Title:	Roadmap to MaRIE November 2015
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Intended for:	Newsletter Web
Issued:	2015-11-23

November 2015
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Roadmap to MaRIE

Inside

As deputy project director for MaRIE, John Tapia oversees project planning for the Laboratory's proposed experimental facility for the study of matter-radiation interactions in extremes.

John Tapia

Projecting success through hard work and experience

A willingness to take on challenging professional roles and to seek out supportive mentors—it's a quality John Tapia advises newcomers to cultivate if they want to leverage the career possibilities offered at Los Alamos National Laboratory.

He speaks from experience. "There's nowhere else besides a national lab I can imagine I'd become what I am today," said Tapia, who is deputy project director for MaRIE. "Los Alamos offers enormous opportunity for people who want to take advantage of what it has to offer."

> *"I believe MaRIE will change Los Alamos and I think I can help (the Lab) eventually realize it."*

MaRIE (Matter-Radiation Interactions in Extremes) is the Laboratory's proposed billion-dollar-class experimental facility for the discovery and design of the advanced materials needed to meet 21st century national security and energy security challenges.

To meet its mission of solving national security challenges through scientific excellence, the Laboratory relies on more than researchers, said Tapia. Scientists, engineers, technologists, and operational and administrative staff are all essential in fulfilling the Lab's purpose.

Tapia was an undergraduate studying business administration at Eastern New Mexico University when he accepted an internship in the Laboratory's business operations.

That decision has had far-reaching consequences as it has allowed him to play critical roles supporting the development of large, scientific facilities through positions in Washington, DC and southern France, and at Los Alamos. Along the way, he has

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Moniz: Sustained investment in innovation is critically important to national security needs

Experimental facilities such as MaRIE will help meet that need

During an event marking the 20th anniversary of Stockpile Stewardship, Secretary of Energy Ernest Moniz stressed the critical role innovation played in making that program a success and its enduring importance to meeting the nation's nuclear security needs.

The public event, hosted by the Department of Energy's National Nuclear Security Administration and held in Washington, DC, celebrated the science and engineering breakthroughs that have allowed the country to maintain a safe, secure, and effective nuclear weapons stockpile without explosive nuclear testing. The event also included remarks by Secretary of State John Kerry and Under Secretary for Nuclear Security and NNSA Administrator Lt. Gen (retired) Frank G. Klotz.

"[Stewardship] is a story of incredible innovation. Nothing about this program was guaranteed to succeed. There was nothing off-the-shelf about it. Science and technology had to be invented to go into completely new domains," Moniz said. "That innovation is what is critically important … to meet our nuclear security needs and our other critical mission needs. That's what comes, not by trying to turn things on and off, but by making a sustained investment over many decades to sustain that innovation."

Using the advanced simulation and computing initiative as an example, Moniz said, "It wasn't just about buying 10,000 of something that existed. It was about, for example, pushing the paradigm of parallel architectures. It was about innovation in the business model … As we now look to this next

Secretary of Energy Ernest Moniz speaks during the Stockpile Stewardship Program's 20th anniversary event in Washington, DC. The program can be seen on YouTube.

push, to exascale, we are looking again at a paradigm shift in how this is going to be achieved."

Just as at the start of Stockpile Stewardship, this is going to be again the same kind of innovation challenge we need, he said. "In fact, it wasn't long ago that we are now hearing about MaRIE—can we reach a whole new generation of imaging [of] materials from very small ranges to mesoscale in terms of materials dynamics under extreme conditions."

"That kind of innovation," Moniz said, such as "incredible new capabilities from x-ray FELs, such as under construction at SLAC, … these are the kind of capabilities that are just really extraordinary and important."

Tapia cont.

earned two master's degrees and become a certified Project Management Professional and a recognized expert in managing projects, frequently participating in DOE project peer reviews.

With encouraging mentors behind him—"ones who supported me and said 'you can do more,' " he said, Tapia took on positions of increasing responsibility. After his internship, he briefly served as a budget analyst in the Lab's environmental management programs before becoming a mentoreee for the chief financial officer. As chief of staff for Los Alamos's Spallation Neutron Source Project, he was the Lab's point-of-contact on all business functions with the project office at Oak Ridge National Laboratory, where the $1.4 billion facility was being built. As the acting section leader for Project Controls at ITER, a large-scale experimental science facility now under construction in France that is designed to prove the feasibility of fusion as an energy source, Tapia developed the initial project control and risk management standards for the international organization.

