

Los Alamos Materials Strategy update

Delivering materials solutions for national security missions, advancing materials discovery science

Los Alamos National Laboratory's newly refreshed Materials Strategy was highlighted at the recent Materials for the Future capability review. The strategy's goal is to enable the Laboratory to meet current and future national security mission needs by providing transformative materials research.

Several factors, including the need to more clearly articulate connection to the Lab's mission and to emphasize actions that help inform investments, prompted a re-examination of the original document that was drafted in 2010.

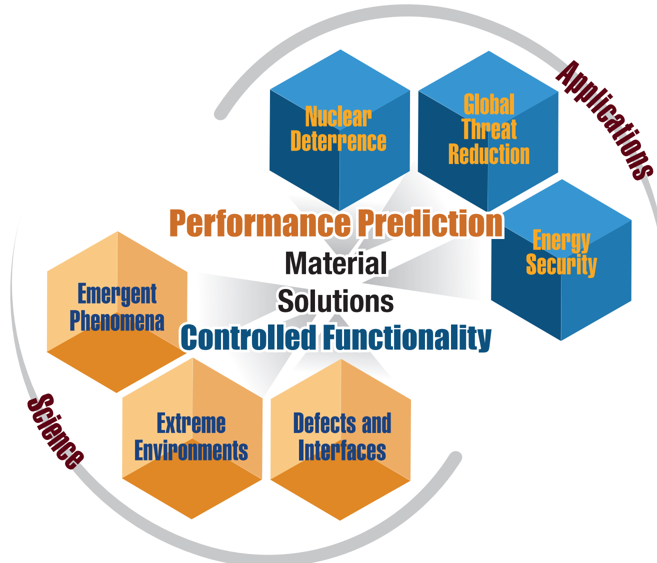
Since 2015 diverse groups representing all aspects of the Laboratory's materials community have contributed to reviewing and identifying the key science and engineering challenges that will exist over the next decade for materials critical for the success of Los Alamos's missions.

Identified are seven Areas of Leadership in which the Laboratory must excel to successfully meet its mission. They are Actinides and Correlated Electron Materials, Energetic Materials, Integrated Nanomaterials, Complex Functional Materials, Manufacturing Science, Resilience in Harsh Service Conditions, and Materials Dynamics. The Areas of Leadership are connected through common Science Themes—Defects and Interfaces, Extreme Environments, and Emergent Phenomena.

The strategy's overarching goal is to support the Lab's mission by providing materials with controlled functionality and predictable performance while ensuring the Lab's materials capability remains agile for future emerging national security mission needs. To that end, the strategy advocates support of basic science to enable a forward-looking science profile that will attract a new wave of bright and energetic scientists.

Mesoscale science and the opportunities presented by the phenomenal advances in light source user facilities are already key to many of the Areas of Leadership and will remain central elements of the Materials Strategy for the next decade. The strategy explicitly acknowledges that close coupling between experiment, theory, modeling, and simulation is essential for success in developing robust, validated, and verified predictive tools of stockpile performance.

This enhanced definition of the co-design process depends on advanced models and algorithms, next-generation codes, appropriate experimental tools such as MaRIE (Matter-Radiation Interactions in Extremes), and sophisticated, next-generation architectures and platforms as developed for the Exascale Computing Project. This broad co-design also requires bridging both time and length scales—from the atomistic, through the mesoscale, up to the continuum—and from kinetic through quasi-equilibrium.



Our Materials Strategy enables Los Alamos to provide national security solutions through controlled functionality of materials. Our strategy maintains a dynamic balance of advancing science in our three theme areas with supporting the applications in the Laboratory's three mission areas.

The Materials for the Future science pillar is one of four such pillar concepts the Laboratory uses to manage its multidisciplinary scientific capabilities and activities. The Laboratory uses external peer reviews to measure and improve the quality of its science, technology, and engineering.

During the out-brief following the review, committee chair Julia Phillips, a member of the National Science Foundation's National Science Board and executive emeritus of Sandia National Laboratories, said the first thing the committee noticed was the major progress to the Materials Strategy document and noted it looks forward to seeing continued refinement on it and an implementation plan next year.

