MSTe NEWS
December 2018
Approved for public release; distribution is unlimited.

INSIDE

Saryu Fensin studies a projection of molecular dynamic simulations of tantalum where the colors indicate local crystalline orientation. These atomistic simulations guide her experimental work.

Saryu Fensin

Driving experiment and simulation for national security solutions

By H. Kris Fronzak

> *"My unique background has helped me ask questions about dynamic behavior of materials that sometimes end up being new and exciting."*

As an enterprising materials scientist, Saryu Fensin leverages both experiments and simulations to improve understanding of how materials behave when subjected to extreme forces. Her aim is to use the complementary techniques to design and develop innovative materials for use in extreme conditions such as stockpile-focused applications.

"To certify our stockpile with confidence, we need to understand the role a material's microstructure plays in determining its dynamic properties," Fensin said. "I'm hoping to solve this puzzle and improve our predictive capability to model material response in extreme conditions. Achieving this kind of specific, controlled functionality of materials could have a big impact on the Laboratory's national security science mission."

continued on next page

Los Alamos NATIONAL LABORATORY EST. 1943

Fensin cont.

Fensin (Materials Science in Radiation and Dynamics Extremes, MST-8), who earned her Ph.D. in materials engineering from the University of California, Davis, first made an impact on the field of dynamic materials research as a Los Alamos postdoctoral researcher. Recent research had shown that not all grain boundaries in materials were equally susceptible to damage and failure. The common belief was that boundaries with low energy did not fail. Fensin used molecular dynamics simulations of copper to show grain boundary energy wasn't the phenomenon preventing failure. The way boundaries dissipate stress dictated their susceptibility to failing.

The project's success enhanced communication between experimentalists and modelers in the group, said Steve Valone, an MST-8 guest scientist and Fensin's former mentor. Combining the two approaches helped the researchers to better predict failure and develop damage-tolerant materials.

Fensin takes pride in using both approaches: her experiments inform computational models that, in turn, inform experiments, in a process called codesign. With MaRIE, the Laboratory's proposed capability for studying matter-radiation interactions in extremes, Fensin could directly validate both her simulations and experiments to further certify the stockpile.

In a recent study published in *Nature Communications*, Fensin and collaborators used Argonne's Advanced Photon Source synchrotron-radiation light source to measure strain in a loaded copper film. They modeled the atomic structure and showed that the measured strain field corresponded to a specific kind of dislocation in the lattice structure. This experiment could help determine how defects cluster and contribute to strain in a material.

She also contributes to a joint experimental and modeling study of the instabilities that affect materials' strength and ejecta. The project, sponsored by the Primary Assessment Technologies science campaign, will also simulate molecular dynamics to explain the mechanisms that drive differences in materials' behavior.

"My unique background has helped me ask questions about dynamic behavior of materials that sometimes end up being new and exciting," said Fensin, whose undergraduate degree is in chemistry. The complex, systematic experiments she and her teammates perform are leading to "innovations in both materials science and shock physics, which is really exciting."

Fensin, who has received a young leaders professional development award from The Minerals, Metals & Materials Society (TMS) and is a leader on the organization's scientific committees, sets an inspiring example for those she mentors. "Saryu is extraordinarily resourceful and certainly an expert in the materials field, and her ability to explain concepts and to direct research truly sets her apart from other mentors I have had," said Rachel Flanagan (MST-8), a Ph.D. candidate at the University of California, San Diego. "What really impresses me about Saryu is her dedication to her work, her resourcefulness, and her ability to connect with other researchers. As a fellow woman in engineering, she sets an amazing example for the type of scientist I hope to someday become."

Saryu Fensin's favorite experiment

What: Incipient spall experiments with recovery coupled with molecular dynamics modeling

Why: To determine if adding a second soft phase (Cu-1%Pb) alters the damage and failure response and uncover the mechanism that contributes to the change, if any

Who: Saryu Fensin and Rusty Gray III (MST-8) and Ellen Cerreta (Explosive Science and Shock Physics, M-DO)

When: 2011

Where: Materials Science Laboratory at Los Alamos

How: We performed recovery shock experiments on Cu-1%Pb in the Materials Science Laboratory, varying both the peak stress and the pulse duration. The recovered samples were analyzed using electron backscatter diffraction and scanning electron microscopy to provide both qualitative and quantitative insights into material strength and the mechanisms that contribute to it.

The "aha" moment: Coupling of the metallography with the molecular dynamics simulations helped us determine that the mechanism responsible for causing a decreased spall strength in this two-phase material was linked to super heating and softening of the second phase. This led to cavitation-type behavior in the second soft phase.

