

Roadmap to MaRIE

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Science and technology delivering to the stockpile today

We are doing science and technology today on the “Roadmap to MaRIE,” delivering to the mission of the nuclear enterprise.

We need to enhance our predictive capabilities in key areas, especially in control of the materials with which we make our stockpile.

Above, an illustration of MaRIE (Matter-Radiation Interactions in Extremes) Los Alamos National Laboratory’s proposed experimental facility that will be used to discover and design the advanced materials needed to meet 21st-century national security and energy security challenges.

After the decision to end nuclear testing and the inception of the Stockpile Stewardship program, the condition of the stockpile was the primary mission driver. During the first two decades of stewardship, the primary program goal could be described as underwriting the Stockpile-to-Target Sequence (STS), the military requirements on the conditions the nuclear warheads needed to survive and still operate. This created an emphasis on performance and reliability of the stockpile systems that we were left with at the end of testing. The dominant concern was to avoid hubris, or over-confidence that the systems would continue to perform and be reliable in the face of evidence of imperfections and aging. This effort was successful as we developed improved predictive capability for simulation “from button to boom” on the performance of stockpiled systems.

However, by 2020 and beyond, the nuclear enterprise will be well into a necessary effort to modernize the aging stockpile. The primary program goal will be to underwrite the entire life cycle of our stockpile systems, from production and manufacture through the possible button-to-boom phase to eventual disposition. This is needed to meet the national policy goals of enabling a smaller total stockpile while maintaining confidence, all in support of reducing global nuclear dangers in the future while sustaining a strong deterrent. To afford this mission, the way we do the mission must change. We need to enhance our predictive capabilities in key areas, especially in control of the materials with which we make our stockpile. This has the added benefit of building the enterprise’s unique science, technology, and engineering capabilities to address broader national security needs and to help the nation protect against technological surprise.

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Science and technology ... cont.

This science can deliver certifiable, flexible, and low-cost product-based solutions to the materials problems of the enterprise.

Much of the science that is needed is being done today.

To meet the NNSA Defense Program mission of “sustain a safe, secure, and effective nuclear arsenal,” there is a mission need to accelerate the qualification, certification and assessment of materials. This includes “dynamic materials performance” of materials such as high explosives, metal alloys such as plutonium pits, or materials having undergone solid-liquid phase transitions (or solid-to-plasma!) during the STS. It also includes “process-aware manufacturing” issues of whether old materials can still be used (aging), what new materials are possible (with controlled functionality such as for safety or security), and what new processes can be used (using advanced techniques such as additive manufacturing). Science is needed to support lifetime extension programs (LEPs) including those planning re-use of key parts such as pits. This science can deliver certifiable, flexible and low-cost product-based solutions to the materials problems of the enterprise.

Much of the science that is needed is being done today. This newsletter contains recent examples of science highlights that are addressing how to improve predictive capability for materials and accelerate the qualification, certification, and assessment of those materials for national security missions. The MaRIE 1.0 project will fill a capability gap identified for this mission need; meanwhile, much progress is being made with current theory and experimental tools. I hope you enjoying reading these highlights!

MaRIE Capture Manager Cris Barnes

MaRIE provides the materials science that supports other thrusts:

Pu Strategy; Sub-critical experiments; Advanced Manufacturing; Exascale for Materials ...

The Mission Need:

Sustain a safe, secure, and effective nuclear arsenal
Through accelerated qualification, certification, and assessment.



Strengthen the ST&E base
Energize the people of the nuclear enterprise

Drawn from the 2015 NNSA SSMP

Science and technology on the roadmap to MaRIE

Advancing Stockpile Stewardship science by combining theory with new, advanced experimental capabilities

Los Alamos National Laboratory experimental and theoretical materials scientists are developing a new generation of experimental and theoretical tools in support of the nation's Stockpile Stewardship program. Continued evolution in computing architectures is changing the way researchers perform physics calculations for the nation's Stockpile Stewardship Program—evolutions that encourage higher fidelity representation of highly coupled complex physics events. In turn, advances in experimental capability at these present-day light source facilities are enabling never-before-achieved views of materials physics behavior under extreme loading conditions of interest to the Stockpile Stewardship Program. Higher fidelity models might be used in an adaptive physics refinement approach as illustrated in the figure below, and only be applied by a simulation when needed. Development of these models are the result of advances in both computing architectures and new experimental capabilities available at the Argonne National Laboratory Advanced Photon Source and the SLAC National Accelerator Laboratory.

