MST eNEWS

Summer 2023
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INSIDE

David Andersson named ANS 2023 Mishima Award winner

David Andersson (Materials Science in Radiation and Dynamic Extremes, MST-8) is the recipient of the 2023 American Nuclear Society (ANS) Mishima Award. The award recognizes outstanding contributions of an individual in research and development work on nuclear fuels and materials.

"I am very happy and honored to be awarded the Mishima award from the American Nuclear Society," Andersson said. "I would like to acknowledge my colleagues at Los Alamos National Laboratories and other collaborators for enabling the work that underpinned the award. Thank you."

Andersson is a staff scientist on MST-8's Modeling of Radiation Effects team. An expert in atomistic modeling of nuclear fuels—both traditional UO_2 light water reactor fuel and advanced accident-tolerant fuel concepts—he has been involved in numerous international and national multiscale simulation efforts to develop models for use in nuclear fuel performance simulations.

In particular, his work has used atomistic simulations of fission gas behavior and thermal conductivity to inform mesoscale simulations designed to capture the fuel's evolving microstructure under irradiation.

Andersson is the deputy lead for the materials and fuel technical area of the DOE's Nuclear Energy Advanced Modeling and Simulations Program, which aims to develop simulation tools for nuclear reactors. He previously held a similar position with the Consortium for Advanced Simulation of Light Water Reactors Program, a DOE Energy Innovation Hub that aimed to develop modeling and simulation technology for a virtual version of existing operating nuclear reactors.

As of 2022, Andersson is also the deputy national technical director for DOE's Advanced Materials and Manufacturing Technologies Program. He is the author of more than 110 published papers, which have been cited more than 5,000 times.

> "I would like to acknowledge my colleagues at Los Alamos National Laboratories and other collaborators for enabling the work that underpinned the award."

Andersson, who received his PhD is in materials science and engineering from Sweden's Royal Institute of Technology, joined the Laboratory in 2007 as a Glenn T. Seaborg Postdoctoral Fellow.

Technical contact: David Andersson ■

Los Alamos NATIONAL LABORATORY

"In my mind, the transition from summer to fall is always concomitant with the push to meet year-end deliverables. While I absolutely appreciate the drive and ambition to deliver for sponsors, it is also just as important to carry out our work thoughtfully and responsibly."

From Matt's desk . . .

Dear MST,

As summer draws to a close, I hope this letter finds you in good health and you have taken some much-needed time to spend with family and friends. For many of us with change to the PTO model, the hours tend to accumulate faster, providing additional motivation to take the time needed to rejuvenate from work. In my mind, the transition from summer to fall is always concomitant with the push to meet year-end deliverables. While I absolutely appreciate the drive and ambition to deliver for sponsors, it is also just as important to carry out our work thoughtfully and responsibly. Taking a thoughtful and responsible approach to work is in alignment with the message at the core of the ALDPS-initiated pause focused on disciplined operations, which I am sure most of you participated in on August 14. To be clear, I believe we have a strong safety culture in MST. The uptick in work-related injuries across the Laboratory, and reflections on events from Laboratory staff, should only strengthen our resolve to keep safety in the forefront of our minds while executing work.

On a different topic, with the unprecedented growth of the Division, it is important to have discussions on the importance and the relevance of the work we do. We support some of the biggest and most visible efforts at the Laboratory: MST-16's support of first production units; MST-7's support of the W93; and MST-8's support of the Low-Enriched Fuel Fabrication Facility just to name a few. With many new folks in the Division, it is important to impart the relevance to those supporting our missions. I would encourage the more experienced folks to have frequent dialog with the students, postdocs, technicians, and junior staff across the Division to help build understanding of how their individual contributions fit into the broader Laboratory and national strategies. For those of you looking for more information on the relevance of your work, or are curious about a particular program or mission, please find the time to talk to your team, group, or division management.

Finally, in looking to FY24, an exciting place to start is LDRD-DR new starts. These projects are often a window into the future direction of the Laboratory, and this year I had a unique vantage point—being on the strategy team—to observe the great work that was put in by a number of MST PIs, co-PIs, and researchers. I would like to congratulate Topher Matthews (PI, MST-8) "ZiaCore: Enabling materials driven reactor design;" Amanda Graff (PI, MST-7) and Cindy Welch (Co-PI, MST-7) "Achieving high fidelity vibrational information with an ultra-thin, self-powered sensor;" and Blas Uberuaga (PI, MST-8) "M3ONARCH: Making, measuring, and modeling optoelectronics for next-generation applied radiation-hard components and hardware." I would also like to offer a job well done for the excellent leadership on the DRs coming to a close and transitioning into program space: Jeremy Mitchell (PI, MST-16) and Sarah Hernandez (Co-PI, MST-16) "Aging and metastability of delta-phase plutonium" and David Andersson (Co-PI, MST-8) "Advanced characterization to enable prediction of actinide-molten salt behavior." If you are looking for great scientific discussion, reach out to any of the leaders of a new or ending DR!