MST staff in the news

Hehlen elected Fellow of The Optical Society

Markus Hehlen (Engineered Materials, MST-7) has been named a Fellow of The Optical Society (OSA). The OSA's board of directors cited him for "major contributions to the field of rare-earth-doped optical materials for scintillators, upconversion phosphors, and optical refrigeration."

Hehlen, who received his Ph.D. in inorganic and physical chemistry from the University of Bern in Switzerland, is a member of MST-7's materials performance and characterization team. He has published more than 80 papers and holds 8 patents, with 6 pending. Hehlen is also the recipient of a 2013 LANL Distinguished Performance Award for his contributions to the National Explosives Engineering Security Sciences project on homemade explosives. His current R&D interests include next-generation sensors for agile space applications, materials for solid-state optical refrigeration and radiation-balanced lasers, and advanced X-ray screens for computed tomography.

He joined Los Alamos as a postdoctoral research associate in 1994 and returned as a scientist in 2003, after performing a postdoctoral fellowship in the Optical Sciences Center of the University of Michigan and leading a development team at the start-up company Gemfire Corporation.

At Los Alamos, Hehlen has initiated, developed, and led numerous projects at the interfaces of applied physics, material science, and photonics and contributed to the Laboratory's goals of creating and modifying materials to achieve advanced, controlled functionality and predictive performance.

The OSA, which was founded in 1916, is a professional organization for scientists, engineers, students, and business leaders who make discoveries, create applications, and accelerate achievements in the field of light. The society aims to promote the generation, application, and archiving of knowledge in optics and photonics. Its fellows number no more than 10% of the total OSA membership.

Technical contact: Markus Hehlen

El-Atwani receives Acta Materialia's Outstanding Reviewer Award

Osman El-Atwani (Materials Science in Radiation and Dynamics Extremes, MST-8) received the 2017 Outstanding Reviewer Award from *Acta Materialia* in recognition of his work assessing manuscripts for publication in the journal. The Outstanding Reviewer awards for excellence in reviewing are selected by the editors of *Acta Materialia*, *Scripta Materialia*, and *Acta Biomaterialia*.

El-Atwani received his Ph.D. in materials science and engineering from Purdue University in 2012 for research on ion beam irradiation on hard material surfaces, particularly the nanopatterning of gallium antimonide and silicon substrates and irradiation damage of tungsten. He was a postdoctoral researcher and a visiting professor at Purdue from 2012–2014 and became a Director's Postdoctoral Fellow in MST-8 in 2016. At Los Alamos, El-Atwani works on multiscale studies in advanced structural materials for nuclear energy. His work supports the Laboratory's Energy Security mission area and its Materials for the Future science pillar.

Acta Materialia is a peer-reviewed journal that publishes original papers and commissioned overviews that further understanding of the relationship between the processing, the structure, and the properties of inorganic materials.

Technical contact: Osman El-Atwani

Gray granted Rinehart Award at 2018 DYMAT conference

George T. "Rusty" Gray III (Materials Science in Radiation & Dynamics Extremes, MST-8) has received the DYMAT association's John S. Rinehart Award, based on the recommendation of an international jury of DYMAT members. The award recognizes outstanding and creative work in the science and technology of dynamic processes in materials.

The award is granted to one or two people every three years; Gordon Johnson, a program director at Southwest Research Institute in Minneapolis, is the other 2018 recipient. The award was presented at the 12th International DYMAT Conference, held recently in France.

continued on next page

MST staff cont.

Gray leads critical science projects for the Lab's Stockpile Stewardship efforts; publishes Laboratory research on materials science advances; and advises institutions on materials dynamics in defense and manufacturing areas, acting as a liaison for the Laboratory. He is the only active Los Alamos scientist elected to the National Academy of Engineering. He is a fellow of the American Physical Society, ASM International, Los Alamos National Laboratory, and the Minerals, Metals and Materials Society, having served as its president in 2010.

DYMAT is a European association created to promote research into the dynamic behavior of materials and related applications. Its Rinehart Award is named for John S. Rinehart, who has actively developed the field of dynamic deformation in materials.