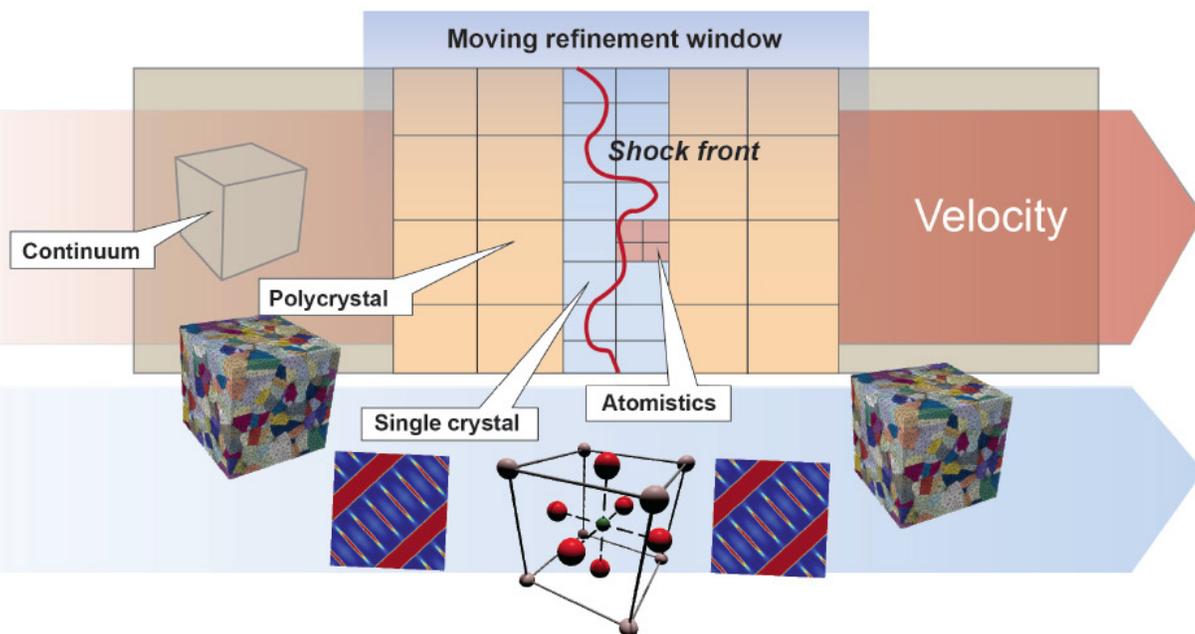
By combining theory with experimental data, new materials behavior theory is being developed at the material meso-scale to take advantage of these new experimental insights and to anticipate adaptive physics refinement strategies to computing in the future. For example, Los Alamos researchers recently made advances in three key areas: representing the mechanics of dislocation motion and twinning; equation of state representation at the single crystal level; and

coupling of phase transformation and plasticity processes. These will allow a greater physical basis for weapons calculations where these highly coupled problems are, today, under-resolved.

The work is an example of science on the roadmap to MaRIE, the Laboratory's proposed experimental facility for control of time-dependent material performance. Using MaRIE's advanced capabilities, similar studies could be performed that provide multiple images in a movie format of the evolution of materials at the mesoscale in situ under dynamic conditions. This would be an unprecedented achievement and significantly advance our knowledge of the physics at these spatial and temporal scales.

The research, which supports the Laboratory's Nuclear Deterrence mission and Integrating Information, Science, and Technology for Prediction science pillar, is funded by Science Campaign 2 (LANL Program Manager Rick Martineau). Participants include LANL scientists Curt Bronkhorst and Francis Addessio (both Fluid Dynamics and Solid Mechanics, T-3), Turab Lookman (Physics of Condensed Matter and Complex Systems, T-4), Ellen Cerreta, Don Brown, and Paulo Rigg (all Materials Science in Radiation and Dynamics Extremes, MST-8), Cindy Bolme (Shock and Detonation Physics, WX-9), and Carl Greeff (Physics and Chemistry of Materials, T-1).

Technical contact: Curt Bronkhorst



Adaptive physics refinement incorporates models and data across various relevant scales dynamically.

Toward a new quantification and certification paradigm for additively manufactured materials

Characterization of additively manufactured 316L SS

Additive manufacturing (AM) is an agile model for designing, producing, and implementing the process-aware materials of the future. However, as no “ASTM-type” additive manufacturing certified process or AM-material produced specifications exists, the AM certification and qualification paradigm needs to evolve.

For example, even for small changes in such variables as starting feed material (powder or wire), component geometry, build process, and post-build thermo-mechanical processing, the qualification cycle can be complicated—leading to long implementation times.

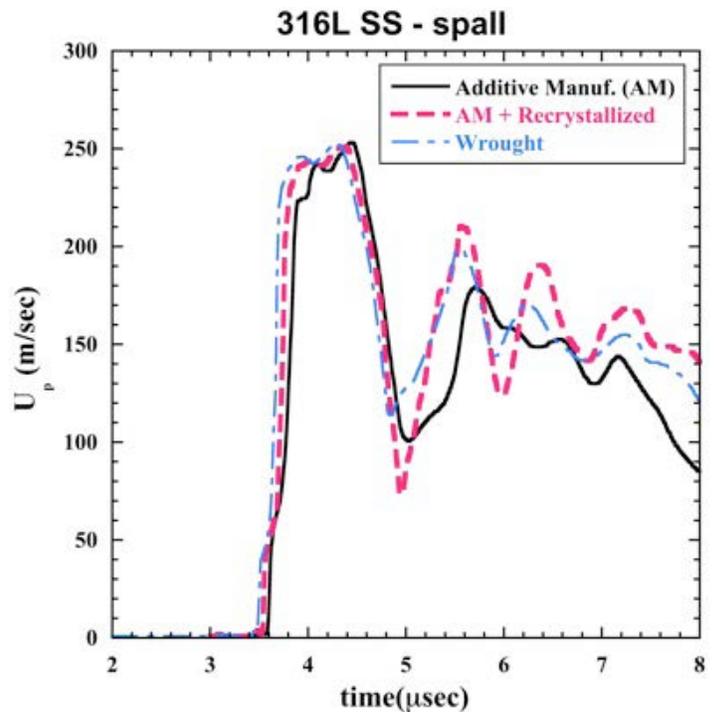
In large part, this is because researchers cannot predict and control the processing-structure-property-performance relationships in additively manufactured materials at present. Metallic-component certification requirements have been documented elsewhere for specific materials, but generally involve meeting engineering and physics requirements tied to the functional performance requirements of the engineering component, and finally—process and product qualification. Key microstructural parameters and defects need to be quantified in order to establish minimum performance requirements.