"You can't be afraid to take risks," he said, referring to his time at ITER, which meant uprooting his family to another country. He said he's had to ask plenty of questions, read several textbooks, and "get past the vernacular … You have to walk in knowing you don't know everything and find a way you can contribute."

The result has been a rewarding professional career. "I learn something new every day," he said. "I've been around some of the most complex projects on the planet."

For MaRIE, Tapia oversees the project's planning, is responsible for developing the project's standards and procedures, and works closely with the technical leads as well as colleagues at the Department of Energy and other laboratories to benchmark the best practices to ensure the MaRIE project is effectively managed. His experience with large, complex experimental science facilities has cemented in him the desire to make a lasting contribution to the Laboratory. Tapia said he has seen what happens, "how (these facilities) can change a Lab. The best thing about the project is it brings all the best skills to build this facility, the technical staff and the support staff," he said. "I believe MaRIE will change Los Alamos and I think I can help (the Lab) eventually realize it."

Science and technology on the roadmap to MaRIE

A key development to implementing the next generation of high brightness x-ray sources: phase preserving diamond optics

In a promising advance in the development of the high-quality optics needed by the MaRIE project, the Laboratory's proposed facility for time-dependent materials science at the mesoscale and other high-energy x-ray light sources, Los Alamos researchers, in collaboration with Brookhaven National Laboratory and Modern Microsystems, have successfully designed, fabricated, and tested a new x-ray lens made from diamond.

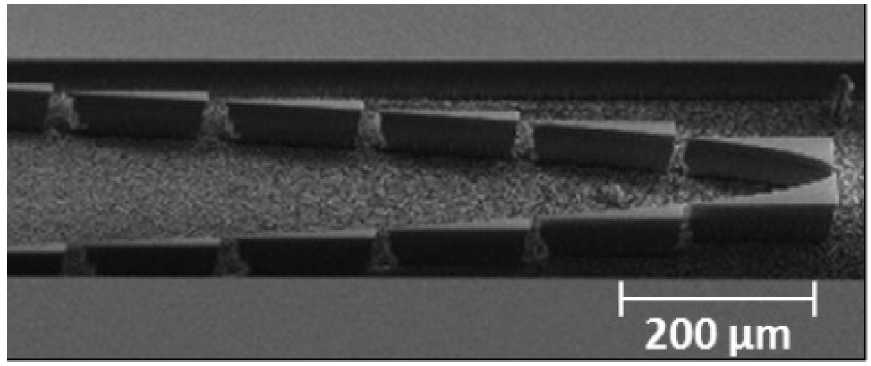

Figure 1: A prototype kinoform x-ray optic formed in single-crystal diamond by deep reactive ion etching.

MaRIE (Matter-Radiation Interactions in Extremes) will ultimately provide a bright source of high-energy x-ray photons; but without focusing elements to concentrate the x-rays on the region of interest, the full potential of the source will not be realized. From the point of view of x-ray optical properties alone, beryllium is one of the best lens materials available, and a large fraction of the existing refractive x-ray lenses in use around the world are made from beryllium. Unfortunately, beryllium has some drawbacks. It is usually produced as polycrystalline material, cannot handle high heat loads, and is hazardous to work with. The polycrystallinity degrades perfection of the photon phase profile that is produced by the source, and the poorer thermal quality of beryllium precludes its routine use as the first optical element facing the source.

Diamond has long been realized as an excellent material for x-ray lenses. Diamond has good optical properties for x-ray photons, but more importantly, has an order of magnitude higher thermal conductivity and lower thermal expansion compared to beryllium, as well as excellent hardness that will allow its use in the high heat-load present at the new high brightness sources like the planned MaRIE.