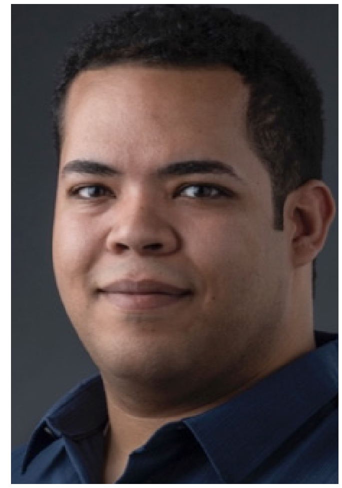
Technical contact: Rusty Gray

Zepeda-Alarcon, Santiago Cordoba receive Seaborg Postdoctoral Fellowships

Eloisa Zepeda-Alarcon (Materials Science in Radiation and Dynamics Extremes, MST-8) and Miguel Santiago Cordoba (Engineered Materials, MST-7) received 2018 Seaborg Postdoctoral Fellowships, based on the technical merit and the strategic importance of their proposed research in actinide science.

Zepeda-Alarcon, a member of the MST-8 Scattering Science team, is mentored by Sven Vogel (MST-8). She outlined a novel method to measure the stresses that happen during the highly anisotropic thermal expansion of uranium. Zepeda-Alarcon will apply neutron diffraction and imaging to a novel experimental technique that provides access to crystal lattice strains in mechanically constrained polycrystalline and unconstrained α-uranium powder. Combining these two techniques will provide unique data for thermomechanical models and will, for the first time, quantify thermal residual stresses in uranium.

Zepeda-Alarcon received her Ph.D. in earth and planetary science (with a focus in mineral physics) from the University of California, Berkeley. She focuses on materials characterization using diffraction with a special focus in texture development in polycrystalline materials.



Santiago Cordoba, who is mentored by Miles Beaux and Igor Usov (MST-7), is a materials chemist with experience in enhanced optical sensing and surface science techniques. He will explore the surface of a δ-phase plutonium alloy using atomic force microscopy to simultaneously acquire mechanical, electronic, and topographical information from the nanoscale to mesoscale. If successful, the work will demonstrate that atomic force microscopy can provide fundamental information about plutonium in high-dimensional resolution.

Santiago Cordoba received a Ph.D. in chemistry from Penn State University in 2016. He develops strategies to design functional materials and to understand matter-interactions from surface to bulk across multiple length scales.

This year's Seaborg recipients also included Jordan Evans (National High Magnetic Field Laboratory-Pulsed Field Facility). Recipients participate in the Actinide Science Lecture Series, and have their work featured in *Actinide Research Quarterly*.

The Los Alamos branch of the Glenn T. Seaborg Institute serves as a national center for educating and training students, visiting scientists, and faculty in transactinium science. Its research programs investigate properties of the lighter actinide elements as fuels for energy and as nuclear weapons. Support for Seaborg Postdoctoral Fellowships comes from the Laboratory Directed Research and Development program, the Principal Associate Directorate for Global Security, and the Science Campaigns in the Principal Associate Directorate for Weapons Programs.

Technical contacts: Eloisa Zepeda-Alarcon and Miguel Santiago Cordoba

continued on next page

MST staff cont.

Torres receives 2018 Distinguished Mentor Award

Joseph Torres (Engineered Materials, MST-7) has won a 2018 Distinguished Mentor Award. The annual awards program is sponsored by the Student Programs Advisory Committee and the Student Program Office.

Torres was nominated by Sendin Bajric (Nuclear Materials Science, MST-16), whom he mentored from post-master's through graduate research assistantship and conversion to a full-time staff position. In his nomination, Torres was commended for his care in explaining how projects tied into the Laboratory's mission and for his advice about becoming successful at the Lab.

Torres began mentoring students in January 2017 and has served as the student coordinator for MST-7. He has actively recruited students at his alma mater, the University of Oregon; more than 75% of the students he recruited to the Lab stayed for a post-master's internship and about half have been hired as research technologists in MST-7 and other groups.

Torres joined the Laboratory as a post-baccalaureate intern and became staff in 2014. He is a research technologist focused on synthesizing and characterizing polymeric materials. His research focuses on polymer processing, additive manufacturing, and polymer characterization. Torres received a large-team Los Alamos Distinguished Performance Award in January 2014.

Technical contact: Joseph Torres

Wilson wins outstanding poster award at Lab's 2018 Student Symposium

Tashiema Wilson (Materials Science in Radiation and Dynamics Extremes, MST-8) won an outstanding poster award in the materials science category at the 18th Annual Student Symposium—her second such award in two years.

Her research, "Understanding uranium silicide fuel and the effects of fission products," focused on the need for new fuel types in light water reactors, which is driven by the need for accident-tolerant fuels with better operational and transient safety. Uranium-silicide compounds are among the candidates for accident-tolerant fuels. Wilson used arc-melting to fabricate compositions between U_3Si_2 and USi_3 and systematically studied the impact of the dominant fission products that form during the lifecycle of a fuel element. The data from her study allows for a new interpretation of the U-Si phase diagram.