As part of a National Nuclear Security Administration complex-wide effort researching techniques toward a certification and qualification process for additively manufactured materials, Los Alamos researchers compared and quantified the constitutive behavior of an additively manufactured stainless steel in the as-built condition to that of the same that had undergone recrystallization and yet again to a conventionally manufactured annealed and wrought stainless steel.

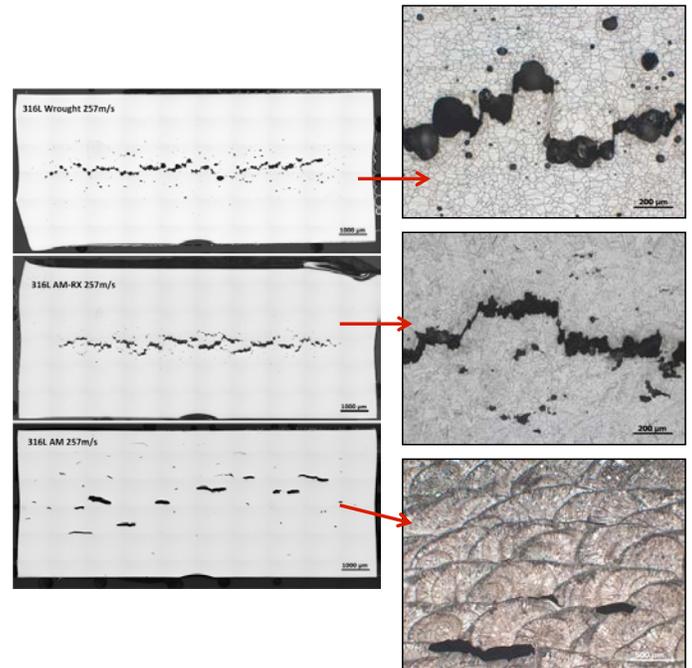
The results of their mechanical behavior and spallation testing reinforce that additive manufacturing will force a shift from “material” qualification (ASTM) to science-based qualification and certification.

The work is part of the qualification and certification research thrust of a Department of Energy additive manufacturing initiative that includes Los Alamos National Laboratory, Sandia National Laboratories, Lawrence Livermore National Laboratory, Kansas City Plant, and Savannah River Site. Using materials additively manufactured at these sites, Los Alamos is conducting further fundamental dynamic spall tests and characterizing the resulting structure/property relations.

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Initial spallation testing indicates significant dynamic ductility.



The results of flyer-plate impact-driven spallation on (from top) conventionally manufactured annealed and wrought stainless steel, additively manufactured stainless steel that has been recrystallized, and the as-built additively manufactured 316L SS. The optical microscopy results show void formation and damage along solidification boundaries in the as-built additively manufactured steel; classic spherical void nucleation, growth, and shear coalescence in the wrought steel; and reduced void formation and shear in the recrystallized additive steel.

Additively cont.

In this initial study, cylinders of 316L stainless steel (SS) were produced using a LENS MR-7 laser additive manufacturing system from Optomec (Albuquerque, New Mexico) equipped with a 1-kW Yb-fiber laser. The microstructure of the additively manufactured-316L SS was characterized in both the as-built condition and following heat-treatments to obtain full recrystallization. The constitutive behavior as a function of strain rate and temperature was measured and compared to that of nominal annealed wrought 316L SS plate. The dynamic damage evolution and failure response of all three materials were probed using flyer-plate impact driven spallation experiments at two peak stress levels, 4.3 and 6.2 GPa, to examine incipient and full spallation response.

The spall strength of wrought 316L SS was found to be invariant for the two-peak shock stresses studied while the AM-316L SS spall strengths, in the as-built and following recrystallization, was seen to decrease with increasing peak shock stress. The damage evolution as a function of microstructure and peak shock stress is being characterized using optical metallography, electron-back-scatter diffraction, and scanning-electron microscopy.

The initial results of the spallation investigation on 316L-SS were presented during the complex-wide Joint Working Group (JOWOG) on additive manufacturing held at Lawrence Livermore National Laboratory in October.

Science Campaign 2 (LANL Program Manager Russell Olson, acting) and the Joint Munitions Program (LANL Program Manager Tom Mason) funded the work. The work supports the Laboratory's Nuclear Deterrence mission area and Materials for the Future science pillar.

Future facilities, such as MaRIE, could take this research into linking process-aware materials behavior to performance and thereafter qualification and certification even further by facilitating in-situ quantification of deformation and damage evolution during dynamic loading.

Participants included G.T. (Rusty) Gray III (Materials Science in Radiation & Dynamics Extremes, MST-8) who serves as principal investigator for the complex-wide program and the LANL activities, John Carpenter, Thomas Lienert (both Metallurgy, MST-6), and Veronica Livescu, Carl Trujillo, Shuh-Rong Chen, Carl Cady, Saryu Fensin, and Daniel Martinez (all MST-8).

