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Author(s): Kippen, Karen Elizabeth; Cruz, James Michael; Hockaday, Mary Yvonne P.; Lacerda, Alex Hugo; Wilburn, Wesley Scott; Batha, Steven H.; Bronkhorst, Curt Allan; Brown, Eric; Carnes, Jay Russell; Del Mauro, Diana; DeYoung, Anemarie; Freibert, Franz Joseph; Fronzak, Hannah Kristina; Gray, George Thompson III; Hooks, Daniel Edwin; Martineau, Rick Lorne; Martz, Joseph Christopher; Migliori, Albert; Poling, Charles C.; Prestridge, Katherine Philomena; Schraad, Mark William; et al.

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VISTAS

Performance through Science

Los Alamos
NATIONAL LABORATORY
EST. 1943

For the past three decades, the nation has relied on scientific excellence to sustain a safe, secure, and reliable nuclear stockpile in the absence of weapons testing and new plutonium production.

The Stockpile Stewardship Program has dramatically expanded our understanding of weapon physics and the unique materials that make up our stockpile—and we are not done.

We have learned during the past 20 years of stockpile stewardship that materials matter! But for a more detailed understanding of how–and how much–materials matter, we need to explore the relationships among manufacturing processes, material structure and properties, and ultimately performance in materials science—the classic materials tetrahedron. We develop our science view of this understanding through the prism of controlled functionality—the ability to synthesize and process materials to create unique and defined characteristics. Through this control we connect the performance of these materials to our national security mission, both driven by and expanding material science solutions. Controlled functionality of materials could create new options for sustaining stockpile performance and achieving improvements in safety or security.

We continue to monitor and assess the effects of plutonium aging as we reincorporate old pits into the stockpile.

We use advancements in diagnostics for subcritical experiments to provide increasingly detailed understanding of plutonium properties to help verify and validate computational predictions.

And by exploring the high-energy-density regimes, turbulence and mixing, and high explosive performance, our experiments give us increasing insights into phenomena key to weapons performance.

This issue of *Experimental Physical Sciences Vistas* focuses on the integrated science that plays a critical role in Los Alamos National Laboratory's support of the nation's nuclear deterrent. I hope you will enjoy reading about these accomplishments, opportunities, and challenges.

Associate Director Experimental Physical Sciences
Mary Hockaday

On the cover: Our science is a lens through which the world views Los Alamos National Laboratory and through which our scientists communicate with the world.

A safe, secure, effective deterrent

Los Alamos is solving national security challenges through scientific excellence

The Stockpile Stewardship Program is nearly 25 years old, and the progress made in ensuring the safety, security, and reliability of our stockpile in the absence of nuclear testing is astounding.

On September 23, 1992, the last full-scale underground test of a nuclear weapon was conducted by Los Alamos National Laboratory at the Nevada Test Site. The test, code named "Divider," was the last of 1,030 nuclear tests carried out by the United States. Shortly after Divider, President George H.W. Bush signed Congressional legislation that mandated a nine-month moratorium on U.S. nuclear weapons testing, a mandate that has been extended by every subsequent U.S. President into the present day.

The end of the 1980s saw three remarkable changes that forever changed the future of Los Alamos National Laboratory. First, in July 1989 the United States suspended pit production operations at the Rocky Flats Plant outside of Denver, Colorado. Over the next few years more than half of the U.S. nuclear weapons production complex would close. Second, five months after the closure of Rocky Flats, the Berlin Wall fell on November 9, 1989 and the Cold War was over, with the Soviet Union officially dissolved the day after Christmas 1991. The third momentous change was the cessation of underground nuclear testing. The last U.S. nuclear weapons test was conducted on September 23, 1992, code named "Divider." Little did we know how appropriate that name was. Divider indeed was the delineation between old and new eras at Los Alamos.

Any one of these changes would have meant a very different focus on the work of Los Alamos. Taken together, these three developments completely changed the direction and focus of the U.S. nuclear complex.

The challenge of ensuring a safe, secure, and reliable stockpile in the absence of either new testing or new production was profound. The national laboratories responded with the Stockpile Stewardship Program. Stewardship contained three elements:

1. assessment of weapons from the bottom-up via a combination of better-resolved physics represented in new computing codes running on state-of-the-art platforms;
2. a suite of new small-scale experiments to measure the myriad of parameters and material properties to populate these codes; and
3. a new generation of integral experiments to verify and validate the predictions from our computations.

In this issue of *Experimental Physical Sciences Vistas* we see how far we've come in many of these areas. More than 20 years of effort have dramatically expanded our understanding of weapon physics and the materials that make up our stockpile. We've also learned an enormous amount along the way, especially the source of uncertainty in our weapons performance predictions. Understanding uncertainty drives a tremendous amount of work in the weapons complex and refurbishment of weapons via life extension programs or modifications. These programs add margin to nuclear safety and performance.

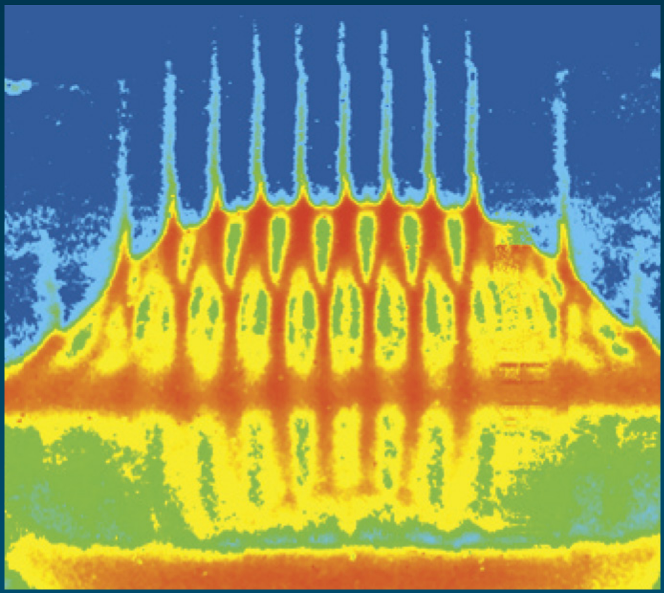
As we look at future challenges in the stockpile, it is clear that we must make continued progress to understand many areas of weapon science that remain poorly understood. As weapons continue to age and as new manufacturing and production processes are employed, we must continue to assess the impacts on weapon performance.

A key lesson from the more than past 20 years of stewardship is that materials matter! Indeed, the majority of our uncertainty in assessment of weapon function arises from uncertainties in material properties, especially dynamic properties at the mesoscale. This issue highlights many of these material challenges and shows how a more detailed understanding of the processing-structure-properties-performance relationship in materials science—the classic materials tetrahedron—will form a key focus in the evolution of stewardship.

Articles in this issue include an overview of controlled functionality of materials, showing how this resolved understanding can be used not just for improved predictions of weapon function, but could be employed to engineer materials at the atomic scale and mesoscale to gain tailored properties for dramatic improvements in safety or security. You'll also find a description of the importance of the mesoscale in materials and why this is such a focus for facilities like MaRIE (Matter-Radiation Interactions in Extremes). Understanding materials at the mesoscale is key to enabling advances in additive manufacturing, a critical tool to improve agility in the National Nuclear Security Administration complex.

Plutonium aging continues to be a focus of stewardship and has become especially important as we consider the use of old pits to meet Department of Defense requirement of 50-80 pits by 2030. These ideas will require a detailed understanding of plutonium properties, a task made especially challenging as new tools and experiments are deployed with plutonium. This includes new types of subcritical experiments diagnosed by neutrons to measure key properties of these integrated systems. In this issue, you'll find descriptions of this and a range of new diagnostic techniques such as resonant ultrasound spectroscopy, various other subcritical experiments, and how the Dual-Axis Radiographic Hydrodynamic Facility uses surrogates to verify and validate computational predictions.

High-energy-density physics—and the experiments conducted to improve our understanding of it—forms another important component of the future of stewardship. You'll find descriptions of a number of facilities where this research is conducted, including work at the National Ignition Facility and OMEGA Laser Facility. Closely related is our work on high explosives and turbulence and mixing.



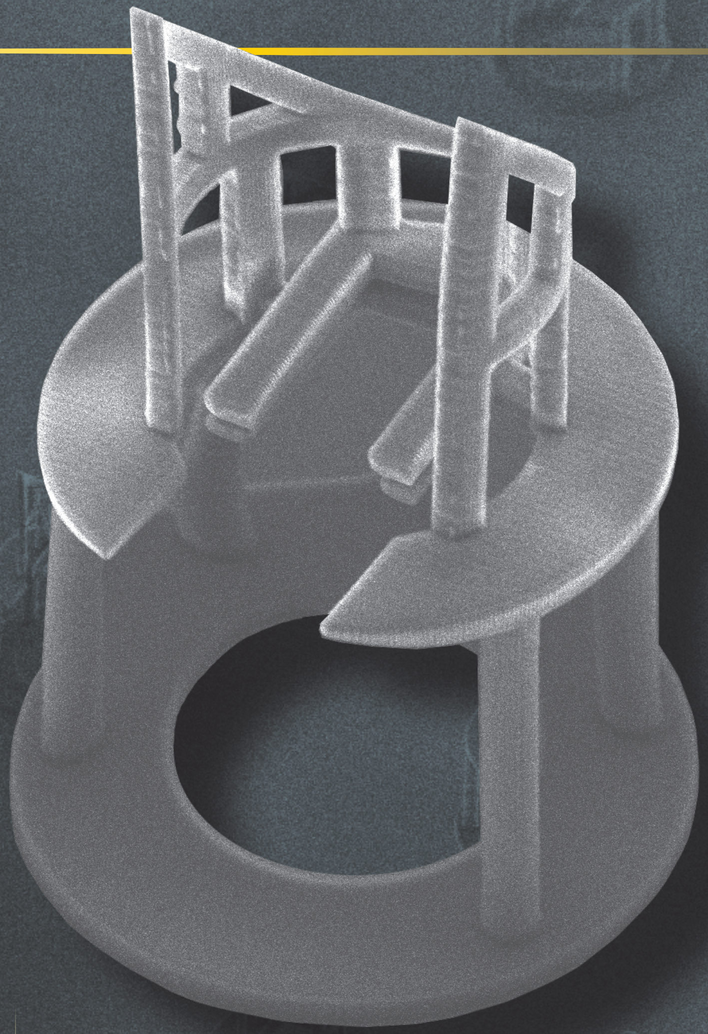
In this proton radiography image, protons penetrate a sample of explosively shocked tin, providing insight into the material's behavior under dynamic conditions.

