PHYSICAL SCIENCES

VISTAS

PERSPECTIVES ON EXCELLENCE IN NUCLEAR SECURITY
AT LOS ALAMOS NATIONAL LABORATORY // SUMMER 2019

Revealing the experimental signatures of dynamic plutonium hydriding

Culture of shared responsibility bolsters safe and secure operations during complex renovation project

Dartmouth science on the horizon for Estrella 'Star' Torres

Los Alamos
NATIONAL LABORATORY
EST. 1943

On the cover, foreground: Laura Wolfsberg (left) (Inorganic Isotope and Actinide Chemistry, C-IIAC) and Brian Scott (Materials Synthesis and Integrated Devices, MPA-11) load a sample holder in preparation for an experiment characterizing and measuring the chemical signatures of plutonium hydriding at ultrafast timescales. Background: atomic force microscope image of tin particles created through laser ablation and collected on a witness plate.

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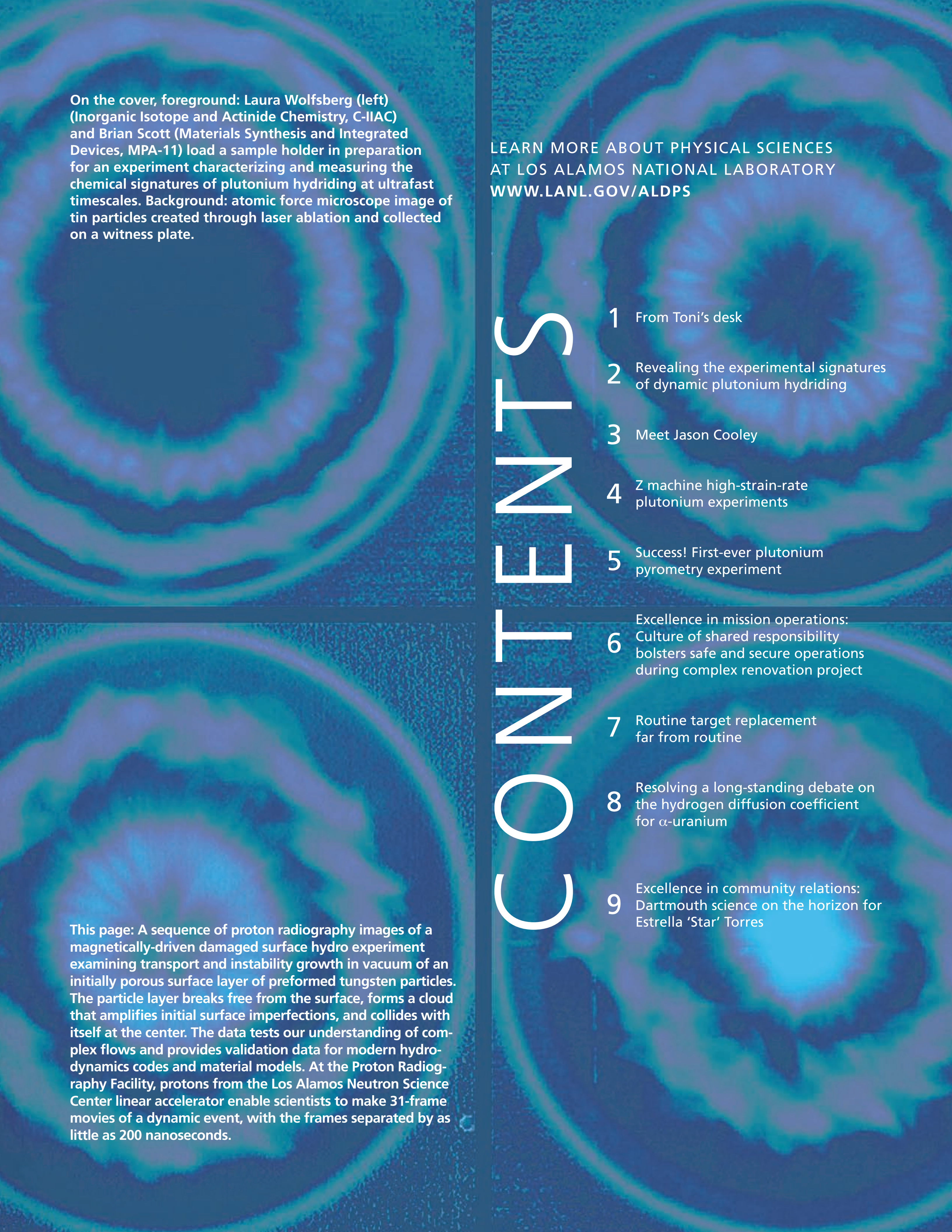


This page: A sequence of proton radiography images of a magnetically-driven damaged surface hydro experiment examining transport and instability growth in vacuum of an initially porous surface layer of preformed tungsten particles. The particle layer breaks free from the surface, forms a cloud that amplifies initial surface imperfections, and collides with itself at the center. The data tests our understanding of complex flows and provides validation data for modern hydrodynamics codes and material models. At the Proton Radiography Facility, protons from the Los Alamos Neutron Science Center linear accelerator enable scientists to make 31-frame movies of a dynamic event, with the frames separated by as little as 200 nanoseconds.