Technical contact: Rusty Gray

New, efficient method for direct embedding of polycrystal plasticity in multiscale materials models

A team of Lawrence Livermore National Laboratory (LLNL), Los Alamos National Laboratory, and Cornell University scientists published new research on multiscale materials modeling that sets forth a framework for embedding polycrystal plasticity models in component-scale simulations—one that overcomes the high computational cost associated with such simulations.

While specific applications in this work are focused on the deformation of titanium specimens, including the effects of deformation twinning, the framework offers an attractive path forward for computationally efficient multiscale embedding of polycrystal plasticity for a very general class of structural materials in simulation codes for engineering applications.

This research, appearing in the journal *Computational Methods in Applied Mechanics and Engineering*, demonstrates the numerical implementation of an efficient way of embedding microstructure-sensitive material models in component-scale simulations of mechanical response. The need for numerically tractable models to capture anisotropic plastic flow, such as in simulations of metal forming, is the driving force behind this effort.

For the above purpose, this work unifies three separate pre-existing models: 1) LANL's viscoplastic self-consistent (VPSC) model, widely used for the prediction of mechanical behavior of polycrystalline aggregates; 2) Cornell's discrete harmonic (DH) representation of crystallographic texture, including the treatment of lattice reorientation due to slip and twinning activity at single crystal level; and 3) LLNL's adaptive sampling (AS) model, a numerical strategy that mitigates the computational cost of direct embedding by building on-the-fly a database of material response, achieving two or more orders of magnitude in wall-clock speedup, compared with direct interrogation of the lower length-scale models. All three models were integrated in LLNL's flagship Finite Element code ALE3D.

This work is also an example of Science on the Roadmap to MaRIE, the Laboratory's proposed experimental facility for Matter-Radiation Interactions in Extremes. The development of such novel theory, modeling, and computation tools, integrated with the wealth of experimental data that will come from MaRIE, will provide an unparalleled capability to understand, predict, and control materials behavior under extreme conditions.

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Additively cont.

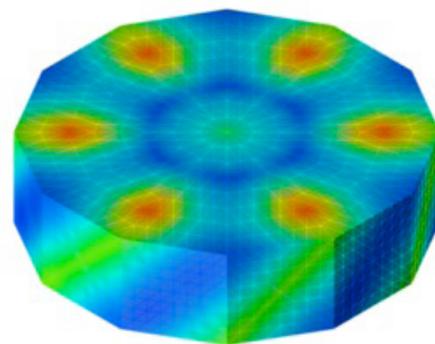
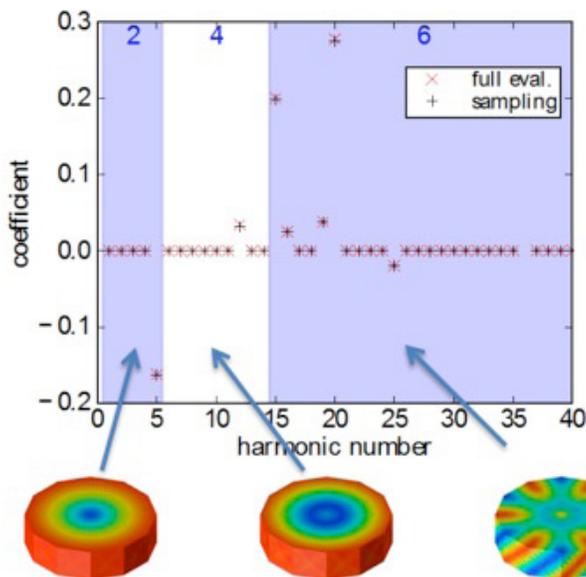
The U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research funded this research through LANL-LLNL's joint Exascale Co-Design Center for Materials in Extreme Environments (ExMatEx).

The work supports the Laboratory's Energy Security mission and Materials for the Future science pillar by providing a new computational tool to enable the science and engineering required to establish novel design principles and manufacturing processes for advanced materials.

Reference: "The use of discrete harmonics in direct multi-scale embedding of polycrystal plasticity," by N.R. Barton and J.V. Bernier (LLNL), R.A. Lebensohn (Materials Science in Radiation & Dynamics Extremes, MST-8); and D.E. Boyce (Cornell University), *Computer Methods in Applied Mechanics and Engineering* **283**, 224-242 (2015).

Technical contact: Ricardo Lebensohn

Results for evolved harmonic coefficients using full fine-scale evaluations versus adaptive sampling, including harmonic modes of degree 2, 4 and 6, over the hexagonal fundamental region of Orientation Distribution Function (ODF) space. Right: ODF predicted for a deformed Ti polycrystal.