Despite nearly 60 years of investigation of high explosives science, elements of explosive function remain poorly understood. A new generation of tools such as MaRIE could be critical to finally measure key elements of high explosive performance. Similarly, the behavior of materials under high strain rates leads to unusual behavior. It is critical to understand these details of fluid flow and how turbulence contributes to mix in high strain rate flows. All of these issues present a challenge for the future of stewardship and our task of assessing and certifying our future stockpile.

We've come a long way since the inception of stewardship. Nonetheless, many challenges remain. It's an exciting time at Los Alamos National Laboratory, as we focus again on the materials in the stockpile and prepare for a new generation of tools, both experimental and computational. These tools will allow a new generation of measurements to provide previously unknown data on structure and properties. These data are key to ensuring we continue to fulfill our mission of ensuring a safe, secure, and reliable stockpile for the United States.

By three-dimensional printing on the nanoscale, Los Alamos researchers are helping to invent novel materials with functionalized and engineered properties. The production of mesoscale and nanoscale materials with engineered structures could provide materials options for the stockpile and other mission areas.

Shown are electron microscope images of a Los Alamos-designed, greatly scaled down, mirror physics package holder for the Cepheus campaign at the National Ignition Facility. Background: an array of holders that can be rapidly printed with various geometries; at right: a close-up of one structure.



At right: a Los Alamos materials scientist uses a focused ion beam/scanning electron microscope to analyze a range of material properties, including looking at the results of dynamic shock loading and at the influence of a material's internal structure on deformation, void nucleation and growth, and ensuing failure. The ultimate goal is to create materials designed for a specific function.

Pursuing controlled functionality

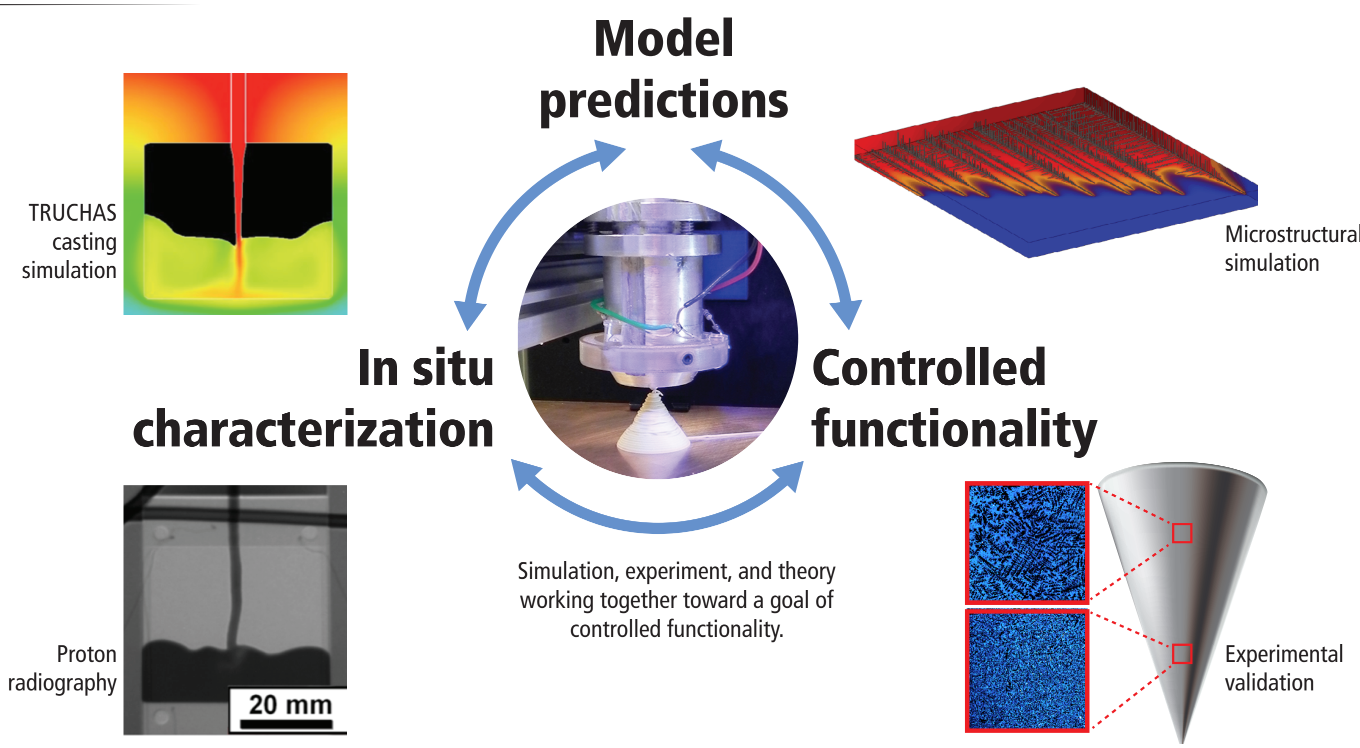
Creating new materials for national security

The objective of controlled functionality is to control or tailor a material's nanoscale and mesoscale features to provide specific properties or performance in a given environment. The challenge lies in the ability to design and manufacture materials with desired functionalities.

Los Alamos is actively pursing this goal to satisfy ever-increasing demands for advanced materials underpinning national security.

Laboratory researchers are contributing to the urgent need to develop design principles accelerating the discovery and application of advanced materials with useful function—a radical departure from traditional discovery of materials and functionality by "informed serendipity."

Initial success is promising. State-of-the-art, first-principles calculations and computational algorithms performed by Los Alamos and collaborators have successfully shown it is possible to reliably predict the chemical stability, voltage capacity, and oxidation state of inorganic compounds relevant for photovoltaic, battery, and thermoelectric applications.[1] These materials properties result from predominantly independent-electron characteristics, which are relatively straightforward to calculate. Even more challenging are the complex functional materials underpinning national security directives, including new metals, higher energy insensitive



Simulation, experiment, and theory working together toward a goal of controlled functionality.

explosives, and multifunctional polymers. Controlling such complex functionality is even more difficult due to the need to bridge our understanding of interactions across multiple time and length scales.[2,3]

To date, the design of functional materials has been restricted to those for which theoretical modeling is an integral component. Additionally, materials for the nation's nuclear stockpile are complex and need continued attention. For example, the nation's stockpile could benefit from new insensitive explosives with higher energy density and functional materials with enhanced performance and age-resistant properties. To maintain the nation's leadership in materials for national security, an effective approach to design materials with complex functionalities is required. Such an approach will directly support life extension programs (LEPs) in the future with new materials and enhanced functionality in response to evolving strategic threats.

The key challenge in certification of components for the stockpile is that many of the important properties a weapon designer must know in order to calculate safety and performance are exceedingly difficult to measure.

The key challenge in certification of components for the stockpile is that many of the important properties a weapon designer must know in order to calculate safety and performance are exceedingly difficult to measure. This challenge is becoming more prevalent as the days of underground testing recede into the past.

Controlled functionality is based on the approach that measurable and quantifiable properties can be sufficiently evaluated to ensure confidence in performance. Relationships between observable microstructure, such as grain size, inclusions, and impurities, would be evaluated in light of the best materials science. With a suitable set of measured parameters, the product would be qualified, and confidence in performance characteristics such as strength will have been established.

A number of components in the current U.S. stockpile systems will need to be replaced and may benefit from materials with controlled functionality. Consider, for example, metals, where the large deformation, damage, and failure processes for polycrystalline metallic materials involve many types of mechanistic and atomistic processes. Environmental influences such as hostile conditions add additional challenges that must be overcome to ensure performance. New functional materials to enhance fire resistance and to function as designed when subjected to high pressure and large plastic deformation will be important in the future stockpile. With controlled functionality, a scientist will be able to design a material with nanoscale and mesoscale features tailored to perform in a given environment.

Controlled functionality is based on the approach that measurable and quantifiable properties can be sufficiently evaluated to ensure confidence in performance.

High explosives materials research continues to be central to Los Alamos National Laboratory's core mission. The challenges of predicting explosives are severe: extreme temperatures, pressures, and statistical responses resulting from fine details of microstructure have been driving advances in experiments for decades. The ultimate goal is to develop a predictive capability that spans from engineering response, accident scenarios, assault, and detonation, to performance in extreme environments. The engineering-style detonation models have reached a pinnacle in their capabilities, and a new generation of models and physics-based understanding is required to capture the interaction between microstructure and chemistry. Future stockpile requirements will drive the need for increased understanding of material processing further removed from nuclear testing and employ insensitive explosive materials and options for enhanced surety. New functional energetic materials with variable-energy-density based on insensitive formulations derived from synthetic chemistry will enable enhanced options to support future LEPs.

Polymers, foams, and organic components are pervasive in our nuclear weapons stockpile. Fundamentally different than metals, these materials require completely different methodologies and theories to describe their behaviors. In the U.S. stockpile, these organic materials exist in a radioactive environment and when called up undergo a number of transitions under dynamic loading that must be captured in our predictive models. The need for advance polymers with controlled functionality is of increasing interest to support LEPs, particularly given that many of the polymers that were certified in underground tests are no longer available.

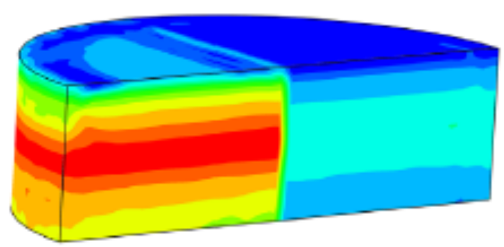
As the nuclear stockpile continues to age and evolve, the nuclear weapons complex requires smarter approaches in the design and fabrication of new and replacement materials that meet stringent constitutive and hydrodynamic performance requirements for long stockpile lifetimes. The materials in the nation's stockpile will benefit from a validated scientific means to connect processing to performance, enabling process-aware material specifications—where no further qualification tests are required once fabrication is complete. This effort will take advantage of recent advances in additive and advanced manufacturing techniques such as hierarchical assembly, application-guided controlled functionality, and multidimensional fabrication methods.

The materials in the nation's stockpile will benefit from a validated scientific means to connect processing to performance, enabling process-aware material specifications—where no furthers qualification tests are required once fabrication is complete.