FROM TONI'S DESK

Toni Taylor, Associate Laboratory Director for Physical Sciences

I am proud to introduce the third issue of *Physical Sciences Vistas,* with a focus on "excellence in nuclear security." Los Alamos National Laboratory overall, and our Physical Sciences Directorate (ALDPS) specifically, is well known for excelling in our nuclear security mission, which is supported by our excellence in science, technology and engineering, as well as our excellence in mission operations.

ALDPS has a very broad and complex footprint in the Laboratory's nuclear security mission, ranging from support of the Experimental Sciences program to the Directed Stockpile program and the Laboratory's Production program. Our facilities within ALDPS, such as the Los Alamos Neutron Science Center (LANSCE), support materials and nuclear science experiments for our nuclear security mission, whereas the Sigma Complex, the Target Fabrication Facility, and our Plutonium Facility enable materials processing and fabrication underpinning nuclear security experiments across the Laboratory. Additionally, ALDPS staff perform experiments across the nation ranging from subcritical experiments in Nevada to inertial confinement fusion experiments at the National Ignition Facility at Livermore National Laboratory and dynamic materials experiments at the Advanced Photon Source at Argonne National Laboratory and the Z Pulsed Power Facility at Sandia National Laboratories.

In this issue, highlights of our outstanding R&D supporting the Laboratory's nuclear security mission include the following.

- The development of a capability to measure the change in the properties of plutonium during exposure to hydrogen—that is a technique to understand plutonium on ultrafast timescales using optical techniques.
- Measurement of the response of plutonium to high-strain-rate drive, providing essential data on the plutonium equation of state and mechanical properties necessary to validate and improve our nuclear weapons models and codes.
- The first successful plutonium experiment providing a dynamic measurement of the temperature in a shocked sample of plutonium. This measurement enables the determination of the equation of state of plutonium under extreme conditions, providing data critical to our nuclear security mission.
- A calculation that sheds light on the anomalous behavior of the hydrogen diffusion coefficient in α-uranium, providing an understanding of the reactivity of hydrogen with uranium.
- Activities at the Sigma Complex to improve and ensure safe and secure operations in a complex environment that encompasses construction in close proximity to multifaceted, experimental R&D.
- A description of the complex operation to replace the tungsten target used to generate neutrons for the Weapons Neutron Research Facility at LANSCE.

Additionally there are profiles of important contributors in ALDPS.

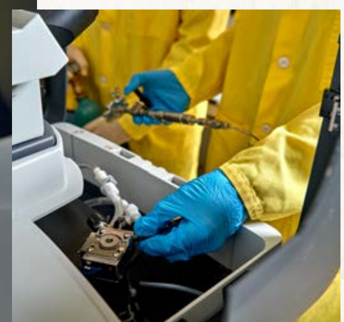
- Jason Cooley is a member of the Foundry and Solidification Science team in Fabrication Manufacturing Science (Sigma-1). He uses his materials manufacturing expertise to solve problems critical to the Lab's nuclear security mission.
- Estrella "Star" Torres is a 2019 Pojoaque High School graduate and a recipient of a Gold Scholarship from the Los Alamos Employees Scholarship Fund who is a student intern working in the Materials Synthesis and Integrated Devices (MPA-11) group on biofuel research. She will attend Dartmouth College in the fall, majoring in chemical engineering.

Finally, I would like to announce the formation of a new group in MPA Division, MPA-Quantum (MPA-Q), combining our quantum materials efforts in Condensed Matter and Magnet Sciences (MPA-CMMS) with the quantum science and applications activities in Applied Modern Physics (P-21). The focus on quantum science will support the national Quantum Initiative, along with the Laboratory's Agenda goal for leadership in this national initiative.

Toni

Revealing the experimental signatures of dynamic plutonium hydriding

Research exemplifies excellence in nuclear security



Brian Scott (far left) (Materials Synthesis and Integrated Devices, MPA-11) and Dmitry Yarotski (Center for Integrated Nanotechnologies, MPA-CINT) flood a plutonium sample with hydrogen gas (below).

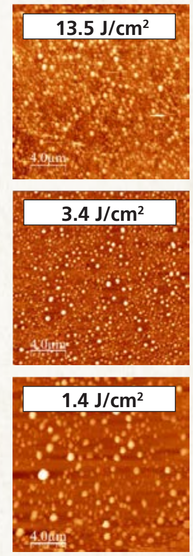


Figure 2. Atomic force microscope images of tin particles created through laser ablation and collected on a witness plate. These data show that particle size can be controlled through tuning of the laser fluence.

In support of the Laboratory's mission to maintain the nation's nuclear stockpile, Los Alamos researchers investigate every aspect of plutonium in every possible environment. This includes plutonium hydriding. In metals, hydriding occurs when hydrogen accumulates in the spaces between the metal atoms. This process changes the physical properties of plutonium metal, leading to embrittlement and a less functional material. The understanding of this process is of importance to many aspects of the Laboratory's plutonium mission.

A team of Lab materials scientists and theorists aims to provide critical insight into this phenomenon using a new capability to characterize and measure the chemical signatures of plutonium hydriding at ultrafast timescales. In particular, the researchers seek to understand how hydriding progresses on the femtosecond-to-tens-of-microsecond timescales and how fast the particles become hydrided. These questions will be answered through production of metal plutonium particles in a hydrogen gas atmosphere followed by measurement of hydriding using ultrafast probes.