I look forward to getting the Division together for broader discussion in the not-too-distant future, but for now have a safe and productive end of FY23.

Best,
Matt ■

Novel deposition technique holds promise in creating ‘reusable’ vessels for use in nuclear metallurgical foundries

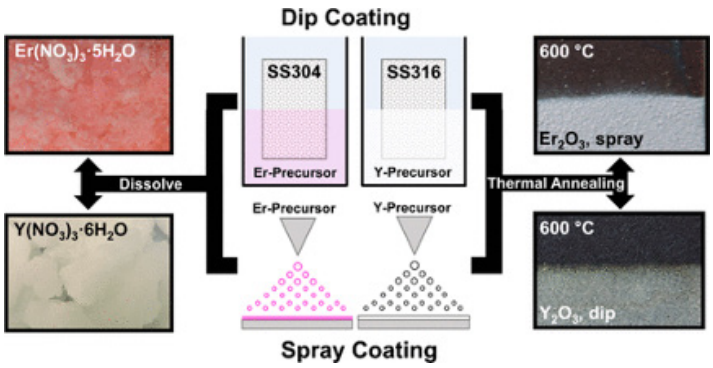
Casting of molten metals, including *f*-table elements, is important for nuclear metallurgical foundries. However, the molds and crucibles used suffer from short lifespans due to corrosion—increasing replacement and waste removal costs.

The creation of a “reusable” mold, by depositing a protective coating onto the melt-containing surface, is one solution—with rare-earth oxides considered strong candidates due to their properties of non-wettability against molten metals.

In *Applied Materials and Interfaces*, Los Alamos materials researchers report on a technique that uses chemical solution deposition to apply rare earth-containing precursors to form thick metal oxide coatings onto low-cost substrates. Their technique relies on solution-based procedures used by others in the area of thin film research. The approach is promising, suggesting its role will be significant for application in the foundry.

Specifically, the researchers deposited protective erbia and yttria coatings on stainless steel coupons. Dip and spray coating techniques were tested and compared to a commercial yttria spray. The team observed that solution concentration, solvent choice, micropowder injection, and annealing temperature and ramp profile were critical to the coating’s physical properties. The work, which provides baseline information enabling further refinement in future studies, leveraged the Lab’s expertise in thin films synthesis and characterization, manufacturing science, and foundry operations.

The work, which supports the Laboratory’s National Security mission and its Materials for the Future capability pillar, particularly



Shown are protective erbia (Er_2O_3) and yttria (Y_2O_3) coatings on stainless steel coupons. Dip coating was shown to yield a higher adhesion strength than spray coating and was further increased if the substrate had preliminary sandblasting.

the Material Resilience in Harsh Service Conditions area of leadership, was funded by Los Alamos’s Laboratory Directed Research and Development Program. It was performed in part at the Center for Integrated Nanotechnologies, a DOE Office of Science user facility operated jointly by Sandia and Los Alamos national laboratories. Researchers: Daniel J. Rodriguez, Alexander S. Edgar, Ashleigh M. Chov, Douglas R. Vodnik, David J. Ross, Victor P. Siller, Igor O. Usov (Engineered Materials, MST-7); Darrick J. Williams (Center for Integrated Nanotechnologies, MPA-CINT). Reference: “Chemical solution deposition of protective Er_2O_3 and Y_2O_3 coatings onto stainless steel for molten metal casting using metal-nitrate precursors,” *Applied Materials and Interfaces* 15 (23), 28649-28663, (2023).

Technical contact: Igor Usov ■

Inclusivity tips

You can help make the Lab a more inclusive place for persons with disabilities by keeping the following tips in mind.

- Ensure accessibility: Accessibility is a common challenge for persons with disabilities. Ensure that workspaces and nearby services (restrooms, lactation pods, parking, etc.) are accessible, and when hosting in-person or virtual meetings, make sure to refer to accessibility checklists like those from Section 508 or Cornell. Creating a handout? Confirm that your PDF is accessible and compliant with Section 508.
- Be respectful: Some disabilities are invisible! Don't assume that your co-workers are able to hike, drink, take the stairs, focus while in noisy settings, etc. Also, be sure to use the correct language when referring to persons with disabilities, both verbal and written.
- Be considerate: Some of your colleagues may have care responsibilities or a flexible work schedule to accommodate their disabilities, so try to give as much notice as possible for work-related requests.