High-energy x-ray diffraction microscopy monitors grain growth in ceramic fuels at operating temperatures

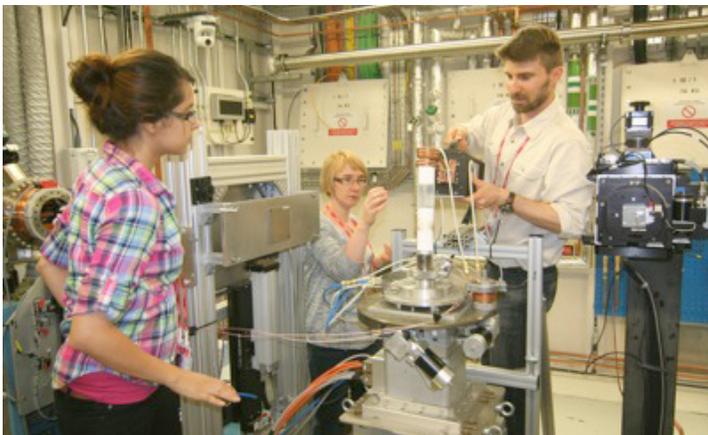
Los Alamos researchers Reeju Pokharel, Bjorn Clausen, Matt Reiche, and Don Brown (Materials Science in Radiation and Dynamics Extremes, MST-8) used the Advanced Photon Source at Argonne National Laboratory to perform experiments aimed at monitoring grain growth in ceramic nuclear fuels at operating temperatures. The data are informing microstructural models of nuclear fuel.

Nuclear fuels operate under some of the most hostile conditions experienced by materials, with temperatures exceeding 2000°C, thermal gradients of several hundreds of °C over millimeters and intense irradiation. Two phenomena—thermal conductivity and the ability of fission products (e.g. xenon gas) to escape the microstructure and be released into the area surrounding the fuel pellet—govern the useful lifetime of the fuel. Both effects are strongly dependent on the grain size and grain boundary morphology.

Near field high energy x-ray diffraction microscopy (nf-hedm), which is essentially tomography with contrast based on crystal orientation (as opposed to electron density contrast of the more familiar medical tomography), provides grain maps nondestructively and at depth even in high-Z material, such as uranium dioxide (UO₂). This technique allows the unique possibility to perform evolutionary measurements on the same sample in 3-D and in the bulk before and after exposure to extreme conditions, such as temperature, or even in situ. The figure (next page) shows grain maps from a single sample assintered (at 1350°C) UO₂ and after 3 hours held at 2000°C. The growth of the grain is readily apparent. These maps come from the area of the same sample representing the evolution of unique grain morphology. The team published early results from this program, and is continuing to analyze the recent data. Future experiments will enlarge the parameter space,

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High-energy cont.



Researchers (Reeju Pokharel, Jette Oddershede (Denmark Technical University), Matt Reiche) at prepare an experiment using high-energy x-ray diffraction microscopy to monitor grain growth in ceramic nuclear fuels at operating temperatures.

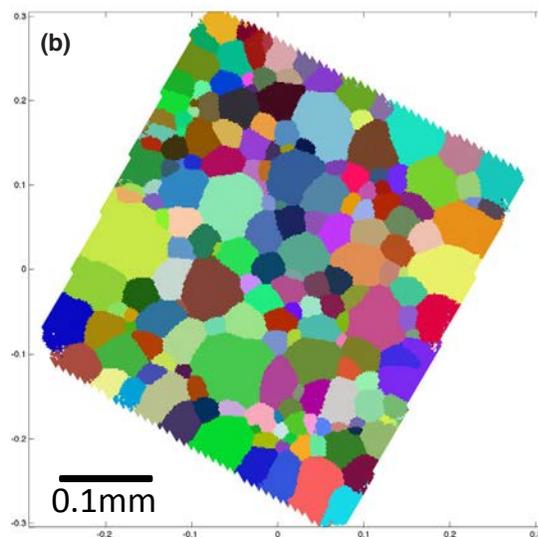
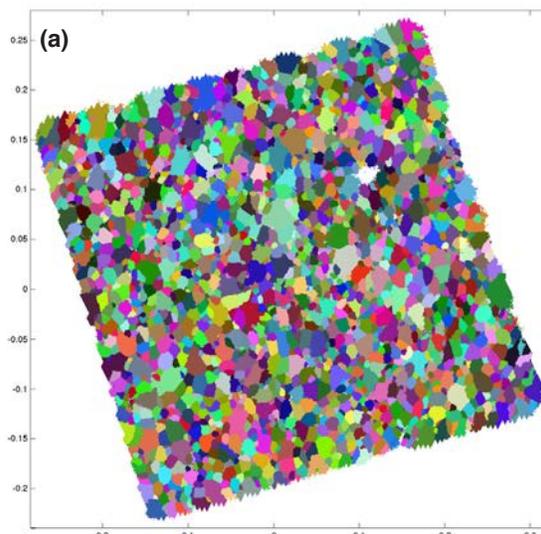
including different oxygen stoichiometry (i.e. UO_{2+d}), which has a strong effect on diffusion, and thus grain growth.

The data are informing microstructural models of nuclear fuel as part of the MARMOT code being developed at Idaho National Laboratory under the auspices of the Department of Energy Nuclear Energy Advanced Modeling and Simulation (NEAMS) program. The technique development is relevant to LANL's proposed MaRIE experimental facility, because grain mapping would be completed on all samples being studied at the Multi-Probe Diagnostic Hall (MPDH) to provide detailed microstructural information for models of the dynamic experiments. This information would increase the fidelity between model and experiment at the advanced facility.