Led by Brian Scott (Materials Synthesis and Integrated Devices, MPA-11), the team plans to generate the particles through laser ablation and monitor the hydriding process by studying the Raman signatures using ultrafast laser spectroscopy. This setup provides the flexibility to quickly change experimental parameters such as temperature and pressure, metal surface, or gas environment while only requiring small samples of plutonium.

To date, the team has made significant progress—designing and fabricating an in situ hydriding apparatus they used to perform Raman spectroscopy on bulk samples of hydrided plutonium and measuring the chemical signature of different hydride species—and thus providing the foundation for identification of plutonium hydride particles as generated in the laser ablation process described above (Figure 1). The spectroscopic signatures of plutonium hydrides have never before been reported, and the experimental data are being used to validate first principle calculations from LANL theorists. While this two-element system (Pu-H) would at first appear to be simple, the chemistry has turned out to be relatively complex. The research team also demonstrated that tin metal particles of sizes ranging from hundreds of nanometers to microns can be created using laser ablation (Figures 2 and 3). This technique

continued on next page

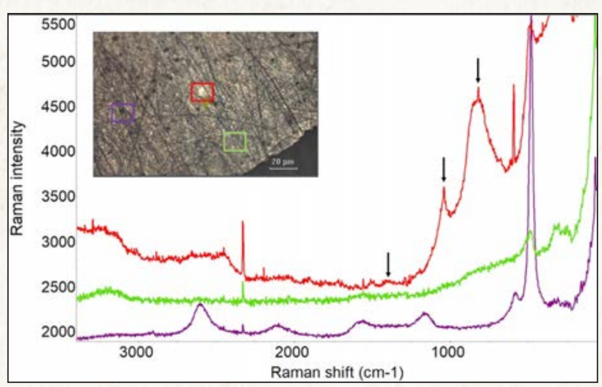


Figure 1. Raman spectrum of PuH_2 and PuH_3 (red), plutonium oxide (purple), and plutonium metal (green). Arrows denote PuH_2 and PuH_3 Raman signatures. Inset: each region enclosed in a colored box corresponds to the spectrum of the same color. Raman spectra provide unique patterns for different molecules, which allows their identification in a similar fashion to a human fingerprint.

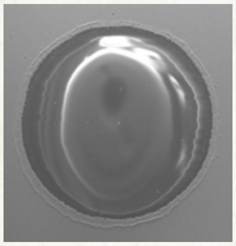


Figure 3. Scanning electron micrograph showing 600-nm-wide hole in tin thin film. The laser pulse, brought in from the back side of a thin film of tin on fused silica, produced the hole and corresponding particles shown on the witness plate in Figure 2.

Experimental signatures continued ...

will be used to generate plutonium particles for the ultrafast experiments.

"Our experimental data will be used to verify theoretical calculations of plutonium hydride phases, with the results benefiting future dynamic experiments," Scott said.

Next, the researchers plan to use Raman and infrared spectroscopy to measure the signature of the particles at different distances from their source. Collectively, this will provide fundamental data about reaction rates of plutonium with hydrogen, what chemical species are being formed, and how those species evolve over time—to ultimately develop a new thermodynamic phase diagram. This will create a detailed timetable of plutonium hydriding.

The work relies on the Laboratory's expertise in plutonium science, materials characterization, and theory and leverages existing capabilities of preparing plutonium bulk samples and thin films with well-defined surface characteristics. Because of the small sample sizes needed for the experiments, the work is being performed in radiological facilities and illustrates the utility of these facilities to executing Lab missions.

Mission connection: The work supports the Laboratory's Nuclear Deterrence and Stockpile Stewardship missions and the Materials for the Future and Science of Signatures science pillars.

GET THE DETAILS

Participants: Brian Scott (Materials Synthesis and Integrated Devices, MPA-11); Robert Chrien (Integrated Design and Assessment, XTD-IDA); Dmitry Yarotski (Center for Integrated Nanotechnologies, MPA-CINT); George Rodriguez (Detonation Science and Technology, Q-6); Laura Wolfsberg (Inorganic Isotope and Actinide Chemistry, C-IIAC); George Goff (MPA-11); Enrique Batista (Center for Nonlinear Studies, T-CNLS); Gaoxue Wang (Physics and Chemistry of Materials, T-1); Paul Dowden and Kevin Baldwin (both MPA-CINT); Troy Semelsberger (MPA-11); and Alison Pugmire (Nuclear Materials Science, MST-16). **Funding:** The work is a Los Alamos Laboratory Directed Research and Development Exploratory Research (LDRD-ER) Reserve project. **Technical contact:** Brian Scott

MEET JASON COOLEY

R&D scientist, Fabrication Manufacturing Science (Sigma-1)

Jason Cooley is a problem solver. As a member of the Foundry and Solidification Science team in Fabrication Manufacturing Science (Sigma-1), he uses his materials manufacturing expertise to solve problems critical to the Lab's nuclear security mission. These solutions require creativity, are often physically and technically demanding, and use specialized tools or materials that necessitate special handling. A quick turnaround is not unexpected. Cooley's specialty is coordinating these complex projects.

"Sigma is the place that has the tools and the critical mass of really smart people to solve those problems," he said, "and one of the things I'm good at is making all of the wheels turn in the same direction."