Learn more! The Lab's DiverseAbility Employee Resource Group has a number of resources on and for persons with disabilities, including member interviews and what it means to have a disability. You can also learn more through the Americans with Disabilities Act (ADA). ■

New guide showcases versatility, robustness of popular materials modeling code

Long-time scientific collaborators Carlos Tomé and Ricardo Lebensohn have co-authored a new book that highlights the theoretical and practical applications of plasticity simulations. *Materials modeling with the visco-plastic self-consistent approach: Theory and practical applications*, published by Elsevier, condenses 30 years of research done by the authors and collaborators.

More than 200 researchers worldwide have employed their approach and associated computer code, which they developed in 1993 as a means to simulate the plastic deformation of polycrystalline materials. Their original VPSC paper[1] has been cited more than 2,200 times.

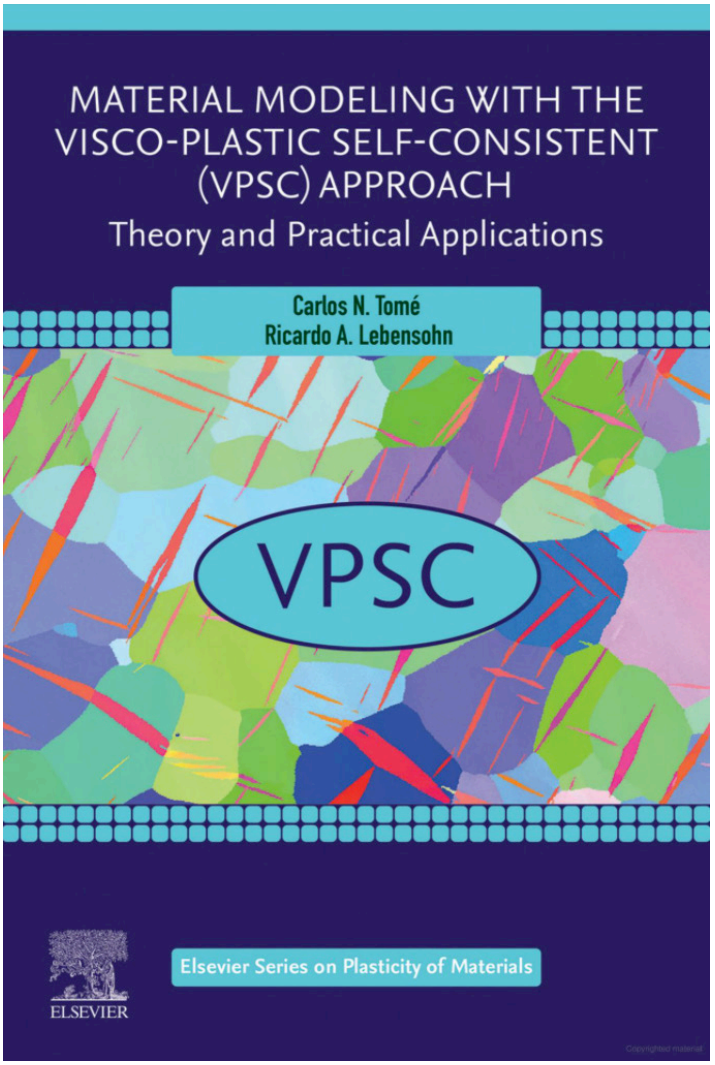
The ability to predict the mechanical response of a material based on its microstructure and its evolution during plastic deformation is key in many technologies, including mission-relevant applications at the Laboratory. VPSC has been adapted for use in a variety of research projects at Los Alamos. These include for programs as diverse as DOE's Basic Energy Sciences, Nuclear Energy Advanced Modeling and Simulation, the Consortium for Advanced Simulation of Light Water Reactors, and Los Alamos's Laboratory Directed Research and Development.

Tomé is a pioneer in the theoretical and numerical development of physically based models of mechanical behavior of polycrystals. In recognition of his contributions to the field, he was named a Los Alamos Fellow and is the recipient of the *International Journal of Plasticity*'s Khan International Medal and the Minerals, Metals, and Materials Society's (TMS) Cyril Stanley Smith Award. Tomé, who has a PhD in physics from the National University of La Plata, Argentina, joined the Lab in 1996.