Diamond solves most of the problems of beryllium, but up to this point it has been difficult to fabricate the precise shapes needed to make high quality x-ray lenses. This research has successfully fabricated the complex shapes in diamond required for x-ray lenses. Shown in Figure 1 is a visible light image of a diamond kinoform lens, etched into a diamond chip of size 4.5-mm x 4.5-mm and 0.5-mm thick. This shape focuses in one direction and produces a line focus. The design and fabrication with electron beam lithography was performed at the Center for Functional Nanomaterials at Brookhaven National Laboratory. Reactive ion etching was performed at Modern Microsystems. The lenses were tested at the CHX beamline at NSLS2 at Brookhaven. Shown in the top panel of Figure 2 is an image of the 280-µm x 55-µm rectangle of light that was incident on the diamond lens shown in Figure 1. In the bottom panel of Figure 2 is shown the one-dimensional focusing effect of the lens, collecting the light into an 8-µm x 55-µm line.

Participants include Richard Sheffield (Experimental Physical Sciences, ADEPS), Kenneth Evans-Lutterodt, Andrei Fluerasu, A. Stein, Lutz Wiegart (Brookhaven National Laboratory), and Craig McGray (Modern Microsystems).

The research, which was funded by MaRIE-related capability development (Cris Barnes, capture manager), supports the Laboratory's Nuclear Deterrence mission and Materials for the Future science pillar.

Technical contact: Richard Sheffield

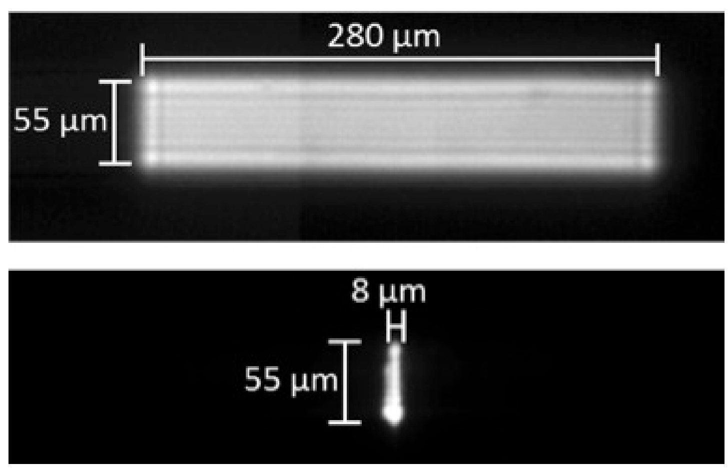

Figure 2: Experimental results on focusing performance of the prototype diamond kinoform x-ray optic. The transmittance of the optic was measured to be 75% ±5%, at a photon energy of 12 keV. Top: The 280-μm × 55-μm rectangle of x-ray illumination that is incident on the lens, as imaged by a YAG crystal. Dark fringes parallel to the aperture edges indicate the coherence of the beam. Bottom: The one-dimensional focusing action of the lens has reduced the 280-μm width of the beam to approximately 8 μm. The resulting line focus has dimensions of 8 μm × 55 μm. (Image brightness and contrast adjusted for clarity of presentation.)

Using cutting-edge lasers to reveal properties of a common Earth material

Los Alamos scientists and collaborators used the high-brightness, short-pulse Linac Coherent Light Source x-ray free electron laser at the SLAC National Accelerator Laboratory to simulate the extreme environment of a meteorite impact and its effects in silica (SiO_2). *Nature Communications* published the research.

Silica is one of the most abundant materials in the Earth's crust. The research revealed its unexpectedly swift transformation to rare stishovite—a hard and dense mineral that is found at bolide-impact craters on the Earth's surface. This study demonstrates the first-ever shock-induced crystallization of an amorphous material observed via femtosecond (10-15 second) x-ray diffraction. These results will lead to a greater understanding of important problems in shock physics and materials science, potentially enabling refined planetary models to provide insight for the impact history of the Earth and solar system, and techniques to design new materials with improved functionality.

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

This method resolved the growth of nanocrystalline stishovite on the nanosecond timescale just after shock compression. The functional form of this grain growth suggests homogeneous nucleation and attachment as the growth mechanism, rather than a diffusion-based mechanism. These are the first observations of crystalline grain growth in the shock front between low- and high-pressure states via XRD.

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

Reference: "Ultrafast Visualization of Crystallization and Grain Growth in Shock-compressed SiO_2," *Nature Communications* (2015); doi: 10.1038/ncomms919. Researchers include Arianna Gleason (Shock and Detonation Physics, M-9 and SLAC National Accelerator Laboratory), Cindy

Arianna Gleason makes final adjustments to detector positions inside the Matter in Extreme Conditions (MEC) target chamber at the Stanford Liner Accelerator facility (SLAC) in California. The MEC facility 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 physic,s and high-energy-density physics.