For example, Cooley and his Sigma colleagues made essential contributions to a Los Alamos–Sandia national laboratories collaboration supporting a U.S. government–sponsored collection of unique signals originating from specific hydrotest-related activities. For their work manufacturing—on a compressed schedule—multiple nonstandard hydrotest devices, the assembly of which required the development, testing, and implementation of new assembly procedures, he and his fellow project members received a Laboratory Large Team Distinguished Performance Award.

Cooley and his team are also working to produce quantities that meet the growing demand for the promising cancer-therapy isotope, actinium-225. Success means overcoming technical, logistical, and regulatory challenges—none of which fazes Cooley. "There's almost nothing we can't do at Sigma," he said.

An impactful exploration under challenging conditions

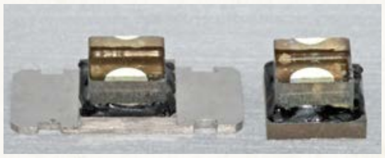
Z machine high-strain-rate plutonium experiments

Dynamically driven high-strain-rate experiments are inherently demanding—ranging from the controlled generation of the shock condition to the meticulous use of optical diagnostics capable of measuring in situ surface velocities with nanosecond resolution. For plutonium and other actinides, high-strain-rate experiments create challenges even greater, with the requirement of high-velocity fragment and particulate containment and the implementation of incompatible materials in intimate contact with radioactive materials.

In a long-standing collaboration between Los Alamos National Laboratory and Sandia National Laboratories, isentropic compression experiments (ICE) and other high-strain-rate experiments have been conducted at Sandia's Z Pulsed Power Facility (Z machine). Since 2006, these experiments, funded by the Science Campaign, have been performed on plutonium to meet NNSA nuclear security and stockpile stewardship mission needs. This series of experiments was recently distinguished as a great success in the *2019 NNSA Stockpile Stewardship and Management Plan*. This collaboration was celebrated for enabling the exploration of plutonium materials equation of state and mechanical properties necessary to validate, test, and improve weapons simulation codes and models. Recent experiments have included ICE evaluations of a 51.5-year-old plutonium sample taken from the stockpile, implementation of shock-ramp experiments, and development of ultrafast pyrometry for sample surface temperature determination.

Over this experimental history not only have Los Alamos and Sandia improved capabilities for safety considerations, but as Z machine platform technology has improved, so has the ability to explore behaviors over greater regions of (pressure, temperature) phase space with greatly improved diagnostics. Furthermore, LANL has reestablished its ability to produce plutonium materials that have not been successfully fabricated for decades as is necessary for control materials against which to assess for aging effects or for multiphase strength, equation of state, and phase transformation kinetics studies. Such results have been employed in the annual stockpile assessment and recently played an important role in the B61 Mod 12 Life Extension Program. These experiments support the Laboratory's Excellence in Nuclear Security strategic objective by transforming nuclear weapons warhead design, production, and certification.

Plutonium metal targets with approximate dimensions of 6.0 mm x 6.0 mm x 0.25 mm glued to LiF windows.



Plutonium-LiF target assemblies glued into platinum holders.

Plutonium-LiF target assemblies in platinum holders glued into a copper panel for shock-ramp experiments. The observable silver round spot on the LiF window is a thin aluminum layer to ensure good return for optical velocimetry diagnostics.

Solving materials compatibility

As an example of a materials compatibility challenge, consider the use of lithium fluorite (LiF) and adhesives in plutonium ICE. Sample surface velocity measurements in high-strain-rate experiments act as a pressure gauge for other measurements, such as reflectivity and temperature. High-quality LiF has been found to remain transparent up to 2.5 Mbar, making it an attractive window material for high-strain-rate use. The different densities and bulk moduli of LiF and plutonium lead to an acoustic impedance mismatch, such that when a shock wave propagates from a plutonium sample to LiF, a weaker shock is propagated forward and a release wave is launched backward into the plutonium. The LiF window material keeps the plutonium sample from releasing to zero pressure for direct observation of highly compressed states of plutonium. These experiments require LiF windows glued in intimate contact with plutonium targets; however, radiation damage and the formation of "color center" point defects are detrimental to LiF optical and physical properties under shock loading conditions. By limiting the target assembly shelf life, neutron irradiation damage and opacity in LiF is reduced and provides predictable performance lifetime in plutonium high-strain-rate experiments.

GET THE DETAILS

Participants: Staff from Nuclear Materials Science (MST-16) provided materials production, sample fabrication, and assembly; Hazardous Materials Management (NPI-7) provided shipping and packaging; and Environment, Safety, Health (ESH/RADCON) provided radiologic protection. **Funding:** Campaign 2: Dynamic Materials Properties (LANL Program Manager Dana Dattelbaum) provided funding for the work. **Technical contact:** Franz Freibert

Success! First-ever plutonium pyrometry experiment

Data critical for nation's Stockpile Stewardship program

The first-ever dynamic temperature measurement on a plutonium experiment was recently successfully completed using the Z Pulsed Power Facility (Z machine) at Sandia National Laboratories. The achievement is part of an ongoing multi-year collaboration between Los Alamos National Laboratory, Sandia, and the Nevada National Security Site, New Mexico Office (NNSS NMO). The data are critical for the nation's Stockpile Stewardship program, which ensures a safe, secure, and reliable nuclear stockpile through science, technology, engineering, and manufacturing.