Wilson, who is a Ph.D. candidate in nuclear engineering at the University of South Carolina, Columbia, is mentored by Joshua White (MST-8). Her work, which supports the Lab's Energy Security mission and its Materials for the Future science pillar via development of fuels for light water reactors, was co-funded by a Nuclear Regulatory Commission fellowship and DOE Office of Nuclear Energy's Advanced Fuels Campaign.

Her poster was one of almost 170 presented at the symposium, which allows LANL students to publicize their research and to network and make professional contacts. The event was organized by the National Security Education Center Student Programs Office and held at the J. Robert Oppenheimer Research Library.

Technical contact: Joshua White

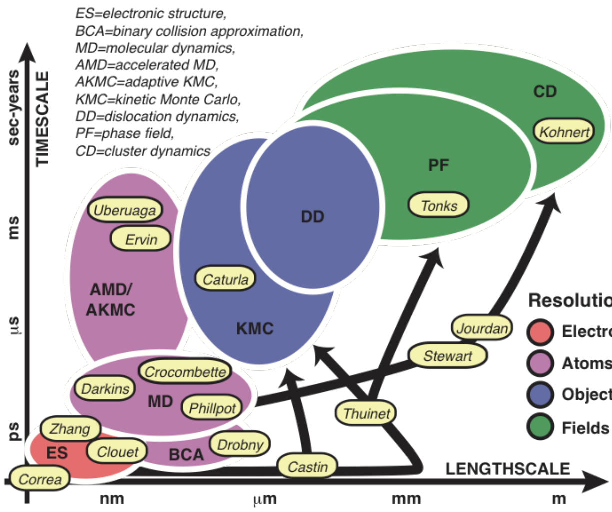
Capolungo, Uberuaga edit special issue of Computational Materials Science *on radiation effects*

Laurent Capolungo and Blas Uberuaga (Materials Science in Radiation and Dynamics Extremes, MST-8) collaborated with Francois Willaime (CEA) to produce a special issue of *Computational Materials Science* that focused on simulations of radiation's effects on materials. Understanding and mitigating the effects of irradiation in nuclear energy systems is a key component of Los Alamos's core mission, which is to maintain a strong nuclear deterrent via stockpile stewardship. Capolungo and Uberuaga were chosen to guest edit the issue because of their extensive experience creating and validating models for materials applications. The issue provided perspectives on the state of the art of the field and introduced common methods used to simulate radiation damage across scales. It included topics ranging from electronic and atomistic scale simulations to mesoscale methods and the coupling between them. The publication featured 16 articles; four of these were studies or commentary by Los Alamos researchers.

"The multi-scale grand challenge of radiation damage modeling" introduced the grand challenge of simulating the ef-

continued on next page

MST staff cont.



This multiscale paradigm shows the length and time scales of modeling methods that show radiation damage in materials.

fects of radiation damage over the decades of relevant time and length scales. It was authored by Capolungo, Willaime, and Uberuaga.

"Design and analysis of forward and reverse models for predicting defect accumulation, defect energetics, and irradiation conditions" weighed in on the challenge of developing predictive models of the effects of radiation on a material's microstructure: a challenge that is made harder because many models use an incomplete catalog of defect energetics and associated reactions. The research was done by James A. Stewart and Rémi Dingreville (Sandia National Laboratories) and Aaron A. Kohnert and Capolungo (MST-8).

"Discovering mechanisms relevant for radiation damage evolution" gave examples of when simulations revealed new and unexpected kinetic mechanisms. It also showed how those mechanisms, when coupled with higher-level models, impacted experimental observables in irradiated materials. The work was done by Uberuaga and Enrique Martínez (MST-8) and Danny Perez and Arthur F. Voter (Physics and Chemistry of Materials, T-1).

"Modeling microstructural evolution in irradiated materials with cluster dynamics methods: A review" discussed the growing need for material models that predict the evolution of microstructures as a function of chemistry, texture, grain size, precipitate content, and irradiation conditions. It reviewed the various cluster dynamics modeling schemes that have emerged from this need for better models. Kohnert and Capolungo (MST-8) and Brian D. Wirth (University of Tennessee, Knoxville, and Oak Ridge National Laboratory) performed the research.

Reference: "Radiation effects," *Computational Materials Science* **149** (2018).