Bolme (M-9), Richard Sandberg (Center for Integrated Nanotechnologies, MPA-CINT), and collaborators from the Linac Coherent Light Source, the Stanford Institute for Materials and Energy Sciences at SLAC, Stanford University; Washington State University; Lawrence Livermore National Laboratory; Carnegie Institution of Washington; and the Center for High Pressure Science and Technology Advanced Research in Shanghai. The Laboratory Directed Research and Development program sponsored the Los Alamos work, and a Reines Distinguished Postdoctoral Fellowship funded Gleason. The research supports the Lab's Nuclear Deterrence mission area and the Materials for the Future science pillar by demonstrating a strategy and methodology to extract phase transition kinetics using time-resolved x-ray diffraction data.

Technical contact: Arianna Gleason

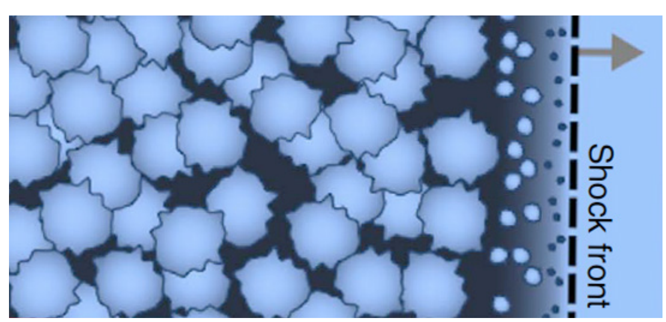

Illustration (for 33.6 GPa at 10-ns delay, grey box) illustrates the researchers' interpretation of grain growth behind the shock front (black dashed line, propagation direction is grey arrow). The distribution of grain size increases with distance from the shock front.

Ultrafast synchrotron 3D imaging during uniaxial loading experiments of 3D-printed specimens sheds light on material damage

Three-dimensional printed materials offer a wealth of possibilities in that unique structures may be printed with geometries that are not possible with traditional molding, extrusion, casting, or machining techniques. Structures may be optimized for weight, strength, or form to improve their overall function. Three-dimensional (3D) printed structures are created through the serial laydown of materials, layer-by-layer. Because of this, inherent discontinuities within the microstructure reduce the overall mechanical strength of a part when compared to traditionally formed materials. Interfacial adhesion through polymer chain entanglement is minimized. Mechanical testing indicates that print orientation as well as the use of print material recycling can affect the ultimate mechanical performance. Due to these problems, there are few demonstrated high-performance applications of 3D-printed materials, especially polymers. To understand the adhesion between the layers and therefore crack initiation, propagation, and ultimately failure, in situ analysis techniques are needed. To further complicate the analysis, these materials are typically hyper-elastic in nature. As such, experiments cannot be paused during data collection, because the material will continue to deform and respond to the applied stress.

Recent experiments led by Los Alamos National Laboratory researchers in collaboration with Arizona State University and Argonne National Laboratory's Advanced Photon Source collected 3D-tomographic data during uniaxial loading of 3D-printed tensile specimens. In order to image them in three dimensions during loading, high-speed, continuous 3D-tomographic data were collected. Using the fastest continuous 3D imaging yet demonstrated, four full 3D images were collected within one second as a loading rig was rotated at 2 Hz while applying a uniaxial load on 3D-printed materials. Eighteen thousand radiographs were collected during this dynamic event to be reconstructed into ~20 tomograms. 3D-printed, glass-bead-loaded nylon polymers (Figure 1) were continuously loaded up to failure, while 901 radiographs were collected for every 180° of rotation while simultaneously recording strain. Dynamic stretching, cracking, failure, and elastic recovery were imaged in these hyper-elastic materials.