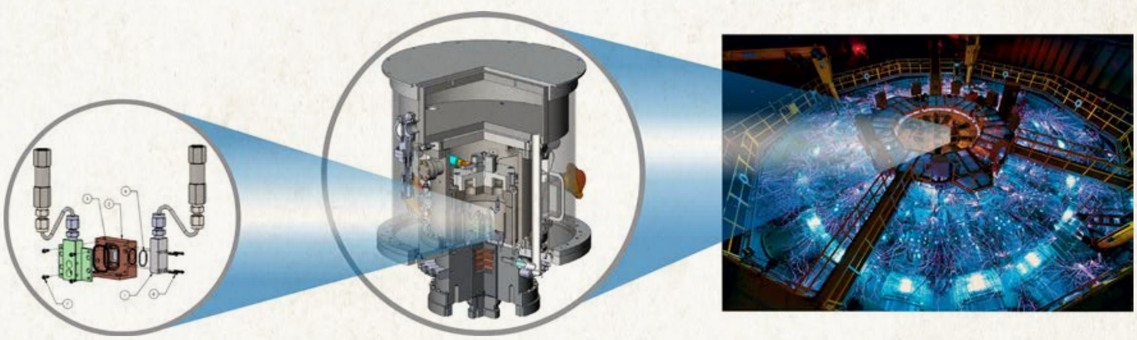
Computer simulations of materials under extreme conditions rest upon equations of state. These equations describe the thermodynamic state of a material, relating its physically measurable properties of pressure, density, and temperature. While the Laboratory has made exceptional progress in dynamically measuring pressure and density with diagnostics such as photon Doppler velocimetry and radiography, measuring dynamic temperature has so far proven too difficult for most experiments. Accordingly, temperature remains poorly understood in many high-pressure conditions.

Pyrometry attempts to infer dynamic temperature by capturing and quantifying the warm glow of light emitted from a heated surface as a function of time. Using a specialized optical system, researchers collect photons from the surface of a target material. They then work to remove sources of optical background to the photon-level and understand the nature of the relative blackbody spectral emissivity—how much that object emits like a theoretically perfect blackbody—to achieve thermometry with nanosecond resolution.

The recent experiment used the Z machine to create these conditions. Z's immense power pulse was tailored to drive a flyer impact, imparting a shock to a plutonium sample. After impact, the pulse continued to squeeze the sample, isentropically compressing it to much higher pressure. The sample was driven through thermodynamic phase-space into novel territory beyond the primary shock Hugoniot of the material. Prior to the Lab's pyrometry development work, measuring temperature under these conditions at Z was impossible. Researchers in Neutron Science and Technology (P-23), in collaboration with NNSS NMO, have developed a portable general purpose pyrometry diagnostic system now being adapted for use at several dynamic shock physics, pulsed power, and explosive firing facilities across the DOE complex, including upcoming subcritical experiments at the Nevada National Security Site.

Implementing low-temperature dynamic pyrometry on Z is extremely difficult: detectors sensitive to single photons must collect light from within the world's most powerful electromagnetic pulse. Further, the state of experimental interest lasts only ~100 nanoseconds, during which time a passively collected signal—one that cannot be amplified relative to background—may vary by as much as four orders of magnitude. The team spent nearly three years developing the specific design for this experiment. Ongoing experiments will continue to test further uncharted regions of thermodynamic phase space to inform models used in the Laboratory's advanced simulations.

To successfully execute the experiment, researchers designed the target (near right), containment vessel (right), and diagnostics to capture the data resulting from the experiment using the Z Pulsed Power Facility at Sandia National Laboratories (far right).



7.5-mm target sample **Z plutonium containment vessel** **Z Pulsed Power Facility**

GET THE DETAILS

Participants: Tom Hartsfield (Neutron Science and Technology, P-23) served as Los Alamos pyrometry principal investigator. Karlene Maskaly (Continuum Models and Numerical Methods, XCP-4); Chris Rousculp (Plasma Theory and Applications, XCP-6); and Carl Greeff (Physics and Chemistry of Materials, T-1) worked on LANL simulations. Dan Dolan, Chris Seagle, and Jean-Paul Davis served as Sandia National Laboratories principal investigators. NNSS NMO principal collaborators were Robert Corrow, Richard Hacking, Carl Carlson, Sheri Payne, and Craig Kruschwitz working under David Esquibel. Nuclear Materials Science (MST-16) members Brittany Branch, Miranda Williams, Carlos Archuleta, Tomas Martinez, Randy Sandoval, and Mike Ramos built the targets for the experiment. **Funding:** Work at LANL was funded by Campaign 2: Dynamic Materials Properties (LANL Program Manager Dana Dattelbaum). **Technical contact:** Tom Hartsfield

Culture of shared responsibility bolsters safe and secure operations during complex renovation project

The Sigma Complex is a mission-critical facility, housing production for the 30 plutonium pits per year institutional commitment, a Hydro Dynamic Test Program Level-2 Milestone, and an Alt 940 Level-2 Milestone. For this more than 50-year-old facility to successfully execute the Lab's mission, refurbishment is underway.

With 30-50 additional non-permanent personnel from several different service providers in the facility executing these upgrades, knowledge of and compliance with safety and security requirements were identified as potential risks.