In addition to the Materials Strategy, the committee was presented with overviews of the state of the Integrated Nanomaterials and Manufacturing Science Areas of Leadership and examples of the research in those fields; an update on the establishment of the MaRIE project, a capability addressing the control of performance and production of materials for national security science at the mesoscale; and a survey of strategic planning and initiatives to expand the Laboratory's capabilities in materials science across the Laboratory-Directed Research and Development program portfolio.

New tools reveal hidden roots of material's post-shock strength

Recent advances in synchrotron diagnostics coupled with dynamic compression platforms have enabled new opportunities for in situ investigations of extreme states of matter on nanosecond timescales. Examining the evolution of material properties at extreme conditions advances understanding of numerous high-pressure phenomena—from natural events like meteorite impacts—to general solid mechanics and fluid flow behavior.

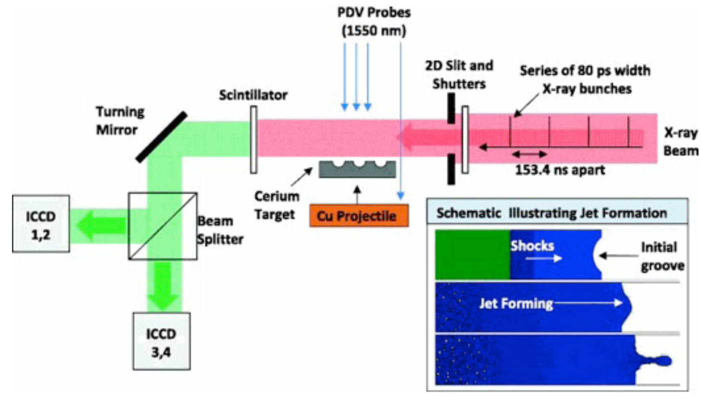
Los Alamos researchers and collaborators used the IMPULSE (for IMPact system for ULtrafast Synchrotron Experiments) gas-gun system at Argonne National Laboratory's Advanced Photo Source (APS) to observe jet formation and evolution with a 2-3 μm spatial resolution in shocked cerium metal. By measuring the jet velocity, using the x-ray images to observe the jets as they evolved, and developing computer simulations to compare the experimental data to calculations, the researchers estimated the yield stress in tension for cerium.

The data and analysis provide insight into material strength during dynamic loading, which is expected to aid in developing strength-aware multi-phase EOS required to predict the response of matter at extreme conditions. This work complements other experiments underway at APS's Dynamic Compression Sector, the Z Machine at Sandia National Laboratories, and explosives loading facilities at Los Alamos. The researchers plan to combine x-ray imaging with x-ray diffraction to correlate microscopic and macroscopic material deformation under extreme conditions; thus fulfilling a persistent scientific challenge.

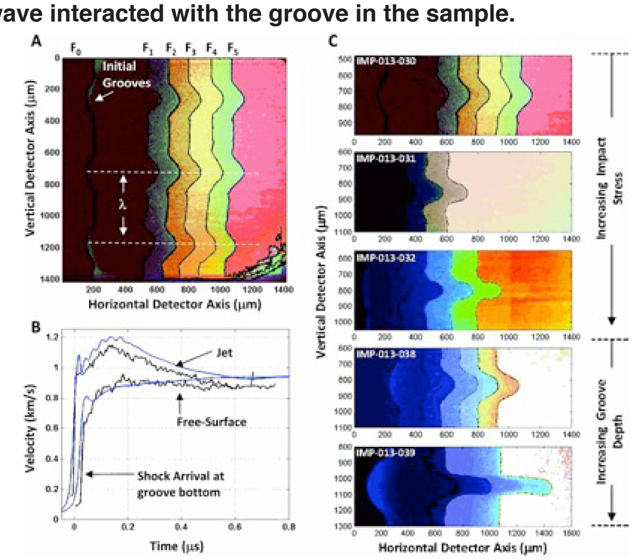
The work is an example of research that will be further advanced at MaRIE (Matter-Radiation Interactions in Extremes), the Laboratory's proposed facility for time-dependent materials science at the mesoscale. With MaRIE's combination of the world's highest energy (42-keV) x-ray free-electron laser and in situ probes, researchers will observe materials deformation in real time at the mesoscale, the region between the atomic and macroscale. Understanding a material's properties at the mesoscale is key to predicting and controlling its performance.