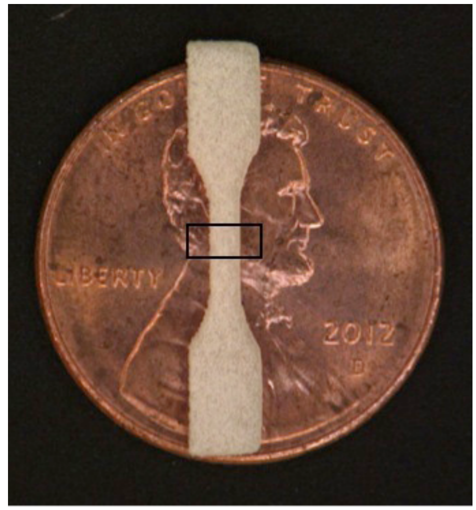

Figure 1: Photograph of a laser sintered 3D-printed tensile specimen. Specimen is 2 cm in length. The field of view imaged at the synchrotron is indicated by the black box.

The micro-specimens of glass-bead-filled polyamide-12 sintered powder (EOS material 3200 GF) were printed on an EOS Formiga P 110 printer. This system sinters the powder using a 30-W CO_2 laser to build the objects layer by layer. Specimens were printed in each of the three orthogonal orientations. During printing, the entire powder bed heated to just below the melting temperature of the polymer. The printed objects were removed from the powder, leaving behind powder that can be used by the next print, however, the material now had a thermal history. To understand the effect of the thermal history during recycling upon layer adhesion and mechanical performance, the tested and imaged specimens were printed with virgin material, 50% virgin-50% recycled, and 50% virgin-50% doubly recycled material.

Figure 2 illustrates a subset of the sequential reconstructed slices through a specimen showing the delamination of the glass microbeads from the nylon, the elongation of the

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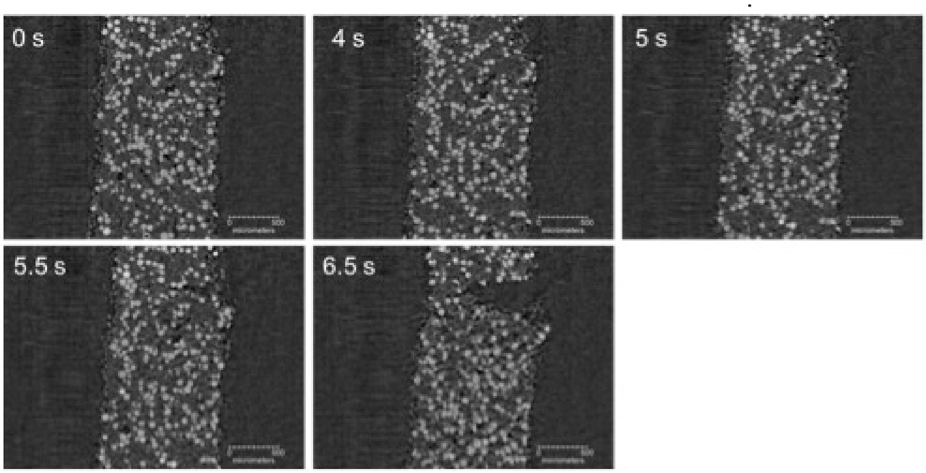


Figure 2: A subset of the sequential reconstructed slices through the glass-bead-filled 3D-printed nylon polymer. 3D images were collected every 0.25 seconds. The material is under uniaxial tension from the bottom. Imaging continued through material breakage. Delamination between the polymer and the beads is clearly seen. The beads become "fuzzy" in the 3D image at 6.5 s due to rapid sample motion.

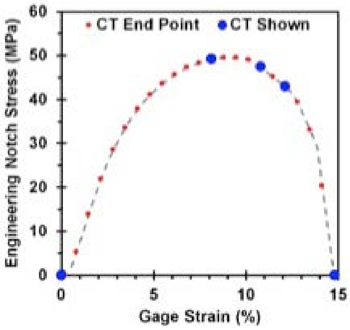


Figure 3. Stress-strain plot for the material shown in Figure 2. Red dots indicate the points at which the continuous imaging for every 180° rotation ended: blue dots indicate the 3D images shown in Figure 2.

Ultrafast cont.

nylon, breakage, and the elastic recovery. Some blurring of the image is seen at 6.5 seconds in Figure 2 due to the high rate of the elastic recovery.