Safe Conduct of Research Principles

- Everyone is personally responsible for ensuring safe operations.
- Leaders value the safety legacy they create in their discipline.
- Staff raise safety concerns because trust permeates the organization.
- Cutting-edge science requires cutting-edge safety.
- A questioning attitude is cultivated.
- Learning never stops.
- Hazards are identified and evaluated for every task, every time.
- A healthy respect is maintained for what can go wrong.

In a demonstration of the Safe Conduct of Research Principles, management worked with programmatic and support staff to come up with suggestions for improving and ensuring safe and secure operations. The results are process improvements that increase the effectiveness of communication and establish consistency, reliability, and predictability, including the following.

- Having more inclusive participation in plan of the day meetings and weekly update briefings, where both support and programmatic personnel can have specific discussions about the impacts of the work taking place and creating a shared fate outlook.
- Sharing lessons learned through post-job reviews and, when appropriate, translating into improvements in the work planning and control process.
- Identifying specific roles and responsibilities to provide clarity for each specific effort, resulting in better working relationships across organizations, including room responsible personnel who are facility residents to help coordinate and de-conflict work within their areas of responsibilities.
- Teaming new craft workers with environment, safety, and health (ES&H) personnel and experienced coworkers to expose them to the complexities of the facility.

Foundry and Solidification Science team member Victor Vargas (left) and Material Control and Accountability (MC&A) lead Chastity Vigil (both Sigma Division, Sigma-DO) prepare uranium components for shipping to another part of the Laboratory for use as part of a larger experiment. This close collaboration between a technical subject matter expert and a trained MC&A representative ensures that the complex safety and security requirements for such activities are met.

The outcome to date has been the creation of a culture that demonstrates shared responsibility, trust, and success.

Routine target replacement far from routine

When the proton beam generated by the Los Alamos Neutron Science Center's (LANSCE) linear accelerator strikes the neutron-rich nuclei of the tungsten target at the Weapons Neutron Research Facility (WNR), the impact shatters the nuclei, releasing copious neutrons. These high-energy neutrons are essential for the defense, industrial, and basic research performed at WNR.

The WNR target requires routine replacement every few years when it reaches the limit of its service lifetime. However, the replacement done during the 2019 accelerator maintenance outage was anything but routine, due to damage to the overhead crane typically used for the job. The work would have to be done using a mobile crane staged behind another building, blocking sight of the target area—and it would take place outdoors as the building's roof was dismantled for repairs to the existing crane.

The procedure was led by members of the Accelerator Operations and Technology target team with support from deployed LANSCE Facility Operations staff. To ensure that radiological standards were in place, several practice sessions were held in a full mock-up of the work area. During these drills, all participants—the target team, the crane crew, and radiological control technicians—perfected their techniques and communications.

Due to the team's careful planning and execution, the successful target replacement ensures experiments critical to the Lab's nuclear science mission using the Time Projection Chamber, LENZ, and Chi-Nu can proceed during the LANSCE run cycle.

In this mock setup, the simulated target, about the size of a D battery, is welded to the target's cooling lines, which will be severed during the removal operation.

To practice, workers constructed a platform to simulate the target and observation holes. Here, one worker guides the strap used to lower the alignment mechanism into the mock observation hole, while an operator rehearses driving the crane.

The crane operator brings the target mechanism toward the shielded container while workers guide it with long hooks. Inside the container, a camera transmits images to a laptop, enabling navigation from a safe distance from what in the actual process will be an irradiated source.

Within the shielded container, workers navigate using a camera (center lower left) as they operate pneumatic bolt cutters (right) to sever the mock target from its holder. During the actual transfer this setup protected them from the used, radioactive target until it was secured in a disposal cask. In the future this work will be handled by robotic equipment.

Teamwork in action

Just as in practice, the crane lowered the new, non-radioactive target as two workers guided the crane's hook and rigging above the target port. Shielded from the sun by an umbrella, the laptop operator watched with cameras from the observation hole as crane crew workers in a hydraulic lift communicated with the crane operator.

GET THE DETAILS

Participants: John Eddleman, Esteban Garcia, Hargis James, Sean Hollander, Jordon Marquis, Joe Shepherd, and Ryan Seltzer (Accelerator Operations, AOT-OPS); James Vigil (LANSCE Facility Operations, DESH-LFO); Pat Padilla, James Martinez, and Chris Garcia (Logistics Central Shops, LOG-CS); Dennis Martinez (Logistics Heavy Equipment Roads and Grounds, LOG-HERG); and Charles Kelsey (LANSCE Weapons Physics, P-27). **Funding:** Maintenance and operations at LANSCE is funded by Weapons Infrastructure. **Technical contact:** Eron Kersteins

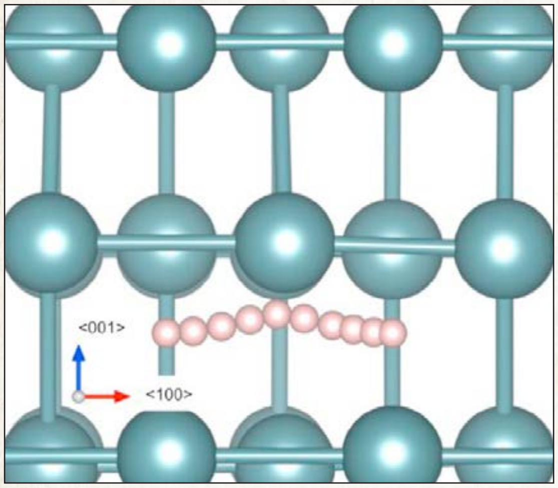
Resolving a long-standing debate on the hydrogen diffusion coefficient for α-uranium