Los Alamos researchers included Brian Jensen, Frank Cherne, John Yeager, Kyle Ramos (all Shock and Detonation Physics, M-9); Dan Hooks (Explosive Science and Shock Physics, M-DO); Jason Cooley (Metallurgy, MST-6); Mike Prime (Advanced Engineering Analysis, W-13); and Guy Dimonte (Materials and Physical Data, XCP-5). Charles Owens and Tim Pierce (M-9) assisted with target and projectile fabrication, gun setup, and shot execution.

Work performed at Los Alamos National Laboratory was supported by the Laboratory's MaRIE concept (Capture Manager Cris Barnes) and NNSA Science Campaign programs. Yeager was supported by an Agnew National Security Postdoctoral Fellowship.



Schematic of the experimental configuration for shock wave experiments using x-ray imaging to observe jet formation in Ce. A Cu plate (2.5 mm thick) impacted the Ce sample located in an evacuated target chamber generating a shock wave that interacted with the machined perturbations at the back surface. The x-ray beam passed through multiple slits and shutters, interacted with the sample and evolving jets, and was incident upon a scintillator. The scintillator light was imaged onto four optically multiplexed intensified detectors that were synchronized to the impact event and the x-rays. (inset) Schematic showing the process of jet formation as the shock wave interacted with the groove in the sample.



(A) Example x-ray images showing jet formation. (B) Corresponding velocimetry data (black curves) obtained using photon Doppler velocimetry showing the jet and free surface velocities. (C) A summary of x-ray images for five experiments showing the effect of increasing the impact stress and groove depth on the jet formation. For the deepest grooves, the jet does not saturate and outruns the free surface.

References: "Jet formation in cerium metal to examine material strength," *J. Appl. Phys.* **118**, 195903 (2015); "Imaged 'jets' reveal cerium's post-shock inner strength," Phys.org, Jan. 29, 2016 (phys.org/news/2016-01-imaged-jets-reveal-cerium-post-shock.html)

Technical contact: Brian Jensen

Enhanced imaging for dynamic physics research at the Proton Radiography Facility

Researchers have successfully installed and operated a new and improved high-speed imaging system at the Laboratory's Proton Radiography (pRad) Facility at the Los Alamos Neutron Science Center (LANSCE).

The imaging system is designed for dynamic experimental studies. These advances significantly enhance the pRad capabilities for users in the materials and shock physics communities.

The Laboratory pioneered proton radiography, which is well suited to the study of dynamic processes in materials. The technology features excellent contrast and the capability to radiograph dynamic events on short time scales (e.g., a few microseconds) multiple times during its evolution.

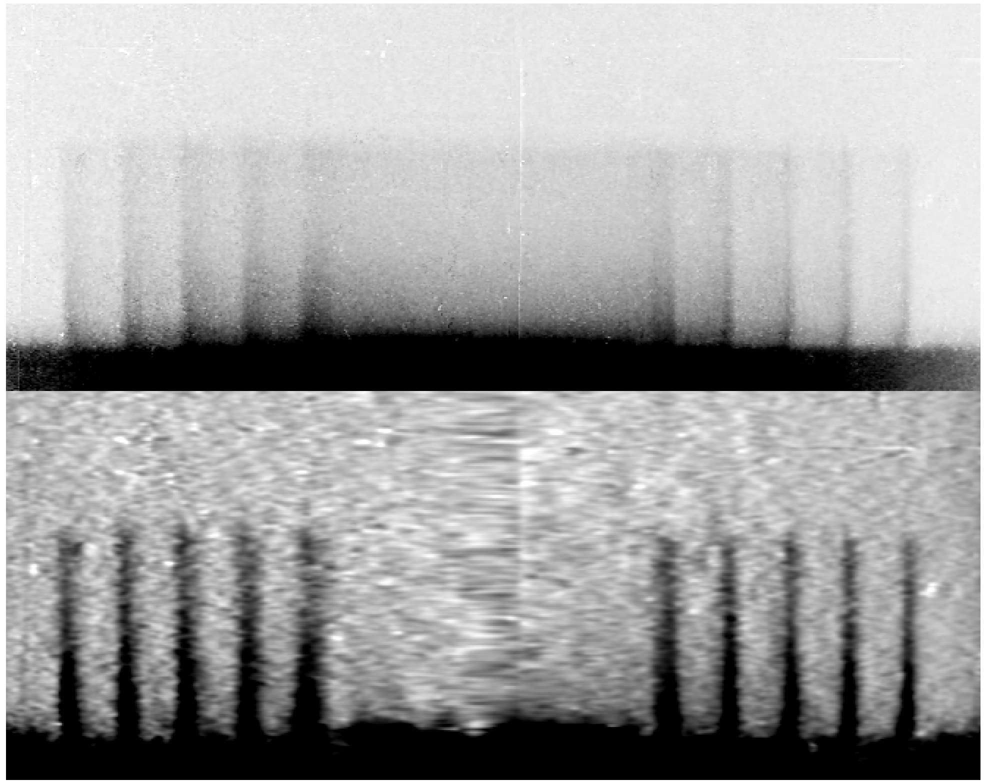
With the LANSCE accelerator's capabilities, the number of radiographs is limited only by the camera technology.