The prediction of structure independent of functionality is, by itself, a grand challenge requiring innovative thinking. And as capturing the materials descriptors that predict the functionality of a material is insufficient to carry out pure materials design, a method is required to invert the correlations to identify which material best meets the design criteria. The co-design approach and materials design strategy will enable future generations to invert the design principles discovered by this approach and enable the discovery of tomorrow's materials by true design.

Microstructure modeling

Properties modeling

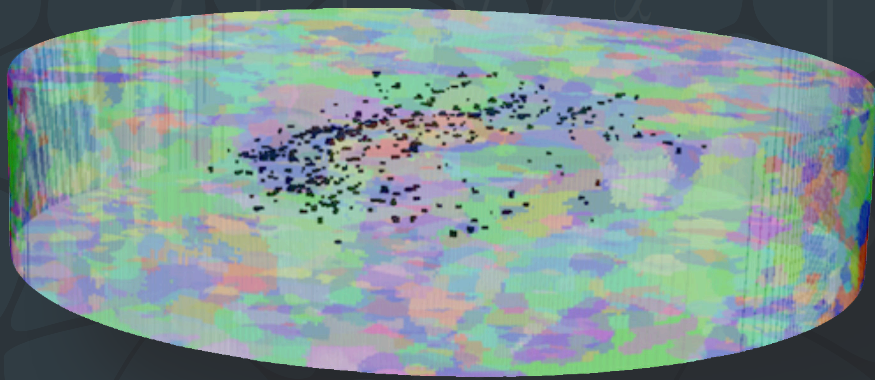


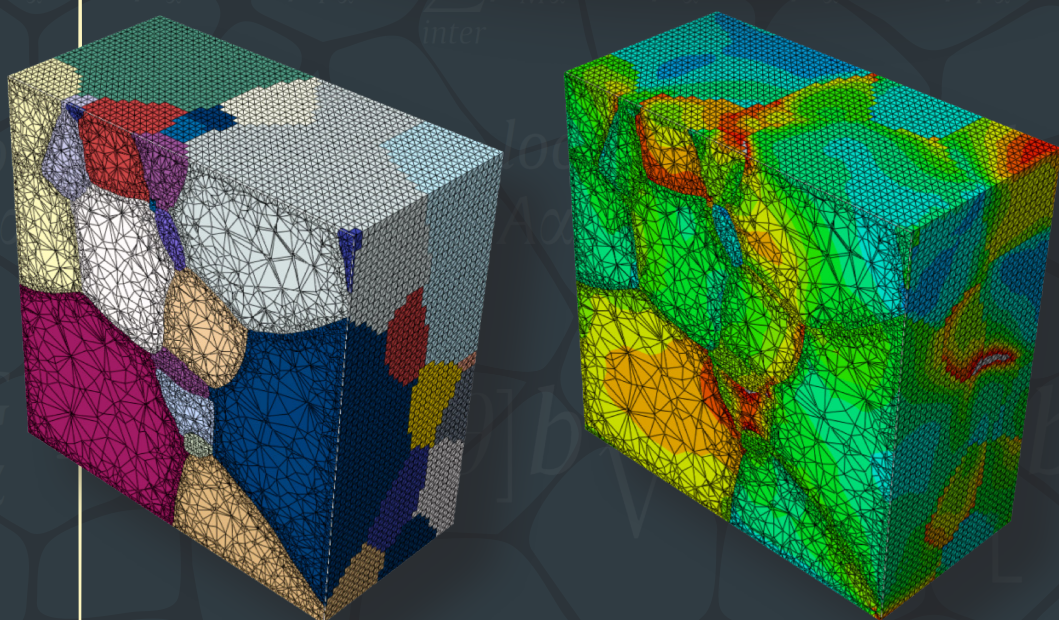
Performance modeling

Controlled functionality for performance requires predictive modeling at multiple length scales. Los Alamos's integrated co-design approach will couple multiscale theory and multi-probe experiments on next-generation computing architectures for future integrated codes. Validated models will reduce uncertainty in integrated codes and provide predictive descriptions of newly manufactured materials and components.

1. Accelerating Advanced Material Development. (www.nersc.gov/news-publications/nersc-news/nersc-center-news/2011/materials-research-in-the-information-age/).
2. Directing Matter and Energy: Five Challenges for Science and the Imagination. (science.energy.gov/~/media/bes/pdf/reports/files/Directing_Matter_and_Energy_rpt.pdf).
3. From Quanta to the Continuum: Opportunities for Mesoscale Science. (science.energy.gov/~/media/bes/pdf/reports/files/From_Quanta_to_the_Continuum_rpt.pdf).

To properly understand the physics of how metals react under extreme loading conditions, researchers must look at the mesoscale. Shown are examples of materials simulations and characterizations revealing the influence of microstructure on materials performance.

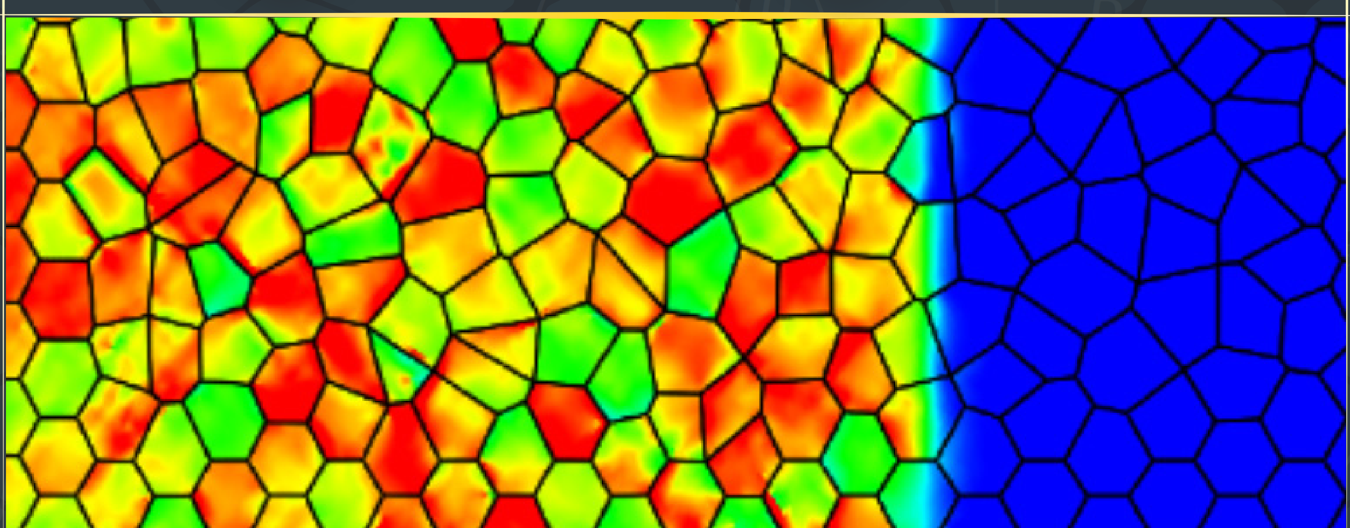




At left: three-dimensional image of a porous copper polycrystal, illustrating emerging in situ techniques to characterize microstructural effects on ductile damage of polycrystalline materials.

Center: statistically representative computational representative volume element of tantalum (far left) microstructure and the internal stress state (left) after applying dynamic loading conditions representative of a plate impact experiment. The deformation due to single crystal heterogeneity leads to highly non-uniform response at the mesoscale and demonstrates the importance of study at this level.

Below: contour plot of shock direction plastic strain field resulting from simulated impact of a polycrystalline energetic RDX specimen. Heterogeneity in field response is due to differing crystallographic orientations for each grain and a sampled distribution of initial dislocation density and slip resistance.



The mesoscale advantage

Exploring the realm controlling how materials react in extremes

The human eye can see sudden changes in metals when two vehicles crash or, less dramatically, when a piece of copper is machined into a part. Although materials studies were once based on such observations, scientists have long realized the limitations of naked eye observations, which take place at the macroscale.

When engineered structures encounter high rates of loading—that is, subjected to an extreme force—it is difficult with controlled experiments to measure the many physical events taking place—for example, to quantify the phase state of materials.

To properly understand the physics of how metals, which are composed of irregular-shaped crystals and contain a variety of defects, react under extreme loading conditions, researchers must look at the mesoscale. The mesoscale is where controlling processes for plasticity, phase change, and damage take place.

From this realization sprang the need for special techniques and instruments to measure properties at the mesoscale. Los Alamos National Laboratory has been at the forefront of single-crystal and polycrystal research for 15 years, developing new experiments, computer simulations, and models. "You need the combination of all three—experiment, model, and simulation—to make headway in understanding materials at the mesoscale," said Los Alamos theorist Curt Bronkhorst.

Imagine if engineers could thoroughly understand the failure mechanisms in metals—the knowledge would benefit vast sectors of the economy. Engineers could develop more reliable components, avoid expensive over-engineering, and prevent certain catastrophic events.

Such insights could also aid Los Alamos's annual assessment of the safety, security, and reliability of nuclear weapons. Metals used in weapons are subjected to extreme forces and thermodynamic states that alter the atomic structure of the materials and, in turn, their performance.

Los Alamos has high-performance computer codes that help guide the weapons assessment process. In the future, the codes will take advantage of exascale computing and will consider both the single-crystal level and the macroscale to predict how the metals will perform over a weapon's service. Phase transformations in plutonium, for example, are likely triggered by stress and temperature, and the next generation of predictive material models must incorporate the role of these fluctuations.

"You need the combination of all three—experiment, model, and simulation—to make headway in understanding materials at the mesoscale."

Los Alamos theorist
Curt Bronkhorst

Los Alamos National Laboratory's predictive capabilities

Plutonium, zirconium, titanium, cerium, and copper are a few of the many metals Los Alamos materials scientists study at the crystal level. Los Alamos researchers use advanced x-ray sources, such as the Linac Coherent Light Source at the SLAC National Accelerator Facility, to obtain information at this level and powerful supercomputer models, such as the Laboratory's SPaSM (scalable parallel short-range molecular dynamics) code, to validate experimental data from the x-ray sources.

Understanding the performance of weapon materials under dynamic loading conditions would be impossible without considering the material's true aggregate nature, in addition to the single-crystal properties. The forces occurring during the stockpile-to-target sequence environment, combined with stress and temperature, can transform the crystallographic structure of metals.