Uranium is central to the Laboratory's mission; however, some of the chemical changes that uranium can go through are poorly understood. Scientists know that as α-uranium (α-U) reacts with hydrogen to form uranium hydride, diffusion of hydrogen through the α-U is a key kinetic step. The only data on this diffusion coefficient comes from experiments performed at temperatures near the α-U stability range, around 500 °C. The data from several independent experiments agree fairly well at these high temperatures, but once they are extrapolated to room temperature, their predictions differ by as much as three orders of magnitude.

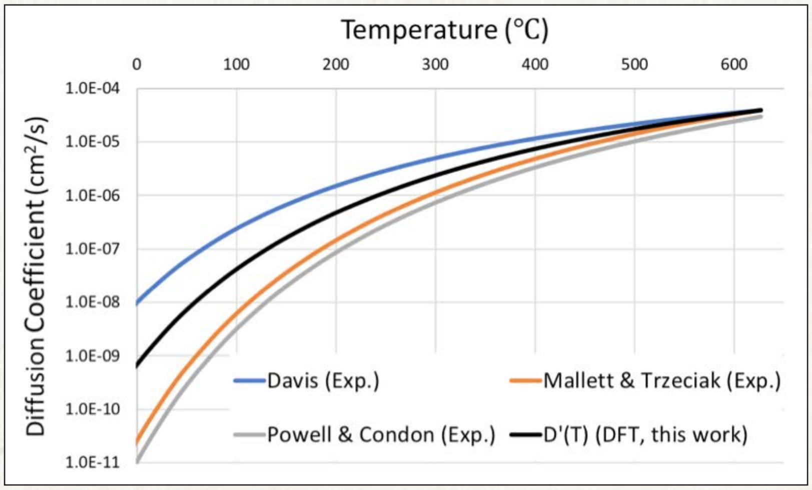
To rectify these differences Edward F. Holby (Finishing Manufacturing Science, Sigma-2) used density functional theory to model the way diffusion would occur in different crystallographic orientations of α-U, including relevant kinetic barriers and vibrational properties. The calculations show that one proposed pathway captures the diffusion coefficient value at experimental temperatures and gives appropriate values at lower temperatures. This pathway, the percolating, low-barrier, bulk hydrogen diffusion pathway (depicted below), was shown in calculations to be not only energetically possible, but also consistent with experimental values. This work proposes an answer to a long-standing dispute regarding the room-temperature diffusion coefficient of hydrogen through α-U.

Published in the *Journal of Nuclear Materials,* this work relied on the Laboratory's institutional computing resources to carry out density functional theory calculations of relaxed structures, diffusion barriers, and vibrational normal modes.

The work supports the Laboratory's National Security Science mission and its Materials for the Future and Information Science and Technology science pillars. It also supports the Excellence in Nuclear Security strategic objective of the Laboratory Agenda by further developing the foundational materials science that underpins the fidelity of the Annual Assessment Reports.



Low-barrier diffusion pathway of hydrogen (white spheres) through the α-U lattice (blue-gray spheres).



Experimental and density functional theory-derived diffusion coefficients as a function of temperature.

GET THE DETAILS

Reference: "Crystallographic orientation effects of hydrogen diffusion in α-uranium from DFT: Interpreting variations in experimental data," *Journal of Nuclear Materials* 513, 293-296 (2019). **Funding:** LANL Enhanced Surveillance, formerly known as Campaign 8 (LANL Program Managers Thomas G. Zocco and Charles R. Hills).
Technical contact: Edward Holby

'It's this type of work that drives me to one day earn a doctorate in chemical engineering and then come back to work for the Laboratory, where I can continue to make a difference to my community and to society.'

Estrella 'Star' Torres
MPA-11 student intern
2019 Pojoaque High School graduate

Dartmouth science on the horizon for Estrella 'Star' Torres

Estrella "Star" Torres yearned to make a difference in her community. Growing up in the Nambé Pueblo, less commonly known as "The Place of the Rounded Earth," she always knew she was different than other kids because of certain circumstances.

"I grew up under the watchful eye of my grandma," Torres said. "This situation has been particularly difficult during my high school years. I mean, I attend all these school functions without either of my parents by my side, but knowing I have my grandma makes me extremely grateful. She has had a hard life battling cancer, but she is strong and independent, a person I have always looked up to."

Discovering chemistry

Located in the foothills of the Sangre de Cristo Mountains, the Pueblo of Nambé in Northern New Mexico is known for its agriculture and traditional textiles.

Although aware of her Pueblo's penchant for agriculture and crafts, Torres preferred the challenges associated with mathematics and the sciences.

"I've always enjoyed math and science," she said. "It wasn't until my sophomore year in high school, though, that I discovered chemistry. With some guidance and encouragement from my science teacher, Ms. Vigil, I found that I liked the many branches of chemistry, so much so that I want to pursue the scientific discipline in college."