Technical contact: Laurent Capolungo

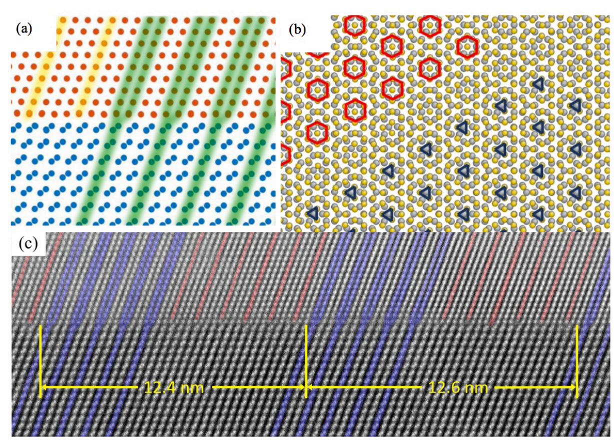
Understanding the atomic interfacial structures of quantum-computing materials

Knowing the atomically precise arrangement of atoms at epitaxial interfaces is important for emerging technologies—such as quantum-computing materials—whose function and performance are dictated by bonds and defects that are energetically active on the microelectronvolt scale. Furthermore, ordered and dislocated interfaces between dissimilar materials may have important roles in improving emerging quantum-computing materials.

In a study that combined atomistic modeling and dislocation theory with scanning transmission electron microscopy (STEM), a multidisciplinary team pinned down the nature of secondary interface misfit dislocation networks using a thin-film prototype (metamorphic epitaxial aluminum [Al] on silicon [Si] interface) that is used in a superconducting qubit device for quantum-computing applications.

The results are a key step in explaining the role of material interfaces in microwave loss in quantum coherent superconducting devices. One area that could benefit from such material research is quantum computing and its applications.

Their work indicated that the lattice misfit at the interface structure was relieved by both primary and secondary dislocations. Detailed examination of the interface structure reveals that there are two domains at the interface with 3-fold and 6-fold symmetries and a relationship between the two domains by a stacking fault. The secondary interface misfit networks are validated by atomic resolution STEM observation, which clearly shows primary interface misfit dislocations for the majority of the strain relief and evidence



(a) Cross-sectional slice of the simulated volume with selected Fourier-filtered planes. (b) High-resolution plan view of the simulated structure across a domain boundary with the yellow atoms being Al and the grey atoms being S. (c) Superposed image of cross-sectional STEM image and Fourier-filtered planes showing the periodicity of the layers of approximately 12.5 nm indicating the existence of secondary dislocations.

continued on next page

Understanding cont.

of a secondary structure allowing for complete relaxation of the Al–Si misfit strain.

The study was performed, in part, at the Center for Integrated Nanotechnologies, a DOE Office of Basic Energy Sciences user facility jointly operated by Sandia National Laboratories and Los Alamos National Laboratory. The work supports the Laboratory's Energy Security mission and its Materials for the Future science pillar. Los Alamos contributed to the research via atomistic modeling and interface dislocation analysis.

Researchers: Xiang-Yang Liu (Materials Science in Radiation and Dynamics Extremes, MST-8); Ilke Arslan and Bruce W. Arey (Pacific Northwest National Laboratory); Justin Hackley and Christopher J. K. Richardson (University of Maryland); Vincenzo Lordi (Lawrence Livermore National Laboratory). Reference: "Perfect strain relaxation in metamorphic epitaxial aluminum on silicon through primary and secondary interface misfit dislocation arrays," *ACS Nano* **12** (2018).

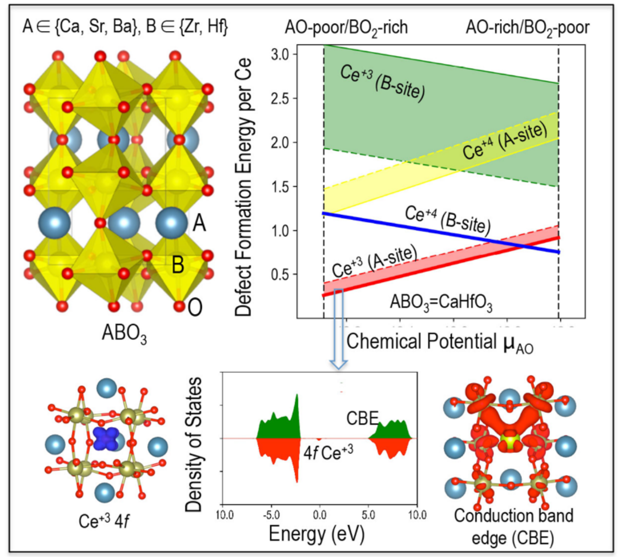
Technical contact: Xiang-Yang (Ben) Liu

Theoretical study could help design better radiation detection materials

Materials researchers across the globe are working to refine and develop scintillators—materials that emit light when struck by radiation. These scintillators can be used to detect high-energy radiation and have applications in fields including space research, oil-well logging, medical imaging, and detection of nuclear materials for homeland security. Their performance hinges on a complex interplay of a number of interrelated factors, such as host chemistry, details of crystal structure, the nature of prevalent defects, and synthesis conditions. In *Physical Review Applied*, researchers from Los Alamos National Laboratory and the Academy of Sciences of the Czech Republic reported how these factors affect the ability of perovskite scintillators to convert radiation into visible light.