Los Alamos has made substantial advances in understanding processes such as dislocation motion (imperfections affecting how the atoms are stacked in the single crystal), deformation twinning (i.e., crystal transformation contributing to plastic deformation), and phase transformations. Each process is critically linked to the other processes, and all are equally important to the single-crystal research effort.

Within a piece of metal, each individual single crystal is oriented differently. How it moves and interacts with other crystals during high-rate loading, including shock loading,

Tools, capabilities, and expertise

- Los Alamos Neutron Science Center's Manuel Lujan Jr. Neutron Scattering Center and Proton Radiography Facility
- Supercomputers at Los Alamos such as Trinity, which makes complex three-dimensional simulations of nuclear detonations
- Linac Coherent Light Source, an Office of Science User Facility operated for the U.S. Department of Energy by Stanford University, provides data on changes in microstructural reorientation
- SPaSM (scalable parallel short-range molecular dynamics) computer code, developed at Los Alamos, enables large molecular calculations for studying how shock waves force materials to break apart
- Elasto-viscoplastic deformation computer code, based on fast Fourier transform for mesoscale modeling, was developed at Los Alamos for predicting the elastic-plastic deformation of polycrystals
- Crystal plasticity finite element-based polycrystal plasticity modeling, for mesoscale plasticity and damage modeling
- Phase field modeling, for high resolution mesoscale and single crystal behavior simulations
- Electronic structure models and computer codes, to simulate detailed atomic interactions within single crystals
- New experiments combined with mesoscale mechanical behavior models
- Single crystal research, a strong and unique capability of Los Alamos involving a broad group of people
- Mesoscale materials damage and failure modeling and computer codes
- Broad modeling and simulation experience and expertise

is dictated by the nonlinear elastic stiffness represented by the equation of state. A non-uniform internal stress state will begin to develop with deformation. At the same time, the density increase also will cause an increase in temperature due to the imposed mechanical work. As loading increases with time, irreversible plastic deformation processes are triggered. These physical processes are called dislocation mediated plasticity and deformation twinning.

In a multiscale modeling study of magnesium, funded by the Department of Energy (DOE) Office of Basic Energy Sciences, Los Alamos gained insights into deformation twinning, which affects the amount of energy a metal can absorb before breaking. The tools and techniques were standard, but the results were leveraged in unique and important ways. This work has been at the forefront of performing innovative experiments and developing predictive models to understand and represent these phenomena in simulations.

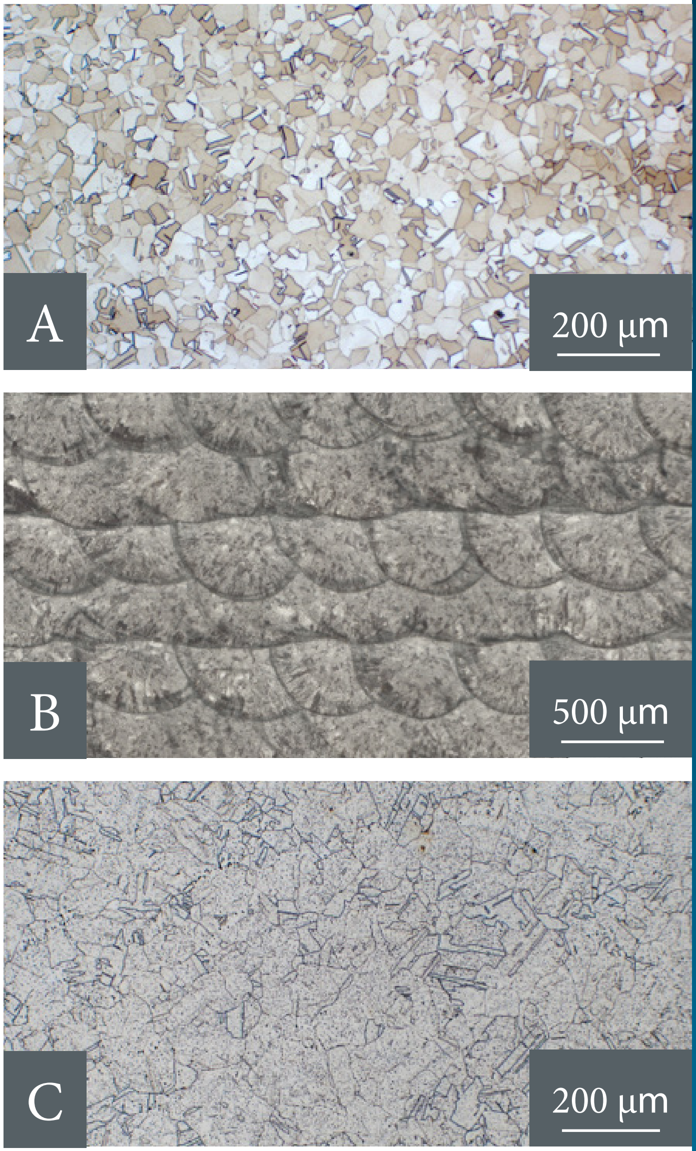
Damage and failure

Under conditions of dynamic loading, where the internal energy can be extremely high, certain conditions of shear and tension loading can lead to damage and the ultimate failure of materials. In general, damage can take three forms: localized shear, ductile voids, and brittle cracks.

Advanced damage models must be based on a physical understanding of these complicated dynamic deformation and failure processes. The models must capture the interaction between microstructure and loading history.

Los Alamos has a long history of studying damage and failure in materials. Researchers drew from that history when they developed a workhorse computer model in 1993 to capture the process of what happens when a material experiences ductile damage, softens, develops voids or cracks, and loses its load-carrying capacity. Standard rate-independent material models were unable to simulate the entire localization process. By applying the rate-dependent ductile failure model, Los Alamos researchers were able to study the physics of how tantalum breaks up when subjected to three different shock-loading conditions. The results demonstrate the significance of loading conditions to the way in which polycrystalline metals respond. The three experimental conditions spanned the regions of nucleation, growth, coalescence, and failure for the porosity-based damage response of polycrystalline metals. The model performed well for regions of response dominated by porosity growth but also showed more research is to be done. The U.S. DOE and the Joint Department of Defense/DOE Munitions Program and the DOE Advanced Simulation and Computing Program funded the study.

To continue solving problems at the single-crystal level, researchers look forward to new and advanced experimental facilities such as MaRIE (for Matter-Radiation Interactions in Extremes), Los Alamos's proposed experimental facility for the study of time-dependent materials science at the mesoscale under extreme conditions. Parallel advancements of new supercomputers, models, and codes that can represent in unprecedented ways the mesoscale physics important to the nation will be needed. Also essential are the dedicated scientists with the drive and expertise to understand complex phenomena for the weapons program as the Laboratory continues to steward the nation's stockpile.



Micrographs of 316L stainless steel (SS): a) annealed wrought plate; b) additive manufactured (AM) (as-built); c) AM following recrystallization heat-treatment at 1060 °C for one hour. Research showed that the spall strength–the ability to resist damage–of additively manufactured 316L SS was similar to that of the annealed wrought or AM-316L SS following recrystallization for high shock pressures, but all three were significantly different for lower loading pressures.

Towards qualifying additively manufactured materials

Even small changes in a material's make-up can have a big impact on how it performs.

For example, the early Liberty ships of World War II experienced hull and deck cracks, some breaking in half, due to impurities in the steel used, which when exposed to the cold waters of the North Atlantic turned brittle and fractured. Yet, with the right chemistry and heat treatments in place, the disastrous consequences came to an end.

Traditionally, this has meant materials manufactured in a process exactly mimicking one developed from successful, full-scale tests. Each step is tightly controlled to be the same as before, thus being described as "process-based manufacturing."

Additive manufacturing, the technique of creating three-dimensional objects by adding layer-upon-layer of material, is a revolutionary method for designing, producing, and implementing the process-aware materials of the future, presenting opportunities for rapid prototyping, free-form and net-shape manufacturing, and local production at a global scale.

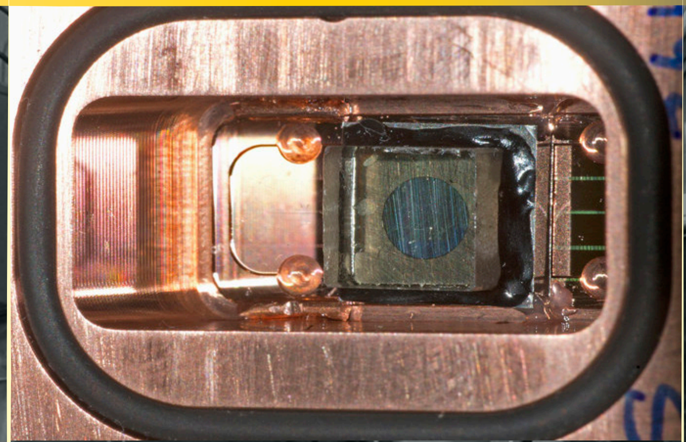
Yet, such advanced manufacturing methods require confidence in the performance of the material. If a process is different, will the material behave differently?

For additively manufactured (AM) materials or components to supplant conventional manufactured materials and processes, the certification and qualification paradigm needs to evolve, as there exists no standard additive manufacturing certified process or AM-material produced specifications.

To help develop that qualification and certification process, Los Alamos National Laboratory researchers in collaboration with the Institute for Shock Physics at Washington State University investigated[1] key microstructural parameters and defects that must be quantified and quantitatively linked to processing and equipment parameters to establish minimum performance properties. The work is part of a National Nuclear Security Administration initiative.

In a set of experiments, researchers compared 316 stainless steel (SS), a ubiquitous austenitic stainless steel often used in marine and medical environments, to 316L AM and to annealed wrought 316L. They discovered that the spall strength—the ability to resist chipping—of additively manufactured 316L SS was similar for the peak shock stress studied to that of annealed wrought or AM-316L SS following recrystallization.

1. "Structure/property (constitutive and dynamic strength/damage) characterization of additively manufactured 316L SS," *EPJ Web of Conferences* **94**, 02006 (2015).



Above: plutonium alpha-phase metal samples prepared for dynamic experiments at Sandia National Laboratories' Z machine are mirror-finished, 250-μm thick, 6-mm x 6-mm squares sandwiched between platinum sample holders and transparent lithium-fluorite windows, and mounted in Z target copper panels. The target assemblies are made at Los Alamos National Laboratory.