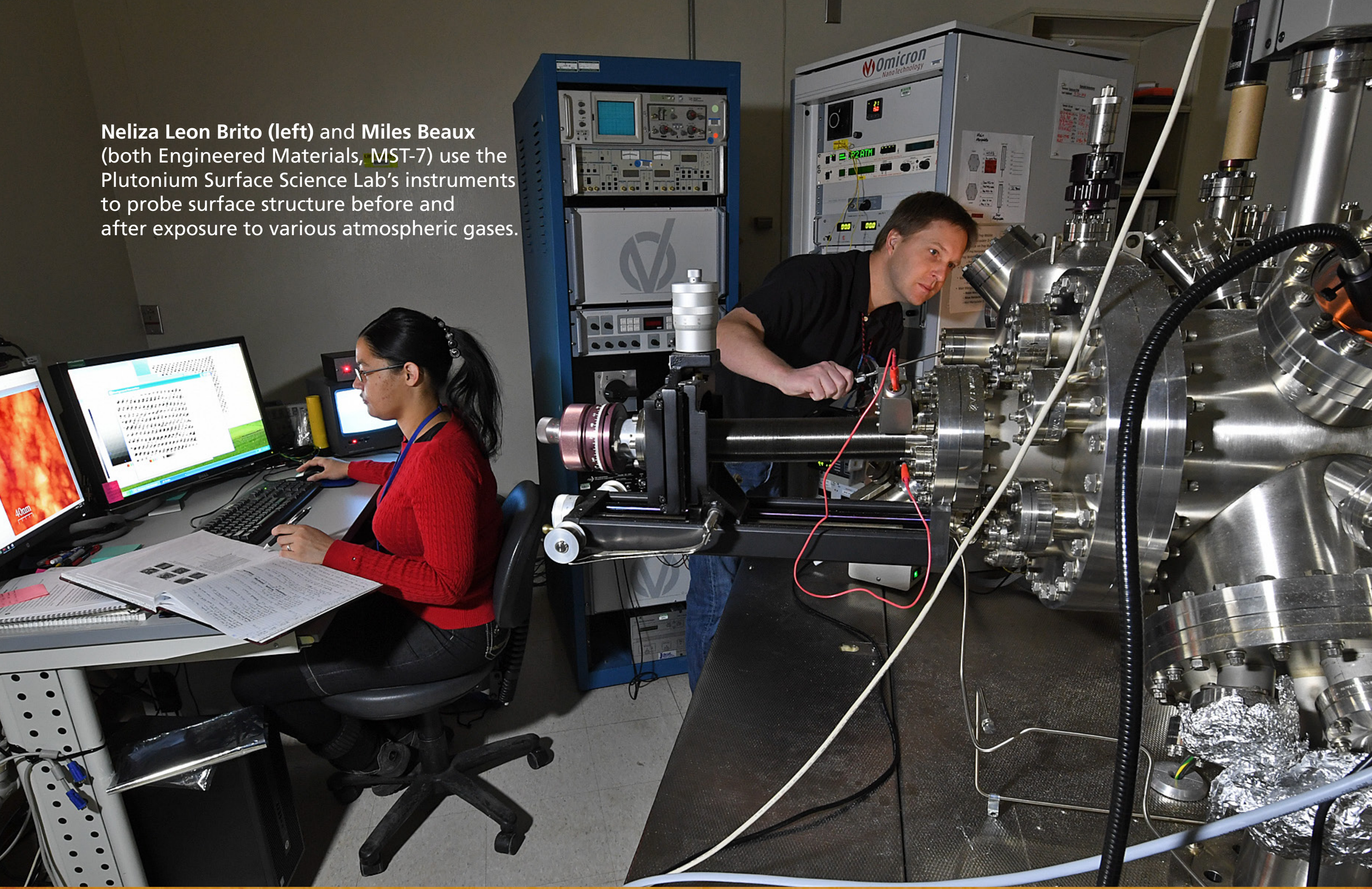
A 2019 graduate of Pojoaque Valley High School, Torres is the recipient of a Gold Scholarship from the Los Alamos Employees' Scholarship Fund, which provides $5,000 per year for up to four years. She plans to use the scholarship while attending Dartmouth College, located in Hanover, New Hampshire.

Shifting to chemical engineering

At first wanting to earn a degree in chemistry, Torres has since decided to study chemical engineering. "It's a great combination," she said, "a balance between the many facets of chemistry and the mathematics and problem solving of engineering."

Influencing this shift in study has been a High School Internship Program position at Los Alamos National Laboratory. Torres started working at the Laboratory in January with her mentor Troy Semelsberger, himself a chemical engineer who works in Materials Synthesis and Integrated Devices (MPA-11).

"I am part of a team working on the development of an alternative energy source," she said. "It's very exciting—for the first time ever I am using science to make a difference. It's this type of work that drives me to one day earn a doctorate in chemical engineering and then come back to work for the Laboratory, where I can continue to make a difference to my community and to society."



Neliza Leon Brito (left) and **Miles Beaux** (both Engineered Materials, MST-7) use the Plutonium Surface Science Lab's instruments to probe surface structure before and after exposure to various atmospheric gases.

Associate Laboratory Director for Physical Sciences:
Antoinette J. Taylor

Physical Sciences Vistas, produced by Karen Kippen, Efrain Garcia, and Madeline Bolding, is published by the Physical Sciences Directorate at Los Alamos National Laboratory.

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