Reference: "Demonstration of Near Field High Energy X-Ray Diffraction Microscopy on High-Z Ceramic Nuclear Fuel Material," *Materials Science Forum* **777**, 112 (2014). Authors include D.W. Brown, D. Byler, and J.F. Hunter (MST-8); L. Balogh (Queens University, Ontario); C. M. Hefferan (R J Lee Group); P. Kenesei (Argonne National Laboratory); S.F. Li (Lawrence Livermore National Laboratory); J. Lind and R.M. Suter (Carnegie Mellon University; and S. R. Niezgoda (The Ohio State University). Peter Kenesei and Jun-Sung Park were the responsible instrument contacts at the Advanced Photon Source. Darrin Byler (MST-8) and Pallas Papin (Metallurgy, MST-6) made the samples.

The Laboratory Directed Research and Development (LDRD) program funded the Los Alamos research to focus on the effect of temperature alone on the microstructure of nuclear fuel. The work supports the Laboratory's Energy Security mission area and the Materials for the Future science pillar.

Technical contact: Don Brown



Grain maps of UO_2 (a) after processing (sintered at 1350°C) and (b) after an additional 3 hours at 2000°C . Grain growth is readily apparent. The sample is $\sim 0.4 \times 0.4 \text{ mm}^2$.



A sample of sintered ceramic UO_2 nuclear fuel material undergoes high temperature grain growth in the x-ray hutch.

Dynamic density field measurements of an explosively driven α - ϵ phase transition in iron

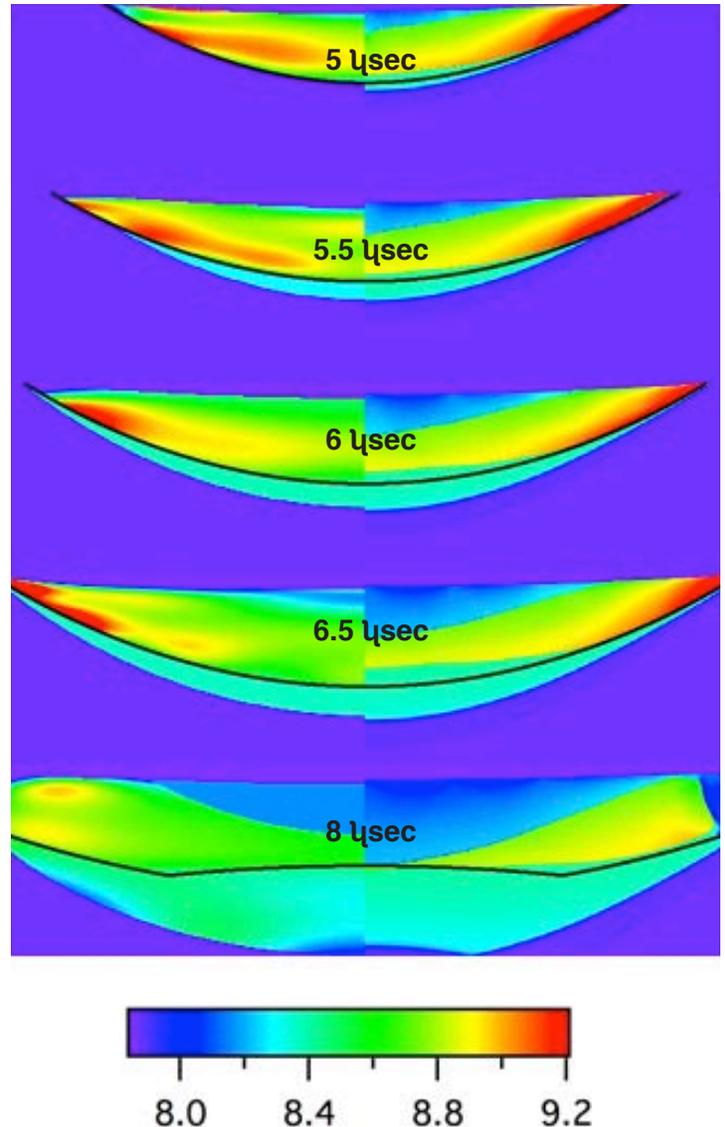
Los Alamos researchers recently completed a novel experiment providing quantitative density and kinetic data for comparison with advanced physical/computational treatments, either existing or in development, of a first-order shock-induced phase transformation.

Most studies of the α - ϵ phase transition have employed uniaxial shock wave loading. For a given material subjected to a uniaxial shock (plane, one-dimensional shock wave), the shear stress throughout both any elastic precursor and the plastic wave are uniquely related to the amplitude. This phase transition in iron has been well studied due to the element's prevalence in the earth's crust and its use in steel and its various alloys.

In this work, Los Alamos researchers provided measured density distributions, dynamically measured at 5 times using the Dual Axis Radiographic Hydrodynamic Test Facility (DARHT) at LANL, of an iron sample undergoing the α - ϵ phase transition from loading induced by a detonation wave sweeping along one surface. This loading path differs from one-dimensional shock wave loading because there are regions of shear developed in the sample that are an evolving function of the obliquity with which the detonation wave interacts with the sample, and consequent shock and elastic wave reflections from the free surface of the iron.