Los Alamos National Laboratory's ability to more fully understand the aging stockpile continues to rest in part on understanding delta phase plutonium-gallium alloy aging.

At right: a Los Alamos chemist uses an x-ray diffractometer loaded with a plutonium sample.

Background: a wide variety of actinide research and development is performed at Los Alamos's Plutonium Facility.

Science of plutonium aging

Answering questions critical to stockpile stewardship

Science-based stockpile stewardship is the U.S. policy that has enabled effective management of the nation's aging nuclear stockpile using leading-edge science and technology. Reusing aged components from current stockpile weapons makes good economic sense and is the current underlying theme of life extension programs (LEPs). But in the case of plutonium pits—the nuclear fuel inside a warhead that initiates a thermonuclear explosion—the use of aged pits for many decades beyond their original design lifetime raises a host of scientific questions.

"Pit reuse is now a certification 'grand challenge,' one of the most complicated we have ever faced," Los Alamos National Laboratory Director Charlie McMillan told employees in 2012.

Los Alamos National Laboratory's ability to more fully understand the aging stockpile continues to rest in part on understanding delta phase plutonium-gallium alloy (δ-Pu) aging—that is, to recognize the underlying physical and chemical processes and to predictively bound potential effects. Direct reuse of δ-Pu components, expected to be in service for many decades, requires physics and engineering performance assessments with firm scientific bases.

As such, significant concerns remain regarding aging of plutonium, to include surface chemical reactivity and corrosion, crystallographic phase and dimensional stability, and self-irradiation and daughter product ingrowth. For example, if δ-Pu behaves under irradiation conditions like austenitic structural steel, another metastable metal with face-centered cubic (fcc) crystalline structure, then when plutonium pits age these alloys could exhibit problematic void swelling and solute segregation leading to density reduction and phase instability, respectively. If this were currently the case, the United States would be focused on manufacturing and certifying new pits, rather than reusing old ones. And while evidence of these changes in δ-Pu have not been observed, the scientific explanation for this circumstance remains poorly understood. Furthermore, it is completely possible that changes in environmental and use conditions for aging pits or manufacturing changes in the chemistry and/or processing of new pits may introduce the mechanisms that initiate void swelling, phase instability, or a host of other problems. Therefore, it is necessary to develop a scientific-based experimental and theoretical capability that scales from atomic structure to bulk components and explores materials performance over a broad range of extreme conditions.

What we've learned about the aging material

For decades, scientists have studied how radioactive plutonium isotope α-particle decay inflicts self-radiation damage on host materials. However, plutonium metal, with its complex electronic structure, phase instabilities, and chemical reactivity, has proven to be a challenging system in which to access a microscopic view of radiation damage behavior. Thus, scientists haven't yet succeeded in validating theories of defect production, lattice recovery, and daughter product ingrowth—of special importance for plutonium-based materials used in nuclear weapons and nuclear reactors.

"Pit reuse is now a certification 'grand challenge,' one of the most complicated we have ever faced."

Los Alamos National Laboratory Director
Charlie McMillan

In 2000, Los Alamos and Lawrence Livermore national laboratories jointly initiated the Accelerated Aging of Plutonium Project within the Enhanced Surveillance Campaign to address the question of expected pit lifetime age and determine the necessity, timing, and capacity for a large Modern Pit Facility. Through the use of the shorter half-life isotope plutonium-238, researchers observed changes in four years that would otherwise require 60 years to evolve. While this extensive experimental project suggested a functional pit lifetime well beyond design based on physics performance, it did not elucidate the extent to which microscopic mechanisms can drive plutonium-aging-induced changes at a bulk scale.

Over the past decade, continuing efforts at Los Alamos and Livermore have sought to understand radiogenic processes in δ-Pu. These studies have revealed crystallographic and bulk distortions, helium bubble evolution, thermal expansion changes, mechanical strengthening and reduced ductility, damage-induced density decreases, and changes in compressibility and phase stability. A more fundamental understanding of defect formation and thermo-kinetic evolution is being developed to guide experimental and theoretical observations into a cohesive physical picture that is usable in age-aware models.

Tools, capabilities, and expertise

- Plutonium handling and characterization capabilities at Los Alamos
- Plutonium Facility at Los Alamos
- Los Alamos radiological facilities
- Z Pulsed Power Facility, Sandia National Laboratories
- Nevada National Security Site
- Joint Actinide Shock Physics Experimental Research Facility, Lawrence Livermore National Laboratory
- X-ray absorption fine-structure technique
- Supercomputer modeling

For example, Los Alamos and Livermore researchers in collaboration with Lawrence Berkeley National Laboratory addressed this knowledge gap by employing extended x-ray absorption fine-structure technique at the SLAC National Accelerator Laboratory, a national user facility. These researchers explored local structure damage introduced in the nascent state (i.e., the "frozen in" damaged state existing at extremely low temperatures with no defect thermal migration). They observed that δ-Pu held at temperatures less than 20 K for over two months accumulated more than 60 % elimination of fcc crystallinity. They witnessed that with time and increasing temperatures, the accumulated damage was mostly annealed by 300 K and that gallium atoms influence local structure differently than plutonium atoms in the crystalline recovery process. These experimental conditions were chosen to best understand the radiogenic energy deposition process occurring as damage accumulates in the lattice and the thermo-kinetics of damage recovery.

That's just one piece of the puzzle. Ultimately, such experiments will examine how damage accumulates as extensive local structure disruption with resultant electronic and vibrational changes impacting thermodynamic, structural, and electronic properties—giving scientists the means to develop and validate theories about aging δ-Pu and explain the absence of void swelling.

Physics performance questions to address

The annual National Nuclear Security Administration Stockpile Stewardship and Management Plan provides a thorough description of the national goals for the nuclear stockpile. In part, Defense Programs such as Science Campaigns have the goal of continued assessment of the potential effects of plutonium aging and their impacts on pit lifetimes and reuse.

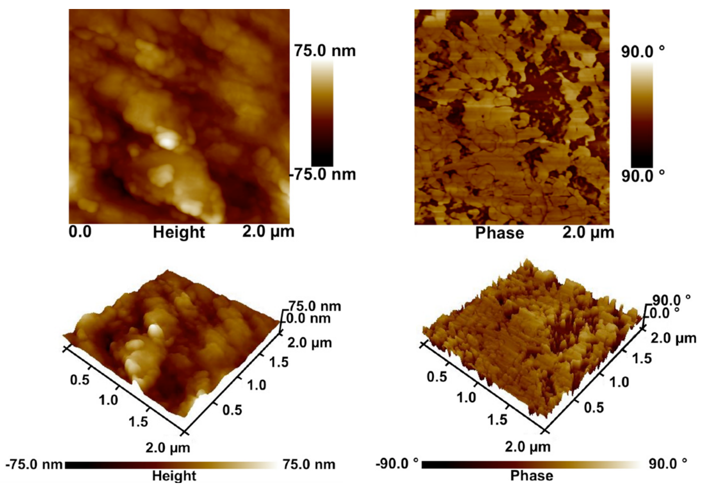
Current physics-based lifetime estimates for plutonium pits are approximately 100 years. These estimates were developed within a quantifying margins and uncertainties (QMU) formalism for primary physics performance. However, the physics models are not the complete composition of fundamental physics. The scientific work of understanding the effects of δ-Pu aging must continue; otherwise today's solution to the LEP could possibly be subject to unforeseen problems in the future.

Aging-related plutonium experiments and small-scale testing and characterization are conducted at Los Alamos's Plutonium Facility and its radiological facilities. Small-scale plutonium experiments play an extremely important role because they connect material structures and physics and chemical properties. Furthermore, experimental collaborations such as those with Sandia National Laboratories researchers on the Z machine have led to improved multiphase plutonium equations of state and strength measurements of new and aged plutonium materials. These data have been and will continue to be used in improving the fidelity of physics performance models.

Integral subcritical experimental collaborations between Los Alamos and Livermore conducted at the U1a facility of the Nevada National Security Site provide the tie between materials properties and component performance. Successful simulation of component performance depends upon small-scale experiments and model development. Expanding and building on such research provides the essential data and computational capabilities to support development and certification of advanced theories and models for nuclear weapon performance. Furthermore, materials data are also applied to validate models and simulation codes used to identify and develop new material options to support component reuse and LEPs.

In the future, as experimental platforms enable higher fidelity data collection over a greater variety of extreme conditions and computational capabilities facilitate better physics models, QMU determinations will become more predictive. Capabilities such as MaRIE are being established with the primary goal to understand the condition of the nuclear stockpile and to extend the life of U.S. nuclear warheads. MaRIE is Los Alamos's proposed experimental facility for the study of matter-radiation interactions in extremes. MaRIE will provide the ability to predict how microscale and mesoscale materials properties evolve under weapons-relevant extreme conditions (including aging) and impact performance, and the ability to predict the microstructure of new materials and materials resulting from new manufacturing processes and how this microstructure will affect weapons performance.

Ultimately, science-based stockpile stewardship requires the ability to provide validated predictive models of materials behavior in weapons-relevant regimes to support stockpile assessments and life extension program certification in the absence of nuclear testing.



The Laboratory recently established the first-ever scanning probe microscopy capabilities dedicated for plutonium surface studies. This effort is focused on both fundamental atomic-scale plutonium surface science investigations necessary to validate theoretical modeling codes and macroscopic signatures studies of plutonium surfaces relevant to the nuclear weapons engineering community. This capability enables techniques able to nondestructively produce three-dimensional surface topography images with nanometer-scale resolution in all three directions.

Above: three-dimensional atomic force microscopy height (corresponding to surface topography) and phase (representing surface mechanical properties) images of as-received δ-Pu<7at%Ga> taken simultaneously from the same region.

Los Alamos technique reveals how plutonium ages

Using the signature Los Alamos National Laboratory technique of resonant ultrasound spectroscopy (RUS), researchers here have achieved an important breakthrough in understanding the long-term stability of plutonium by recording essential measurements of the nuclear material's compressibility and its sensitivity to temperature and time. That information will refine the equation of state of plutonium, which describes its fundamental properties.