Lebensohn is an expert in the structure–property relationship of materials and crystal plasticity modeling. In recognition of his contributions to the field, he was named a Los Alamos Fellow and is the recipient of the Alexander von Humboldt Foundation's Humboldt Research Award and TMS's Structural Materials Division's Distinguished Scientist/Engineer Award. Lebensohn, who has a PhD in physics from the National University of Rosario, Argentina, joined the Lab in 2003.

The book, aimed at researchers in mechanical engineering and materials science and students in these disciplines, provides readers with a foundational understanding of polycrystal plasticity and details the authors' VPSC formulation. It also describes its computational realization—the open-source VPSC code—together with practical simulations illustrating the code's capabilities, including hardening and texture evolution, twinning transformation, creep response, and irradiation effects in metallic and geologic systems of different symmetries.

The work supports the Laboratory's Energy Security and Nuclear Deterrence mission areas and the Materials for the Future and Information, Science, and Technology capability pillars. Researchers:



Materials modeling with the visco-plastic self-consistent approach: Theory and practical applications **is part of the Elsevier series on the plasticity of materials. The combined book and computer code provides a simulation tool to be used by students and researchers. The cover is a micrograph of a zirconium aggregate exhibiting grains with twins and evokes the realm of application of VPSC. The ellipsoid in the center is a reference to a key assumption of the VPSC formalism, namely, that grains are treated as ellipsoidal inclusions embedded in the surrounding medium.**

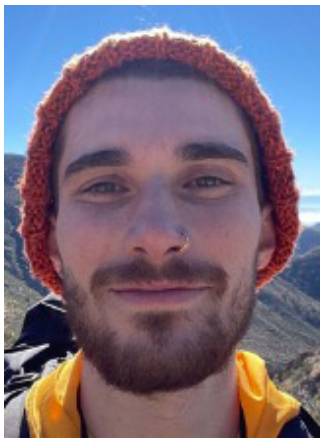
Carlos N. Tomé (Materials Science in Radiation and Dynamic Extremes, MST-8); Ricardo A. Lebensohn (Fluid Dynamics and Solid Mechanics, T-3). Reference: *Material modeling with the viscoplastic self-consistent (VPSC) approach: Theory and Practical Applications*, 1st ed. (Elsevier, 2023).

Technical contacts: Carlos Tomé and Ricardo Lebensohn ■

[1] R.A. Lebensohn, C.N. Tomé, "A self-consistent anisotropic approach for the simulation of plastic deformation and texture development of polycrystals: Application to zirconium alloys," *Acta Metall. Mater.* 41, 2611-24 (1993).

Drewry, Stanfel recognized for Student Symposium presentations

Two MST students earned top marks in the Lab's 2023 Student Symposium. Sean Drewry (Materials Science in Radiation and Dynamics Extremes, MST-8) and Jessica Stanfel (Nuclear Materials Science, MST-16) were recognized for their presentations at the annual event which provides students the opportunity to gain professional presentation experience and network with other LANL personnel and students. The Lab's Partnerships and Pipeline Student Programs Office hosts the event.



Sean Drewry

Jessica Stanfel

Both talks centered on exploring the relationship between a material's processing, its structure and properties, and its performance. This "PSPP" is a central element of the Lab's Materials for the Future strategy, which strives for advanced and new materials with controlled functionality and predictable performance.

In research aimed at developing improved accident-tolerant fuels for light water reactors, Drewry discussed how the addition of chromia affects uranium dioxide bulk behavior. A graduate student at the University of Tennessee, Knoxville, Drewry was mentored by Scarlett Widgeon Paisner (MST-8).

In her talk, Stanfel discussed the effect cooling rates have on the microstructure of and intermetallic formation in a superheated aluminum-silicon-iron alloy. An undergraduate student studying mechanical engineering at the Colorado School of Mines, Stanfel was mentored by Meghan Gibbs and Mathew Hayne (MST-16).

Also presenting from MST were Hope Brown, Jacob Mitchell, Andrew Ahn, Grant Martin, and Cassidy Mazelin (all Engineered Materials, MST-7); Briley Perkins, Thai Hang Chung, Riley Ferguson, Zhangxi Feng, Quinton Geller, Adrian Gonzales, Sangwon Lee, Ashley Lenau, and Geronimo Robles (all MST-8); and Zachary Barker, Joseph Leal, Noah Pearlstein, and Charles Meyer (all MST-16). ■

MST staff get gold for pollution prevention efforts

Members of Engineered Materials (MST-7) were recently recognized with 2023 Gold Patricia E. Gallagher Environmental Awards for their work on two projects, both of which reduced RCRA waste. The Resource Conservation and Recovery Act (RCRA) is a public law that creates the framework for the proper management of hazardous and non-hazardous solid waste.