The large-format, 10-frame hybridized focal plane array design of the new imaging system offers much improved spatial and charge resolution, higher quantum efficiency, lower noise, and faster repetition rate over the current state of the art, with integration times below 50 ns.

The new camera design, slated to replace an earlier 3-frame design, allows experimenters more than 40 radiographs per event as opposed to the 21 provided in the current system, and with fewer cameras.

The goal for the experimental run cycle was to prove that the camera could operate in the harsh ionizing environment of the proton beam. Physics Division researchers made an aggressive push to prepare the camera to take data in a dynamic experiment.

In its first deployment, the camera recorded the evolution of Richtmeyer-Meshkov instabilities at late times (see image). The team will focus on quantitative characterization of the camera's capabilities (i.e., measurements of transfer curves) and integration of the sensor into a production camera design.



The team performed two identical experiments at about 7 atm (atmospheric pressure) of helium. Two shots—one from 0–5.5-μs with an interframe time of 275 ns (21 images and a static) and one from 5.8–13.8 μs (21 images)—will be combined.

The 10-frame camera, which was fielded on the second, from 5.9–9.5 μs with an interframe time of 400 ns, is a link between the two, to verify repeatability. The image taken using the 10-frame camera shows (top) areal density and (bottom) Abel-inverted.

Materials experiments at the Laboratory's proposed Matter-Radiation Interactions in Extremes (MaRIE) experimental facility would demand unprecedented time-resolved imaging capabilities. MaRIE is designed for the study of time-dependent mesoscale materials science.

Many of the technologies featured in this new imaging prototype (e.g., improvements in in-pixel memory and quantum efficiency) are promising additions to the suite of technologies researchers could employ in conceptual designs of MaRIE.

The Lab's Neutron Science and Technology (P-23) and Subatomic Physics (P-25) groups, Teledyne Imaging Sensors, Fishcamp Engineering, and Sandia National Laboratories collaborated to develop this new imaging system.

Billy Buttler (P-23) is the principal investigator. NNSA Science Campaign 3 funded the work, which supports the Laboratory's Nuclear Deterrence mission area and the Materials for the Future and Science of Signatures science pillars through dynamic materials and shock physics investigations.

Technical contact: Johnny Goett

Richard Sandberg elected to leadership of LCLS Users' Executive Committee

Richard Sandberg is chair of the Linac Coherent Light Source (LCLS) Users' Executive Committee. A committee member since 2014, he leads the committee in helping to improve user operations and facility capabilities.

Opened in 2009 at the Department of Energy's SLAC National Accelerator Laboratory in California, LCLS is the world's first hard x-ray laser. It has enabled Sandberg and collaborators to create the first-ever in situ images of void collapse in explosives using an x-ray free electron laser.

Sandberg (Center for Integrated Nanotechnologies, MPA-CINT) holds a PhD in physics, with a certificate in optics, from the University of Colorado Boulder. He joined Los Alamos in 2009 as a Director's Postdoctoral Fellow and became a staff scientist in 2011.

LCLS includes six experimental stations and attracts proposals in a range of disciplines that include biology; soft and hard materials; matter in extreme conditions; chemistry; atomic, molecular and optical; and methods and instrumentations. Sandberg's discipline is matter in extreme conditions. Use of LCLS is supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences.