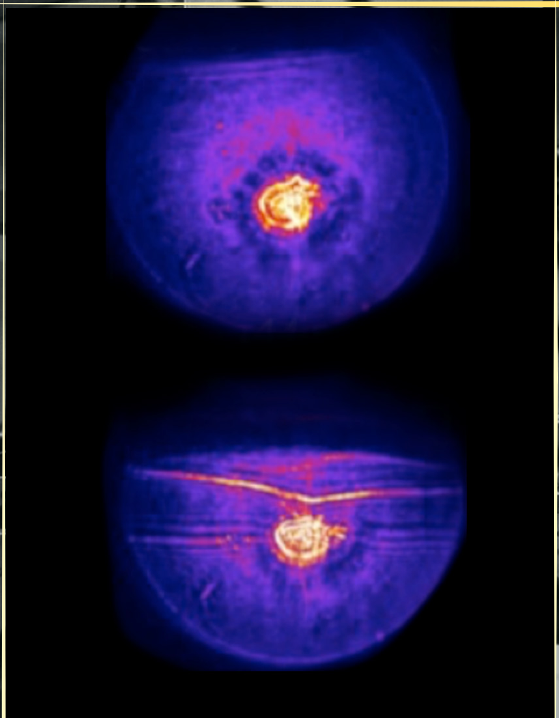
The new results will also improve the predictive codes used in weapons stockpile work, said Albert Migliori, director of the Seaborg Institute for Actinide Science, chair of the Los Alamos National Laboratory Energy Security Council, and Los Alamos National Laboratory Fellow.

The Los Alamos team is measuring the stiffness to hydrostatic compression, or bulk modulus, and the shear stiffness. Both moduli are fundamental thermodynamic quantities like heat capacity. "RUS has the greatest accuracy and most sensitivity of any elastic modulus measurement technique," Migliori said. "With RUS, we're producing, for the first time, quantitative and precise measurements of the change of compressibility of plutonium and its alloys with respect to both temperature and time," he said. "We can watch plutonium-239, similar to that used in the weapons alloy, age in real time over a period of weeks. So we're now engaged in very long-term experiments to look at aging as a function of temperature, of time, and of gallium content so we can provide quantitative baseline information to explain the aging of plutonium."

The work has implications for theoretical models of the electronic structure of plutonium. "We've found an important disconnect between many of the models of plutonium and the measurements we've taken," Migliori said. "The models fail to even get close to the temperature dependence of plutonium's compressibility. These measurements provide an important clue for theorists to go back to work on" as they calibrate the models.

Migliori pointed out that this RUS technique came from fundamental research at the Laboratory, an example of basic science informing the weapons program."It shows how the support of fundamental science at Los Alamos directly benefits the weapons program," he said.

This custom resonant ultrasound spectroscopy stage, designed and manufactured by Los Alamos researchers, exerts minimal stress on the sample while holding it in a stable position for the required long-term measurements. The sample can be measured from 10–700 K. By using a cryogen-free refrigerator, the team is able to make the required long-term measurements.



At left: dynamic x-ray image of void collapse in shocked explosive. The void (bright spot in the center) collapses as the shock wave passes through it. These first in situ images of void collapse in explosives demonstrate a crucial diagnostic for studying how voids affect explosives under shock loading.

Background: Los Alamos has been integral to leading ultrafast dynamic gas gun and contained firing operations at Argonne National Laboratory's Advanced Photon Source. These activities require the Lab's excellence in operational safety and experimental expertise to synchronize the experiment to the beam and the diagnostics.

Below: a Los Alamos explosives scientist demonstrates a flame test to a group of explosive ordnance disposal technicians taking part in the Laboratory's Advanced Homemade Explosives Course. The class made a small batch of an explosive often used in improvised detonators. Exposing a few grams to flame and observing how the substance ignites helps the techs identify it and determine its sensitivity.

Research with high explosives

Designing for performance, safety, and response prediction

Explosives are integral to nuclear and conventional weapons, and are central in many evolving global security issues. The Laboratory has been establishing a new generation of explosive materials and experiments driven by weapons program needs and that will define the materials and predictive tools for the future of the weapons program.

Understanding the intrinsic physical and chemical phenomena governing explosive responses has been a significant challenge for many years due to the extreme time scales, temperatures, and pressures occurring in a detonation. Given the consequences of intentional and unintentional explosive response, there is a constant desire for improvements to the understanding of explosives. More accurate prediction of explosive responses in any scenario remains imperative.

Recent advances in materials and diagnostics have been revolutionary in revealing answers to long-standing questions in explosives. Future diagnostic tools will allow both design of explosives for specific performance and safety and prediction of explosive responses with accuracies never before possible.

"Explosive performance and safety are critical: the explosives need to function and do the work they are designed to do when they are used intentionally, and simultaneously have very predictable safety in any other circumstance," said Los Alamos Explosives Center Director Dan Hooks. Both of these properties have links to microstructural details of explosives, and prediction of both performance and safety have had limitations due to unknown physical and chemical processes in the materials. "Without nuclear testing, it is imperative that we understand each individual physical process in each of these materials. In revealing this physics and chemistry, we also enable the design of better, safer explosives, and make possible large advances in global security, saving lives every day," he said.

"Explosive performance and safety are critical: the explosives need to function and do the work they are designed to do when they are used intentionally, and simultaneously have very predictable safety in any other circumstance."

Los Alamos Explosives Center Director
Dan Hooks

In explosives performance, one long-standing unknown has been how explosives ignite in intentional use. This ignition mechanism is not fully understood at any level—molecular to microstructural. Los Alamos researchers recently designed new materials at the molecular level to receive specific input stimuli to begin detonation. Researchers also performed experiments revealing for the first time the fundamental ignition process in detonators. More broadly, researchers have directly observed the process of microstructural void collapse, theorized since the 1960s as the literal "hot" spots that enable ignition and spreading of reaction to become detonation in explosive materials. Using the x-ray free electron laser at the Linac Coherent Light Source at the SLAC National Accelerator Laboratory, Los Alamos scientists dynamically imaged a 10-μm-diameter shocked void collapse in single crystal PETN (see image, page 16) while simultaneously taking x-ray diffraction data.

Hammer testing of a small amount of homemade explosive. This is a qualitative test to assess the sensitivity of a material to mechanical insult.

Tools, capabilities, and expertise

- Characterizing homemade explosives
- Determining explosive lethality and vulnerabilities
- Developing techniques and technologies to defeat explosives threats
- Determining the short-and long-term effects of explosives aging
- Operations, characterization, and firing with explosives and radiological materials in contact
- Performing core surveillance
- Analyzing blast effects as well as potential mitigation
- Characterizing shock and detonation physics properties of materials
- Open-air and confined firing with many types of diagnostics
- Gas and powder guns
- Flash x-rays, high-speed cameras, interferometric techniques, magnetic gauging, pyrometry, and many more diagnostics
- Research- and pilot-plant scale formulation, powder production, pressing, crystallization, and casting
- Production facility for war reserve detonators, detonator R&D
- Synthetic and analytical chemistry
- Mechanical properties testing
- Thermal response
- Microstructural characterization
- Shock and nonshock initiation
- Dual-Axis Radiographic Hydrodynamic Test Facility
- Proton Radiography Facility
- Manual Lujan Jr. Neutron Scattering Center
- Center for Integrated Nanotechnologies
- Materials Science Laboratory
- National High Magnetic Field Laboratory

Understanding these phenomena will allow the development of a theory of ignition and capture that in a representative way in future models, thereby making prediction of intentional use and unintentional insults possible in ways never before possible. Furthermore, understanding of these phenomena is important to current ongoing efforts to replace "insensitive" explosives in the current U.S. stockpile and to implement safer materials in the future.

Recent advances in imaging and diagnostics have allowed for fundamental measurements in mesoscale solid mechanics, explosive initiation mechanisms, and reactant and product equation of state (EOS)—the evolution of gases from the explosive solid. EOS is critically important to accurate predictions of the work explosives do on their surroundings upon detonation. Recently, Los Alamos researchers made significant refinements to the understanding of both the solid and gas states. Additionally, fundamental measurements to anchor the EOS of the starting solids by many techniques, defining the limits of accuracy and error, were performed. Important developments in both gas gun and laser shock platforms to observe the chemical reactions of a wide range of materials across orders of magnitude variation in time and length scales were part of the research. Recent joint experiments with Lawrence Livermore National Laboratory researchers at Argonne National Laboratory's Advanced Photon Source have been examining fast and slow energy release from detonation product evolution in insensitive high explosives. Slow energy release is due to carbon forming clusters in the hot, high-pressure mixture of product gases, and understanding carbon clustering is essential for accurate modeling of detonation products. Experimentalists recently used small-angle x-ray scattering to provide real-time structural details of carbon clustering forming during the detonation of PBX 9502, Los Alamos's insensitive high explosive charge in use on the B61-12 Life Extension Program.

Safety predictions are also imperative for the stockpile. Accurately answering the question of what happens when an explosive is subjected to an adverse environment, such as a thermal environment, is critical to providing a safe and secure stockpile. "There is almost no limit to the type of 'what if?' questions that need to be answered," Hooks said.

In adverse thermal environments the response of high explosives can span time scales from nanoseconds to hours and is dependent upon the heating profile applied to the material. Recent radiographic experiments have been used to directly observe energetic material response to heating. The reaction of several explosives to heat, spanning slow burning to detonation, has been characterized and these parameters are being incorporated into predictive models. The vast collection of data will be used to constrain models and remove current approximations from how predictions are made.

For broader global security challenges, the science of the nuclear mission makes it possible to address many other threats. There is a growing demand for the development of novel explosives and/or replacement materials that are insensitive to conventional stimuli such as spark, impact, and friction or are motivated by special applications. For the stockpile, this demand is driven by the constant desire for increased safety and security.

A new generation of advanced energetic materials is required for all missions. Replacement materials for the future will be different than materials of the past—even those that are purely replacements—due to changes in sources, methods, and environmental standards. If replacement materials are different, and many new materials offer significant improvements to safety, security, manufacturing consistency, environmental factors, and many more considerations, it is important to provide those options.

New materials of the future will have desired form and function such as performance, sensitivity, and possibly microstructure. Among many new ideas to prepare next-generation explosive materials, co-crystals represent a new method for developing explosive materials with desired properties whereby different explosive molecules are combined at the molecular level to form solids with properties that differ from the parent materials. These materials represent a new path towards producing high-performance, low-sensitivity explosives. Furthermore, new technologies offer wholly new ways to make explosive materials, and these methods offer improvements to what is envisioned as possible in explosive properties. Explosives with specifically defined structures could allow for energetic material property control as never before. Additive manufacturing of explosives could provide control over internal structures of components at a level impossible to achieve through traditional machining techniques.