The team chose to study cerium-activated $A^{2+}B^{4+}O_3$ perovskites, which the scientific community is actively exploring for their potential as scintillators. Using first-principles density functional theory framework, they found that while Ce^{3+} or Ce^{4+} defects can be thermodynamically stable (depending on the choice of the substitutional site, presence of other charge compensating defects, and synthesis conditions), only a Ce^{3+} dopant at the A-site can exhibit scintillation owing to its suitable electronic structure.

The results, which displayed excellent agreement with past experimental observations, explain a number of past experimental observations for perovskites and are expected to be transferable to other chemistries. They also provide new



(*top*) Left: a schematic illustration of the crystal structure of the class of perovskite compounds studied, highlighting the position of the A and B cation sites in the structure. Right: Calculations reveal that, for most synthesis conditions (represented by the chemical potential), Ce^{+3} is the most stable state for Ce on the A site while Ce^{+4} is the most stable on the B site. Overall, Ce tends to prefer residing on the A site.

(*bottom*) Analysis of the electronic structure for Ce^{+3} dopant in $CaHfO_3$ reveals that the Ce 4*f* states lie just above the valance band edge while the conduction band edge is formed by the Ce 5*d* states. The left and right panels show the distribution of electrons in these states. This analysis shows that Ce^{+3} has the minimal required properties to enable scintillation in the material.

avenues for optimizing the performance of scintillators by suggesting co-doping strategies to maximize the prevalence of Ce^{3+} in the material.

This work was funded by the Laboratory Directed Research and Development program and computational support was provided by the Lab's high-performance-computing clusters. It supports the Lab's Energy Security mission and the Materials for the Future science pillar, via the science themes of Extreme Environments and Defects and Interfaces. The research effort also aligns with the Material Resilience in Harsh Service Conditions and Complex Functional Materials areas of leadership. Los Alamos pursues the science and engineering needed to establish design principles, synthesis pathways, and manufacturing processes that advance and create materials with controlled functionality and predictive performance to solve national security science challenges.

Researchers: G. Pilania, S. K. Yadav, B. P. Uberuaga, and C. R. Stanek (Materials Science in Radiation and Dynamics Extremes, MST-8); and M. Nikl (Academy of Sciences of the Czech Republic). Reference: "Role of multiple charge states of Cce in the scintillation of ABO_3," *Physical Review Applied* **10**, 024026 (2018).

Technical contact: Ghanshyam Pilania

Molecular dynamics simulations clarify quantitative link between twinning and void nucleation in BCC metals

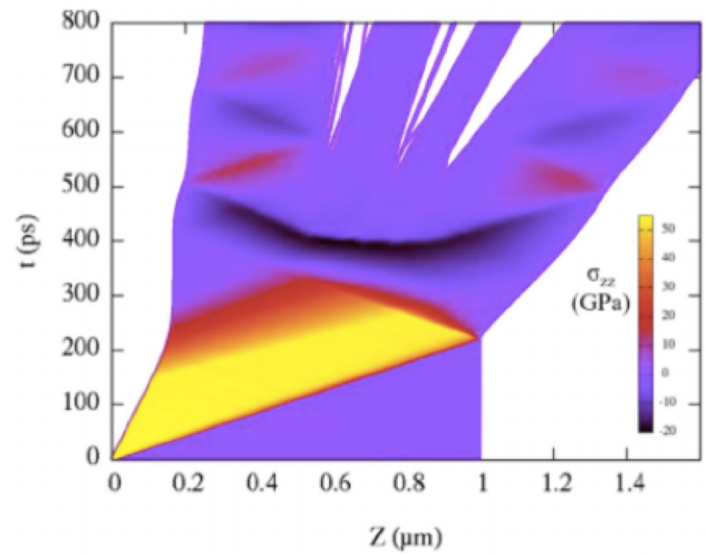
Finding could explain an aspect of material failure in extreme environments

Understanding material failure, especially in extreme environments, is a prominent scientific challenge that can lead to poor physics-based predictions of this process. Many advances have been made in understanding damage and failure in face-centered cubic (FCC) materials, but little comprehensive understanding exists of how deformation mechanisms—specifically twinning—affect spall strength (the quantitative measure of failure under dynamic loading) in body-centered cubic (BCC) metals. Both experimental and computational studies are increasingly being conducted to understand the compressive and tensile behavior of tantalum. However, there is still a lack of data on tantalum that agree on its behavior at high strain rates and are not strongly dependent on material pedigree. High-quality experimental data coupled with insights derived from atomistic modeling are crucial to developing models that can predict damage and failure in BCC materials.