Key technologies originally developed at Los Alamos in the 1980s and 1990s, such as the radio frequency photoinjector and high-brightness electron beams, enabled the x-ray free electron laser (XFEL) facilities currently in use worldwide. Moreover, Los Alamos was part of a multi-laboratory collaboration that designed and built the Linac Coherent Light Source.

Los Alamos's proposed experimental facility MaRIE (Matter-Radiation Interactions in Extremes) will be the world's highest energy hard XFEL. Used for time-dependent materials research, it will help researchers like Sandberg design the advanced materials needed to meet 21st-century national security and energy security challenges.

Technical contact: Richard Sandberg

John Post strengthening scientific community connections

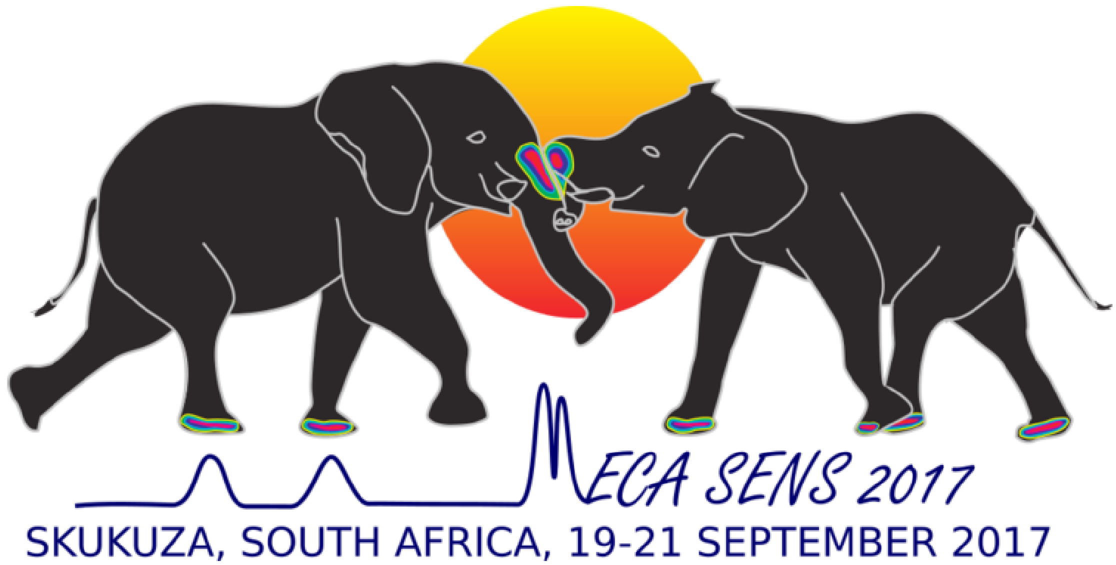
John Post has been working part-time at Los Alamos National Laboratory since the summer of 2015, first spending time with the Principal Associate Directorate for Capital Projects (PADCAP) to help guide the re-certification process for the earned value management system for the Laboratory and then joining the MaRIE (Matter-Radiation Interactions in Extremes) effort last year, with an emphasis on building the collaborations and partnerships with other laboratories that will be needed to deliver the project. Post has extensive experience within the Department of Energy project management community as a senior project reviewer, with an emphasis in the delivery of the Department's large and unique scientific research projects. He is working across the Momentum Initiative this year, in part working with Los Alamos's mesoscale community to help spread the awareness of the mesoscale mission and plans.

Post has worked at Lawrence Livermore National Laboratory for more than nearly 28 years and has experience with program/project management, the federal budget process, and business development. He was most recently a member of the capture team for the High Average Laser System project that Livermore is delivering for the Czech Institute of Physics as a part of the Extreme Light Infrastructure – Beamlines project. He recently moved from the National Ignition Facility/Photon Science PAD to the Operations and Business PAD at Livermore as a senior advisor.

Technical contact: John Post

Laboratory materials scientists lend expertise to international conference on mechanical stress evaluation by neutron and synchrotron radiation

Probes are an ideal tool to explore the mesoscale



MECA SENS 2017, the 9th international conference on mechanical stress evaluation by neutron and synchrotron radiation, will be held in September in Skukuza, South Africa.

As part of the conference's International Scientific Committee, Don Brown (Materials Science in Radiation and Dynamics Extremes, MST-8) and Mark Bourke (MST Division Office, MST-DO) are assisting in developing the event's program. Brown chaired the 2005 MECA SENS, which was held in Santa Fe, New Mexico and hosted by Los Alamos National Laboratory.