Subcritical experiments ensure stockpile's reliability

Every year, the directors of the three Department of Energy weapons laboratories—Los Alamos National Laboratory, Lawrence Livermore National Laboratory, and Sandia National Laboratories—are required by law to write a letter to the President assessing whether the weapons in the U.S. nuclear stockpile are safe, secure, and effective. Since 1992, when the United States ceased testing nuclear weapons, those assurances have rested on highly advanced computer models and simulations of nuclear detonations and on data acquired by the laboratories from an extensive suite of experiments, including from a unique set of real-world tests called subcritical experiments.

A nuclear weapon uses a high explosive blast to compress plutonium into a critical mass, which means the material becomes dense enough to trigger a self-sustaining chain reaction of nuclear fission. In a two-stage process that starts with confirmatory tests, subcritical experiments are the best–and only–way to put plutonium and high explosives together in a real-world test mimicking important aspects of nuclear detonation. That verisimilitude allows researchers to validate and expand the computer simulations backing up design enhancements to existing weapons and their ongoing effectiveness.

Los Alamos is in the midst of a new series of experiments at the Nevada National Security Site. The 2014 Leda experiment tested high explosives compressing a heavy metal surrogate for plutonium. Information from that experiment and follow-on confirmatory experiments in the new Lyra series will inform the planning for a subcritical experiment with classified "weapons-relevant" plutonium materials. High-tech diagnostic equipment will capture how the plutonium behaves under the high temperature, pressure, and radiation levels created by the implosion of the surrounding high explosives.

These experiments probe and challenge researchers' understanding about plutonium as it is driven by high explosives. That understanding helps hold the computer codes and models to experimental reality, which supports confidence in the stockpile as it continues to evolve.

A National Security Technology (NSTec) researcher tests one of several multiplexed photonic Doppler velocimetry systems underground in Nevada. The close collaboration of Los Alamos and NSTec ensures acquisition of high-quality data under challenging experimental conditions.

Enhanced imaging for dynamic physics research

Invented at Los Alamos National Laboratory, proton radiography employs a high-energy proton beam to image the properties and behavior of materials driven by high explosives. The penetrating power of high-energy protons, like that of x-rays, makes them an excellent probe of a wide range of materials under extreme pressures, strains, and strain rates.

Using the 800-MeV proton beam generated by the Los Alamos Neutron Science Center (LANSCE) linear accelerator, the Laboratory's Proton Radiography national user facility provides access to a one-of-a-kind tool for dynamic materials studies, giving users a better understanding of the science and engineering of materials under extreme conditions. This information helps Los Alamos maintain the reliability of the U.S. nuclear stockpile.

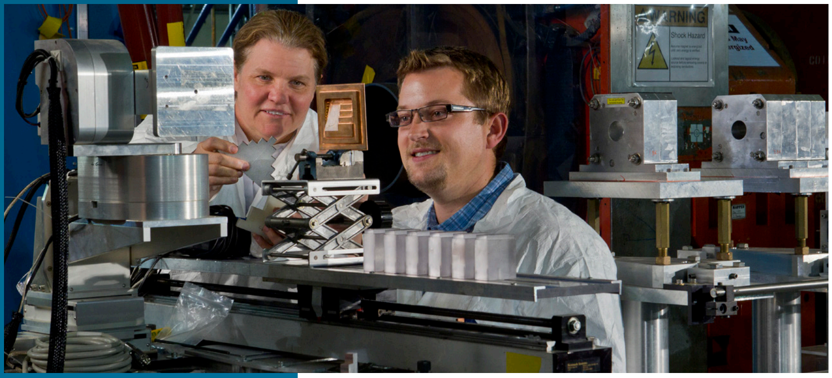
Recently, researchers successfully installed and operated a new and improved high-speed imaging system designed for dynamic experimental studies. These advances significantly enhance proton radiography capabilities for users in the materials and shock physics communities. The technology features excellent contrast and the capability to radiograph dynamic events on short time scales (e.g., a few microseconds) multiple times during its evolution. With the LANSCE accelerator's capabilities, the number of radiographs is limited only by the camera technology. The large-format, 10-frame hybridized focal plane array design of the new imaging system, slated to replace an earlier 3-frame design, allows experimenters more than 40 radiographs per event as opposed to the 21 provided in the current system, and with fewer cameras.

The invention of proton radiography is the direct result of the synergy between the Laboratory's defense mission and basic science research scientists and supports the Laboratory's national security science mission as well as provides for fundamental science discoveries. The proton radiography capability is primarily supported by the National Nuclear Security Administration Science Campaigns.

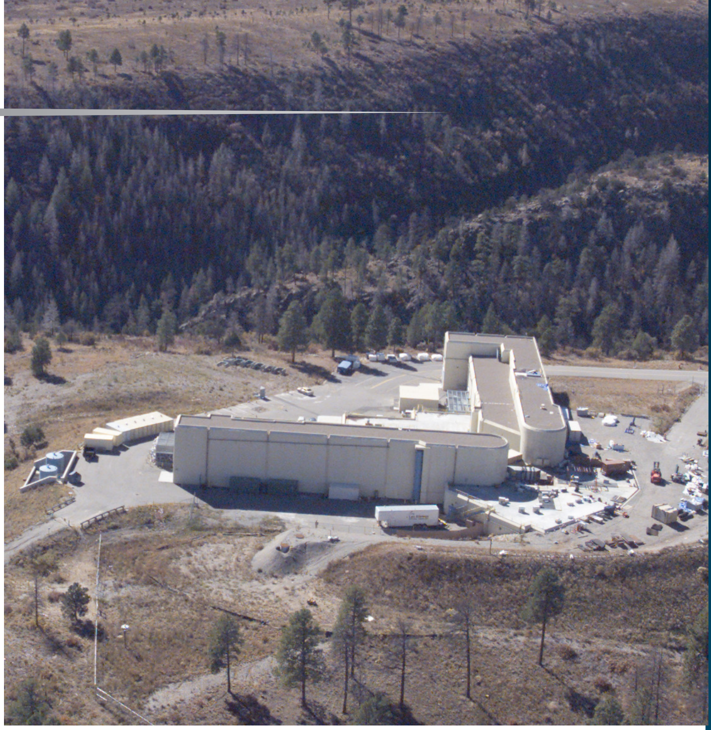
All of the high explosive stockpile focused research—how explosives work and new ways to think about what is possible—has important application to everyday safety. The global security environment of the 21st century is highly dynamic and requires that Los Alamos researchers are responding with critical technologies.

The materials used in terrorist explosive devices are readily available. Homemade explosives are optimal for terrorists because of the inexpensive and unregulated starting chemical precursors. Los Alamos's explosives capabilities allow for evaluation of many threats, and this expertise is regularly exercised. The Laboratory provides training for deploying explosive ordnance disposal technicians that focuses on the safety, sensitivity, and the critical thinking necessary when dealing with these types of explosives, which are sometimes sensitive and unpredictable (see images, pages 16 and 17).

Explosive detection capabilities have excelled over the past 10-15 years due to the demand for quick screening methods to identify threat explosive materials. Recently, Los Alamos developed novel explosive detection techniques, such as MagRay (magnetic resonance imaging- x-ray) and ODD-Ex (optimal dynamic detection of explosives), which might have future applications for homeland security and defense—and may just feed back to the stockpile in developing more active techniques for assessing the health of stockpile materials.



Los Alamos researchers prepare an experiment in the Proton Radiography Facility, where more than 500 dynamic experiments have been performed in support of the weapons program, global security, and other customers since it was commissioned more than a decade ago.



The Dual-Axis Radiographic Hydrodynamic Test Facility at Los Alamos is used to analyze mockups of nuclear weapons.

A shot built from a three-dimensional-printed high explosive part.

Verifying weapons-related computer codes without nuclear testing

The Dual-Axis Radiographic Hydrodynamic Test Facility (DARHT) at Los Alamos is perhaps one of the most impressive firing sites ever built for explosively driven dynamic experiments. Los Alamos scientists built DARHT, the world's most powerful x-ray machine, to analyze mockups of nuclear weapons.

DARHT's two accelerator-based x-ray machines penetrate objects with densities exceeding the center of the earth and with features moving faster than 10,000 miles per hour. At the firing point, where the centerlines of DARHT's two linear induction accelerators converge, sits a spherical confinement vessel containing the materials released during the nonnuclear hydrodynamics experiment. There, surrogates for actual nuclear weapons materials and other components are explosively compressed to the point where they become hot enough to flow like water—thus the name "hydrotest" sometimes used to describe this full-scale mock implosion.

DARHT is a key NNSA (National Nuclear Security Administration) resource for validating nuclear weapon performance simulation codes through its ability to produce high-resolution radiographs of high-density explosively driven experiments at full weapons scale.

As the first facility able to capture multiple, high-resolution images of dynamic, dense-object hydrodynamics experiments, DARHT lends considerable confidence to the computer models the labs use to certify the stockpile to the President of the United States. Delivering five x-ray images from two different angles, DARHT allows Los Alamos and Lawrence Livermore national laboratory scientists to check the implosion symmetry of mock weapon components, observe the time-resolved nature of the implosion, and benchmark supercomputer-based assessments of the actual nuclear weapon.

MaRIE, Los Alamos's proposed experimental facility for time-dependent materials science at the mesoscale, would complement the capabilities of DARHT with x-ray and charged-particle probes revealing fundamental physics operating at the micron, or mesoscale.

On the other end of the spectrum, the Enhanced Capabilities for Subcritical Experiments project at the Nevada National Security Site will be a critical tool to continue to meet requirements without nuclear testing.

Comprehensive energetic materials development, characterization, and testing are key strengths at Los Alamos National Laboratory. An experimental explosive is shown igniting during small-scale impact testing.

Los Alamos firing capabilities and diagnostics in explosives science

Activity at Los Alamos National Laboratory's 12 firing sites—facilities where researchers detonate high explosives—has peaked since the Laboratory invested millions of dollars into extensive site renovations and state-of-the-art data acquisition equipment, including flash x-ray equipment, high-speed cameras, and photon Doppler velocimetry. The upgrades were spurred by the continual demand for better data from experiments, in less time and with fewer interruptions due to inclement weather. Such experiments answer important weapons science questions, support stockpile maintenance programs, and address other national security challenges involving explosives performance.