The annual awards, of which gold is the highest level, recognize individuals or teams for exemplary achievement in waste reduction, improved waste management, innovation that leads to environmental improvement, and environmental education.

In "Process optimization for reduced hazardous waste generation," Erika Guaba-Roldan performed a study that determined the minimal amount of solution needed in a chemical infiltration process without compromising the final product. As a result, Guaba-Roldan's method reduces the amount of hazardous waste used and the hazardous chemicals purchased. The process is being adopted more generally throughout the DOE complex.

In "Environmentally friendly bacteria: A natural substitute for nitric acid leaching of copper," a multidisciplinary team is striving to replace nitric acid by employing bacteria to remove copper used in preparing target components for inertial confinement fusion experiments. The method minimizes hazardous waste, improves worker health, and creates additional opportunities for bacteria in material studies. Participants included Alex Edgar, Brian Patterson, Bryan Hunter, Cassidy Mazelin, Chris Wilson, Derek Schmidt, Ethan Walker, Lynne Goodwin, Patrick Donovan, and Thomas Day (all MST-7); Alex Strickland (LANSCE Facility Operations, LANSCE-FO); and members of the Chemistry, Earth, and Life Sciences (ALDCELS) and Facilities and Operations (ALDFO) directorates.

This year's environmental awards, hosted by the Lab's Pollution Prevention Program, saw the largest number of nominations since its inception, with 30 overall winners. ■

HeadsUP!

Lab's parking policy doesn't have to lead to a bumpy road
Read on for tips on how to meet your workplace transportation needs

With the record number of employees now working onsite, coupled with construction detours and lot closures for much-needed infrastructure updates and mission-related projects, parking violations have skyrocketed. To help curb these infractions and ensure a safe and efficient environment for all employees, the Lab's parking policy was recently updated to encourage everyone to park in designated and legal spaces. Policy updates, which included changes to the fines and penalties for parking violations, are now in effect.

Why the changes?

As noted by the Lab's safety division, the number of parking violations has never been higher. These infractions encompass a variety of illegal parking situations, many of which create serious safety threats. The most common violations include:

- nongovernment vehicles parking in GOV spots
- nonhandicapped vehicles parking in handicapped spots
- vehicles parked in unmarked spots, typically in front of doors, entryways, fire hydrants, and walkways.

When vehicles are parked illegally, it can hinder emergency personnel and vehicle access—and employee egress—to and from buildings.

Likewise, when employees who have handicapped placards and rely on parking in a designated space near their work location are forced seek a parking spot elsewhere, it puts them in danger. Asking them to navigate an excessive distance between an available parking space and their building is unacceptable.

Tips to combat the parking shortage

To plan your parking in advance, consider these tips and resources.

- Schedule extra time between meetings to allow for parking if you must travel between locations.
- Buffer your calendar with enough time on either side of meetings to allow for travel.
- Take a free LANL taxi to meetings at various Lab locations. LANL taxis can take you to any Lab building, including those in townsite and White Rock (except for those located in Santa Fe). Call (505) 667-TAXI to schedule taxi rides.
- Use LANL taxi's regularly scheduled shuttle services to get from one TA to another.
- Eliminate the stress of parking by not driving your car onto campus—which is getting easier to do. Employees have a growing number of commuting alternatives, including a free, new express bus that travels directly from a secured parking lot at Pojoaque's Cities of Gold Casino to TA-35 and TA-55. There are also other transit options that get employees to the Lab's front gate, where waiting LANL taxis take them directly to their building. The taxi service also runs multiple internal routes throughout the day at frequent intervals.
- Sign up for a carpool or vanpool with colleagues and co-workers; designated parking spots are available for registered vanpools.

Celebrating service

Congratulations to the following MST Division employees who recently celebrated a service anniversary.

Joseph Martz, MST-DO	40 years
Kenneth McClellan, MST-8	30 years
Donald Brown, MST-8	25 years
Richard Salazar, MST-16	25 years
Robert Gilbertson, MST-7	20 years
Tarik Saleh, MST-8	20 years
Igor Usov, MST-7	20 years
Gary Gladysz, MST-7	10 years
Amanda Graff, MST-7	10 years
Arul Kumar Mariyappan, MST-8	10 years
Reeju Pokharel, MST-8	10 years
Justin Porto, MST-7	10 years
Najeb Abdul-Jabbar, MST-16	5 years
Simon Barlow, MST-16	5 years
Lynette Casados, MST-16	5 years
Rachel Collino, MST-7	5 years
Mary Knaak, MST-7	5 years
Elisha Willis, MST-7	5 years

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

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NNSA National Nuclear Security Administration