In research published in *Acta Materialia*, Los Alamos researchers used massive non-equilibrium molecular dynamics simulations to investigate the relationship between crystalline orientations in single crystal tantalum and their corresponding susceptibility to nucleate voids under dynamic loading.

The work relied on simulations of six representative orientations that spanned 1 micron in length. Each orientation consisted of about 100 million atoms. The simulations included programming to represent shock and melting behavior and methodology that generated one-dimensional shock-loading conditions that mimic those produced under flyer plate experimental loading in a gun. This work showed a direct correlation between the residual twinning in an orientation and its corresponding susceptibility to spall under dynamic loading conditions. Twins and their intersections function as regions of increased stress localization within the system due to compatibility requirements, and thus operate as critical void nucleation sites. This work also showed the time-dependent evolution of twins and dislocations during shock, highlighting deformation path dependence and the occurrence of de-twinning over picosecond timescales.

The new understanding of this elusive relationship between spall strength and twinning in BCC materials can form the basis of new damage and failure models. Future studies will address the role of grain boundaries in this process, with the logical extension being the study of bicrystals and their relative ability to relieve or amplify stress concentrations.



Position-time-stress diagram shows the propagation of the initial shock wave and subsequent free-surface reflections. Incipient spall occurs in the black tensile stress region at ~380 ps, but full separation/failure is delayed until ~450 ps.

The work supports the Laboratory's Nuclear Deterrence mission area and its Materials for the Future science pillar. It relied on Grizzly, an institutional high-performance computing system located at Los Alamos, and was funded by the Laboratory Directed Research and Development program.

Researchers: E.N. Hahn and S.J. Fensin (Materials Science in Radiation and Dynamics Extremes, MST-8), T.C. Germann (Physics and Chemistry of Materials, T-1), and G.T. Gray III (MST-8).

Reference: "Orientation dependent spall strength of tantalum single crystals," *Acta Materialia* **159** (2018).

Technical contact: Saryu Fensin

Sally Grindstaff

Summer student synthesizes a legacy

Sally Grindstaff said she is reminded of her grandfather every day as she invents and synthesizes new peptoids—a manmade derivative of peptides, the so-called "machinery of life." The reason? Her grandfather, Bruce Merrifield, invented a process that allows peptide chains to quickly assemble through continuous reactions. The technique, called solid-phase peptide synthesis (SPSS), revolutionized the way drugs are made and shortened the complex process of producing peptoids from a matter of weeks to hours. The invention of SPSS earned Merrifield the Nobel Prize in Chemistry in 1984.

The technique also shaped the day-to-day work Grindstaff did as an undergraduate summer student at the Laboratory. Merrifield passed away in 2006, but with his legacy to guide Grindstaff, she is carving out her own space in the field. This summer, as a member of Engineered Materials (MST-7), Grindstaff manipulated and grew new peptoids to have better stability than peptides.

"Sally's sharp and works hard," said Rob Gilbertson (MST-7), her mentor of three years. "I have no doubt she'll be successful in whatever she does,"

One of Grindstaff's main assignments this summer was as part of a Laboratory Directed Research and Development project to develop a foldamer that detects the specific pathogens that cause the Ebola and Marburg viruses. The team is also using a technique called hydrolysis to break down proxy nerve agents, rendering them less toxic. Grindstaff's role was to add solutions, solvents, and resin to one of the Lab's advanced SPPS machines (an automated version of the technique that won Merrifield the Nobel). Once the instrument is turned on, it automatically builds a new peptoid the team can test.

The project, "Foldamers: Design of Monodisperse Macro-Molecular Structure by Selection of Synthetic Heteropolymer Sequence," could be a first step in machining non-biodegradable foldamers that could destroy chemical warfare agents, filter water, catalyze reactions, and manufacture high-specificity sensors and low-dose catalytic drugs.

When asked what her grandfather would have thought of her promising career, Grindstaff looked thoughtful. "I didn't understand the magnitude of the Nobel Prize and what he had done until I was older, but I think he'd be proud of my work so far," said Grindstaff, who is studying chemistry at the University of Oklahoma. "I think he'd be happy that I'm curious about how the world works on a chemical level and that I really enjoy research. Knowing that my work has potential biologic applications and could make a difference is amazing."