Shocked regions and boundaries were measured, as well as regions and boundaries of elevated density (presumed to be the ϵ -phase iron). The formation and dynamics of these regions were captured and are available for comparisons to material descriptions. The researchers also applied 16 photon Doppler velocimetry (PDV) probes to capture the free surface velocity along a discrete set of radially distributed points in order to compare and correlate the density measurements with previous shock wave studies. The velocimetry data are in nearly exact agreement with previous shock wave studies of the α - ϵ phase transition, the density distributions, while generally in agreement with expectations evolved from the shock wave studies, show for the first time quantitatively that the epsilon phase is generated in regions of high shear stress but at hydrostatic stresses below the typically quoted 13 GPa value. The density field measurements are particularly useful for observing the effects of the forward and reverse transformation kinetics, as well as the reverse transformation hysteresis that is also not predicted in current multi-phase equation of state descriptions of iron.

Future facilities like MaRIE will take this research into phase transition kinetics and the importance of stress-state on shock-induced transitions even further by facilitating direct coupling of the shock-induced transition microstructure with the initial starting material microstructure.



The measured density data (g/cm^3 , at times relative to initiation of PBX 9501), are in the left half of the figure and the calculated data are in the right half.

Authors include Larry Hull (Focused Experiments, WX-3), George T. (Rusty) Gray III (Materials Science in Radiation and Dynamics Extremes, MST-8), and Barry J. Warthen (DARHT Experiments and Diagnostics, WX-4).

The execution of an experiment at a large facility such as DARHT necessarily involves large numbers of people and often their predecessors. Various funding sources are also involved. Special recognition is given to the accelerator and operations teams, the gamma-ray camera team, the PDV team, and the mechanical design team, because each fine-tuned its respective contributions to make this particular experiment so successful.

Science Campaign 2 (LANL Program Manager Rick Martineau) and Department of Defense/Department of Energy

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Density cont.

Joint Munitions Program (LANL Program Manager Thomas Mason) funded the work, which supports the Lab's national security science mission and Materials for the Future science pillar. Reference: "Dynamic density field measurements of an explosively driven α - ϵ phase transition in iron," by L.M. Hull, G.T. Gray III, and B.J. Warthen, *J. Appl. Physics*, **116** (2014).

Technical contacts: Larry Hull and George T. (Rusty) Gray III

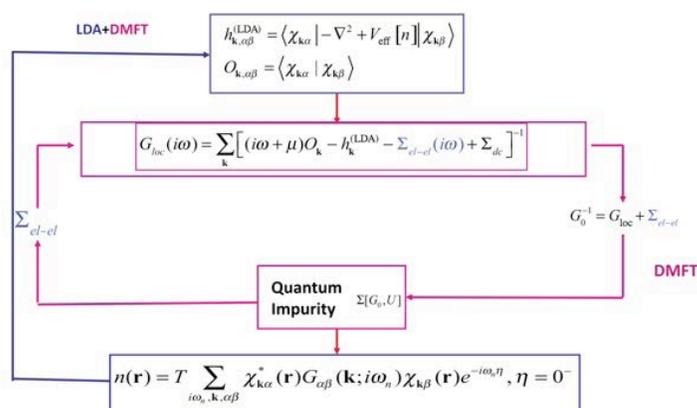
Materials-by-design effort aids search for abundant sources of non-rare-earth magnets

Magnets play a central role in a range of applications—from wind turbines to zero emission vehicles—at the heart of modern technology. As a result, there is a need to find permanent magnetic materials for power generation and energy conversion. Due to the scarcity of heavy, rare-earth elements that are currently filling that demand, scientists are searching for plentiful, non-rare-earth replacements.

By combining theory and experiment, researchers from Los Alamos National Laboratory and Argonne National Laboratory's Advanced Photon Source demonstrate a promising theoretical method for predicting an essential prerequisite guiding the search for these new materials.

In a first-time demonstration, using the yttrium-cobalt compound YCo_5 as a prototype, the researchers prove that electronic correlations play a significant role in determining the magnetocrystalline anisotropy of transition metals. Magnetocrystalline anisotropy is a key property that determines the performance of a permanent magnet. It serves to lock the orientation of the magnetization—that is, the axis that connects the north and south poles of a magnet—along a specific crystalline direction of the material. When the magnetocrystalline anisotropy is high the magnet becomes "hard;" that is, the direction of magnetization remains unchanged when manipulated by external electromagnetic fields, which is critical for use in electric motors or generators.

Key to enhanced predictive power is incorporating the local effects of electronic correlations through dynamical mean-field theory into the conventional band structure theory (LDA+DMFT), the authors conclude. This new approach leads to reliable estimates of the orbital moment, out of which magnetic anisotropy arises, as the authors have confirmed, via x-ray circular magnetic dichroism (XMCD) measurements at the Advanced Photon Source. Their theoretical methods can be used to estimate the electronic correlations and the magnetocrystalline anisotropy of materials containing 3d, 4d, and 5d transition metals, which are natural candidates for replacing rare-earth elements in current permanent magnets.



Schematic description of the dynamical mean-field theory (LDA+DMFT) approach.

This materials-by-design effort in support of discovering non-rare earth magnets is aligned with grand challenges outlined by the Department of Energy Basic Energy Sciences and the Laboratory's Materials Strategy.

This research is also an example of science on the roadmap to MaRIE, Los Alamos's proposed experimental facility that will be used to discover advanced materials needed to meet 21st century national security and energy security challenges. Using MaRIE's advanced capabilities, similar theory and experiment studies could further refine materials-by-design techniques such as the search for non-rare-earth magnets.