The stress-strain curve of the material indicates a tensile strength of 50 MPa (Figure 3). This value is identical to both the orientation-imaging-microscopy-advertised strength of the material as well as the researchers' own full scale mechanical test results. That is, the material does not have a size effect for its mechanical strength. Full 3D renderings of the materials show the movement of the glass particles: a single volume rendering is shown in Figure 4, during elongation of the specimen.

Future efforts include the application of digital volume correlation to understand the flow of material during elongation, as well as faster imaging rates. Imaging rates using a machine spindle to rotate the load cell with rates of 50 Hz (100 tomograms per second) are available. This work addresses the future mission of the proposed MaRIE (Matter-Radiation Interactions in Extremes) experimental facility, in that it advances the tools needed to develop and manufacture next-generation materials for reduced-cost stockpile options through the use of additive manufacturing.

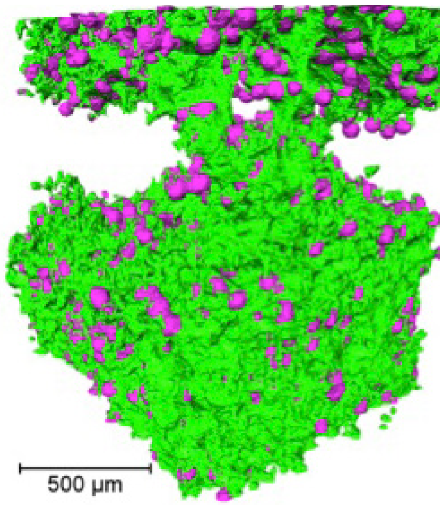
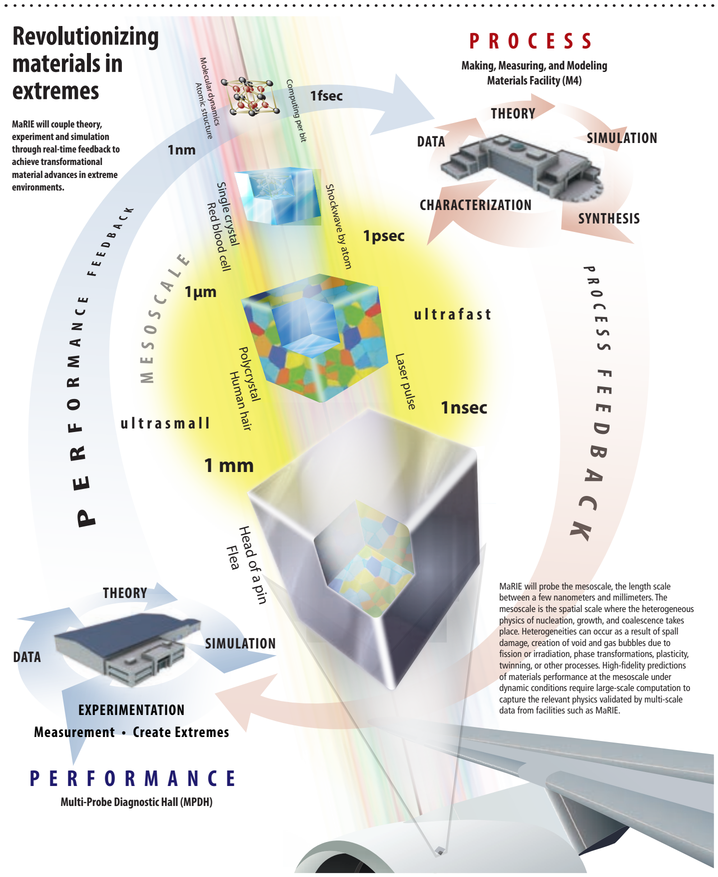


Figure 4: False color 3D rendering of the material during breakage. The glass beads are rendered pink and the polymer green.

This multi-institutional team is composed of Engineered Materials (MST-7) researchers Brian M. Patterson, Nikolaus Cordes, Kevin Henderson, James Mertens, and Robin Pacheco; Arizona State University researchers Nikhilesh Chawla and Jason Williams; and Xianghui Xiao of Argonne National Laboratory. This work is sponsored by the Enhanced Surveillance Campaign (Tom Zocco, program manager) and Engineering Campaign (Eric Mas, program Manager) and supports the Laboratory's Nuclear Deterrence mission and the Materials for the Future science pillar.

Technical contact: Brian M. Patterson



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 adeps-comm@lanl.gov.

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