Article by H. Kris Fronzak; photo by Lindsey Kuettner

Sally Grindstaff sets up a commercial peptide synthesizer to conduct solid-phase peptoid synthesis.

Sally Grindstaff's favorite project

What: Synthesizing and characterizing new peptoids using Bruce Merrifield's solid-phase peptide synthesis technique.

Why: To create materials that can be tested for having secondary structure. These could eventually be used to develop larger materials with intrinsic structure.

When: Summer 2017 and 2018

Where: Los Alamos National Laboratory

Who: Sally Grindstaff, Charlie Strauss (Bioenergy & Biome Sciences, B-11), Rob Gilbertson, Paul Peterson (MST-7), and Jurgen Schmidt (Inorganic, Isotope and Actinide Chemistry, C-IIAC)

How: The solid-phase peptide synthesis machine performs a series of addition and washing steps, creating bonds between amino acids onto a solid resin. The resin is too large to fit through a filter, so excess material can easily be washed away while keeping the growing peptoid intact. Each peptoid is characterized by nuclear magnetic resonance spectroscopy.

The "aha" moment: This technique is exciting because large amounts of excess reagent can be added in order to push the reaction equilibrium toward the formation of the desired product. Since excess reactants can be easily washed away, no lengthy purification is required and material can be synthesized quickly and easily.

HeadsUP!

MST team wins LANL environment award

Project safely disposes of 44 vacuum pumps

Members of the "Bring out your dead" vacuum pump project team have been recognized with a 2018 LANL Patricia E. Gallagher Environmental Award.

For their work in recycling 44 vacuum pumps, the following lab staff were recognized: Iven Gonzales, Mark Lorenzo Ortega, Chris Baxter, and Carlos Archuleta (Nuclear Materials Science, MST-16). Patricia Vardaro-Charles (Waste Management Programs, EPC-WMP), Mike Hundley (Condensed Matter and Magnet Science, MPA-CMMS), and Chris Serazio (Waste Management Services, EPC-WMS).

This project achieved cost efficiencies in recycling a large group of pumps instead of recycling a few at a time. It also furthered the Laboratory goal of reducing legacy equipment.

The Patricia E. Gallagher Environmental Awards program recognizes exemplary achievement in waste reduction, improved waste management, innovation that leads to environmental improvement, and environmental education. Formerly the Pollution Prevention (P2) awards, this program was renamed in 2018 to honor the late LANL environmental steward Patricia "Pat" Gallagher.

Technical contact: Diane Wilburn (MST-DO)

Home heating safety tips

- If you use a portable space heater this winter, ensure it is at least three feet away from anything that can readily catch fire.
- Keep the heater away from drapes, furniture, or other flammable materials.
- Place the heater on a level surface away from areas where someone might bump it and knock it over.
- If you must use an extension cord, make sure it is a heavy-duty cord marked with a power rating at least as high as that on the label of the heater itself.
- Never leave a space heater unattended or running while you sleep. Keep electric heaters away from water.
- Never use them near a sink or in the bathroom.
- Only use clear (1-K) kerosene in such heaters and never use gasoline or any other substitute fuel. Be sure that the wick is set at the recommended height, and the room is adequately ventilated. Always refill the fuel tank outside, and turn off the heater and let it cool before refilling.

Celebrating service

Congratulations to the following MST Division employees celebrating recent service anniversaries:

Joseph Martz, MST-DO	35 years
Terry Holesinger, MST-16	25 years
Kenneth McClellan, MST-8	25 years
Bryan Bennett, MST-7	20 years
Richard Salazar MST-16	20 years
Dominic Peterson, MST-7	15 years
Tarik Saleh, MST-8	15 years
Zachary Smith, MST-7	10 years
John Lamar, MST-7	5 years
Ghanshyam Pilania, MST-8	5 years
Reeju Pokharel, MST-8	5 years
Jesse Salazar, MST-16	5 years
Miranda Williams MST-16	5 years

MST e NEWS

Published by the Physical Sciences Directorate.

To submit news items or for more information, contact Karen Kippen, ALDPS Communications, at 505-606-1822, or aldps-comm@lanl.gov.

For past issues, see www.lanl.gov/org/ddste/aldps/mst-e-news.php.

Los Alamos NATIONAL LABORATORY EST.1943

An Equal Opportunity Employer / Managed by Triad National Security, LLC for the U.S. Department of Energy's NNSA

NNSA National Nuclear Security Administration