This latest in the series of historic conferences on the evaluation of residual stresses in materials will feature both engineering and scientific aspects. Recent developments and capabilities in diffraction-based approaches as well as mechanical and image-based techniques will be presented, with an emphasis on measuring, modeling, applying data.

Hosted by the South African Nuclear Energy Corporation, the conference is attended by scientists and engineers from academia, research facilities, and industry active in the field of neutron, synchrotron, and x-ray strain scanning studies of materials.

Neutron and synchrotron radiation are ideal probes for the difficult to investigate mesoscale, a length scale where a material's features strongly influence its macroscopic behavior and properties. MaRIE, the Laboratory's proposed facility for time-dependent materials science at the mesoscale, will feature the next generation of such probes and the ability to collect in situ data as materials are subjected to extreme environments.

MaRIE will allow researchers to ultimately discover and design the advanced materials needed to meet 21st century national security and energy security challenges—materials that will perform predictable and with controlled functionality in extreme environments.

Registration deadline for MECA SENS is August 8. More information can be found at www.eiseverywhere.com/ehome/mecasens/.

Technical contact: Don Brown

Topics include:

- Stress evaluation using neutrons, synchrotron radiation, and x-rays
- Development of measurement methods and instrumentation
- Material processing with relation to residual stresses
- The influence of residual stresses on physical and mechanical properties of materials and components
- Measurement and assessment of residual microstresses and intergranular stresses
- Residual strains and stresses in complex materials, e.g., multiphase materials and biomaterials
- Residual stresses in thin films and microcomponents
- Industrial applications of residual stress analyses using neutrons, synchrotron radiation and x-rays
- Complementary techniques for residual stress measurements, e.g. mechanical methods vs. diffraction.

Workshop explores solutions to making the most of big data provided by a new generation of light sources

With the advent of third-generation synchrotron light sources, such as the Advanced Photon Source at Argonne National Laboratory, and x-ray free electron lasers, such as the Linac Coherent Light Source at the SLAC National Accelerator Laboratory, nondestructive characterization of new classes of challenging materials is now possible. The high energy and brilliance of the x-rays produced by these light sources can probe high Z, three-dimensional polycrystalline samples at the mesoscale—the domain where materials features have tremendous influence on a material's macroscopic behaviors and properties.

Although new light sources provide previously inaccessible data, the increasing average brightness creates new challenges, such as the generation of extremely large data sets–from gigabytes to terabytes. These unconventionally large data sets are overwhelming experimentalists. This complexity is compounded further by the multi-modal data generation techniques that must be integrated to gain physical insight into a material's behavior.

A day-long workshop, "Even small wavelengths, when bright enough, have big data problems," was held recently as part of the 2017 Advanced Photon Source/Center for Nanoscale Materials Users Meeting at Argonne National Laboratory that brought together experts in the field to explore solutions to this challenge. The workshop's goal was to improve information extraction capability from high-dimensional data and design a real-time feedback framework for driving experiments. The workshop was organized by Reeju Pokharel (Materials Science in Radiation and Dynamics Extremes, MST-8) and Turab Lookman (Physics of Condensed Matter and Complex Systems, T-4).

MaRIE, the Laboratory's proposed experimental facility for time-dependent materials science on the mesoscale, will have at its heart the world's highest energy x-ray free-electron laser with gigahertz repetition ability. MaRIE (Matter-Radiation Interactions in Extremes) will be used to discover and design the advanced materials needed to meet 21st-century national security and energy security challenges.

With current data analysis tools in their infancy, a growing user base, and increasing data collection rates expected when a fourth generation of light sources comes online, there is an urgent need for the development of efficient, fast, and user-friendly software, which has the potential to change how experiments and data mining are performed in the field of three-dimensional materials science.

The workshop focused on identifying and exploring the range of datasets that are currently being produced from experiments at various light sources to solve materials science problems; discussing the latest developments in advanced data analysis tools; and encouraging collaborations between experimentalists, modelers, and data scientists across national labs, academia, and industry.

Technical contact: Reeju Pokharel

A recent workshop explored the new opportunities and challenges faced by materials scientists with the decreasing wavelength and increasing average brightness of the next-generation light sources.