The Laboratory Directed Research and Development (LDRD) program funded the Los Alamos portion of the work, with some theoretical calculations performed at the Center for Integrated Nanotechnologies, a DOE Office of Basic Energy Sciences user facility. The research supports the Laboratory's Energy Security mission area and Materials for the Future science pillar.

Reference: "LDA+DMFT Approach to Magnetocrystalline Anisotropy of Strong Magnets," by Jian-Xin Zhu and Cristian Batista (Physics of Condensed Matter & Complex Systems, T-4); Marc Janoschek, Filip Ronning, J.D. Thompson, Michael Torrez, Eric Bauer (all Condensed Matter & Magnet Science, MPA-CMMS), and Richard Rosenberg (Argonne National Laboratory), *Phys. Rev. X* **4**, 021027 (2014).

Technical contacts: Jianxin Zhu (theory) and Marc Janoschek (experiment)

Sandberg to help steer LCLS x-ray laser user program



Richard Sandberg was recently elected a member of the Users' Executive Committee of the Linac Coherent Light Source (LCLS), the world's first hard x-ray laser, located in California, and a tool that allowed 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 LANL in 2009 as a Director's Postdoctoral Fellow and became a staff scientist in 2011.

The committee's purpose is to help improve user operations and facility capabilities. Since opening in 2009, LCLS has served 2,040 total researchers, leading to 341 journal

publications. It offers 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. LCLS is part of the Department of Energy's SLAC National Accelerator Laboratory operated by Stanford University.

Sandberg team's LCLS research demonstrated a crucial diagnostic for studying how voids affect explosives under shock loading. The in situ data constitute the first experimental step toward developing next-generation, physically based mesoscale models with predictive capability for high explosives. Future facilities like Los Alamos's proposed MaRIE will take this research into next generation of Stockpile Stewardship in order to design the advanced materials needed to meet 21st-century national security and energy security challenges.

Technical contact: Richard Sandberg

To 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.

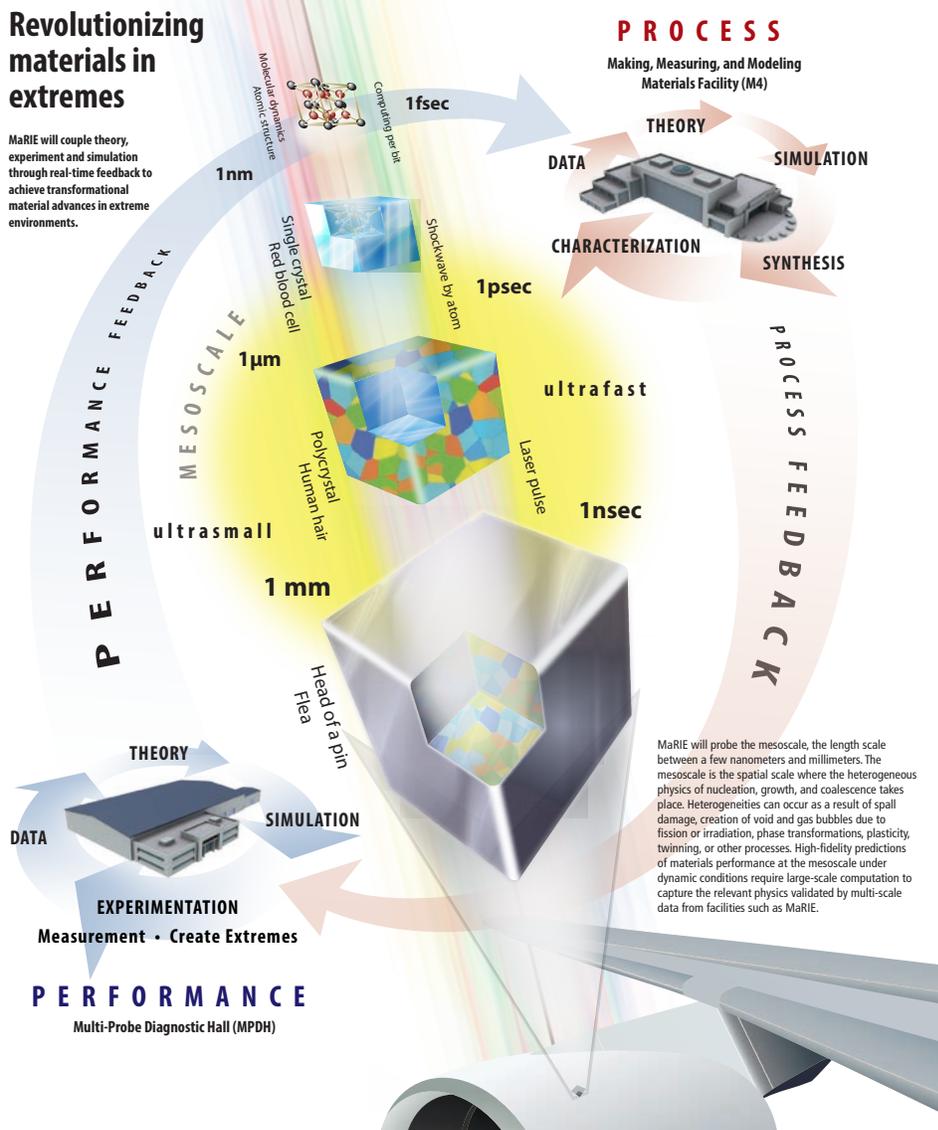


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Revolutionizing materials in extremes

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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