Recently, the high-profile Phoenix experiments, led by Lawrence Livermore National Laboratory, were moved in a collaborative effort with Los Alamos to a firing site in Ancho Canyon to take advantage of its unique capabilities. Packed with more than 800 pounds of conventional explosives, Phoenix's first shot delivered one of the most vigorous detonations in recent experience. These experiments will provide unique physics performance data for the weapons program.

Los Alamos firing sites serve a variety of objectives, from inventing new explosives, to understanding how explosives work, to qualifying weapon parts.

The materials being studied in the extreme conditions created at these firing sites vary. In focused experiments, it might be a piece of metal driven by explosives, with the aim of isolating a particular physics phenomena—like how a material responds to the high explosive shock wave—or to better understand the explosive detonation process. Other times, it's a complete weapons system mock-up without the fissile material.

Cygnus mound (before)

Cygnus mound (after)

Outdoor firing is a unique Los Alamos National Laboratory capability.

Marked with "Caution: High Noise Levels" signs, the Laboratory's firing sites have military-style bunkers, volleyball-court-like sand piles for firing mounds, and small- and large-caliber guns. Many have names from another era, like Daisy Mae, Dogpatch, and Lower Slobbovia from the Li'l Abner comic strip.

Los Alamos's diversity of testing capabilities is an important resource for other National Nuclear Security Administration laboratories. Sandia National Laboratories relies on experiments conducted at Los Alamos to perform engineering qualification tests and assess the impact of certain new or modified weapon parts. Lawrence Livermore National Laboratory brings experiments to the Dual-Axis Radiographic Hydrodynamic Test Facility, an open-air firing site, to validate weapons performance without nuclear testing (see "Verifying weapons-related computer codes without nuclear testing," page 21). The Pantex Plant in Texas, where nuclear weapons are assembled and disassembled, looks to explosives research at Los Alamos to help answer safety questions important for protecting workers.

Ten firing sites are located outdoors, in the pine forests and canyons of Laboratory property. During the Lab's ongoing revitalization project, all open-air firing sites were gutted of old equipment, cleaned of legacy waste, and given new berms and fencing. The Ector firing mound, when configured as defined in the "Vegas" Project, for example, is a new vessel-confined configuration to allow safe firing operations during red flag and stage 3 wild fire restrictions or adverse weather.

Two firing sites are indoor firing facilities: the Proton Radiography Facility at the Los Alamos Neutron Science Center and Chamber 8 at Technical Area 40. Strategic plans call for more indoor firing capabilities, which can muffle earthshaking explosions and operate in adverse weather conditions.

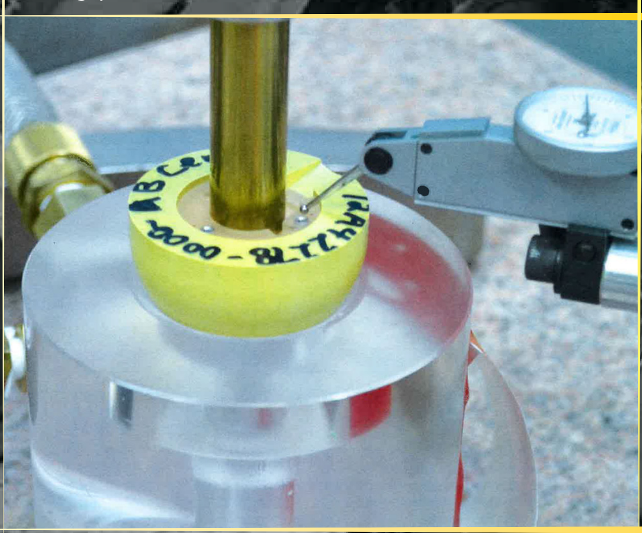
Tests at the firing sites help Los Alamos determine year after year whether the B61, W76, W78, and W88—and their components—are safe and will work as intended, or if it's time to manufacture replacement parts. The B61 Life Extension Program and the Los Alamos Weapons Directorate funded the restoration of an abandoned firing site, which now features two standalone firing mounds instead of one, a new shot racking system, and a new camera house.

The firing sites are part of a full-spectrum explosives science effort across the Laboratory. For more details about these efforts, see the story on page 16.

At right: centrifuge for testing materials and engineering response design under re-entry conditions (high G force). The first live high explosives test was completed in 2016.

Background: diagnostics connections being made to an explosives device via confinement vessel feedthroughs.

Below: high explosive assembly, held in a vacuum fixture. Potting material is used to seal gaps.



Material engineering

Evaluating options, informing decisions for possible stockpile changes

Imagine advanced nuclear materials with built-in security, rendering the material useless, or engineered weapon materials that predictably change color as they deteriorate. Imagine new materials guaranteed to be identical in every way, even as they age, as the certified original legacy weapons materials.

Such a material would solve a "sticky" problem being faced right now. An adhesive used for decades in assembling weapons is no longer being manufactured, and finding a suitable substitution isn't a straightforward matter. Despite the small amounts used of this adhesive, its performance details, especially extrapolated over decades, are critical to certifying the weapon as safe and reliable.

As the Laboratory advances the stockpile—with safer, more secure, more reliable performance, while incorporating increased efficiency in production, surveillance, and maintenance of the weapons themselves—materials science is an important contributor towards that advancement.

Materials engineers must evaluate existing performance data from previous qualification and aging studies, and then design and execute experiments sufficient to provide confidence in the selection of an alternate material. The nation can't afford to assume any change in materials or processes or equipment is too subtle to discount, and Los Alamos researchers must assess and validate that material changes don't negatively impact safety, performance, or reliability of the materials, components, and systems utilizing the alternative material.

Los Alamos National Laboratory is the Design Agency for the nuclear explosives packages in four of the nation's seven nuclear weapon systems, the W76, W88, B61, and W78. The Design Agency role requires that Los Alamos also qualify the manufacturing processes for the parts made at the National Security Campus (Kansas City Plant), Y-12 National Security Complex, and the Savannah River Site, and how the components are assembled into weapons systems (and disassembled) at the Pantex Plant. Any new production technologies, materials, and processes are evaluated by Los Alamos before they are deployed at the Production Agencies.

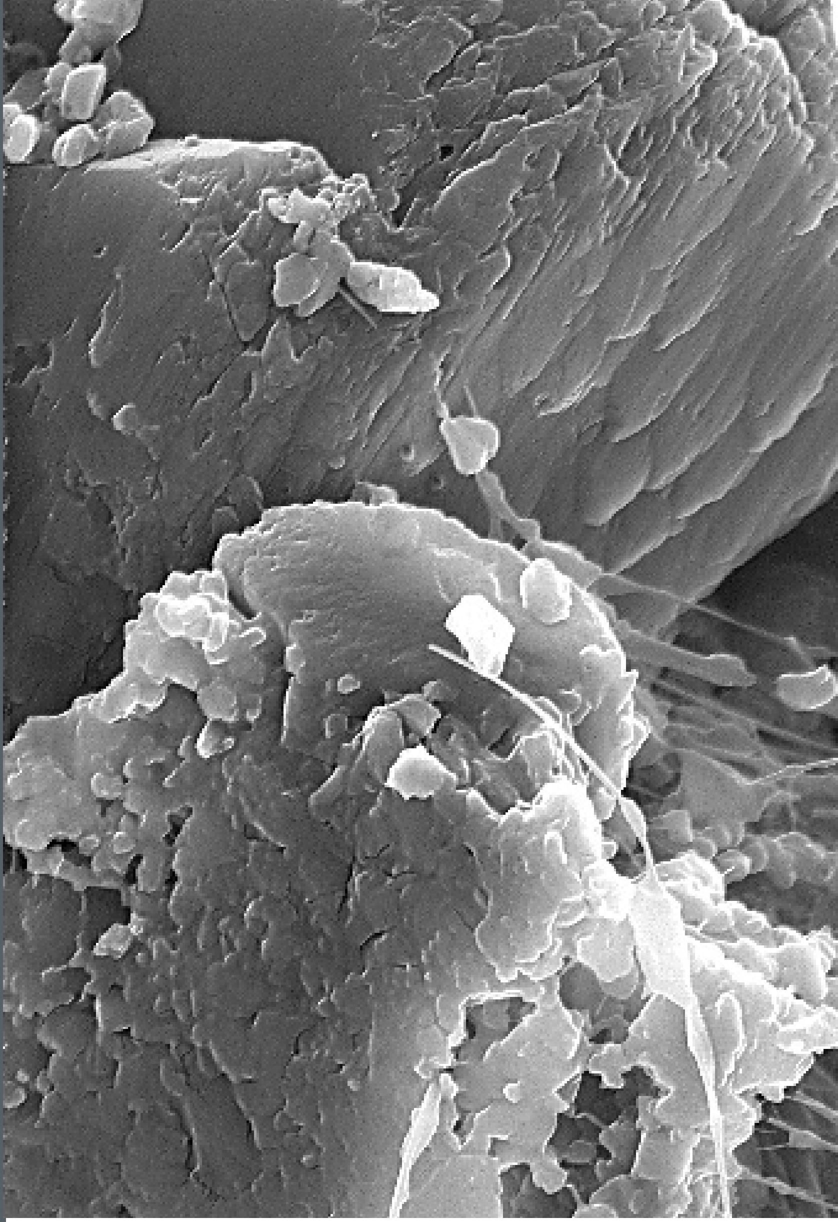
When engineers design a bridge, they must quantify the risk that the bridge could fail. Likewise, weapons engineers and scientists strive to understand the margins and uncertainty of materials and designs in order to support nuclear stockpile decision-making. While establishing how one component will perform at one point in time is relatively simple, defining margins of uncertainty (i.e., how far away from failure is the material/component) for that component—or for the entire weapon assembly—over a decades-long time span is daunting. The answer lies in a full understanding of the materials' properties under the conditions the materials will experience in the weapons' life cycle and in our confidence regarding how far away the material/component is from its failure boundary.

Currently, the Los Alamos weapons program's busiest efforts revolve around the B61 and W88 programs as changes are being introduced to those systems, partly to account for the material challenges through life extension and alterations. But with change also comes opportunity to transform the future stockpile—a challenge for Los Alamos engineers and scientists to embrace and drive. Materials science is an important contributor towards that advancement.

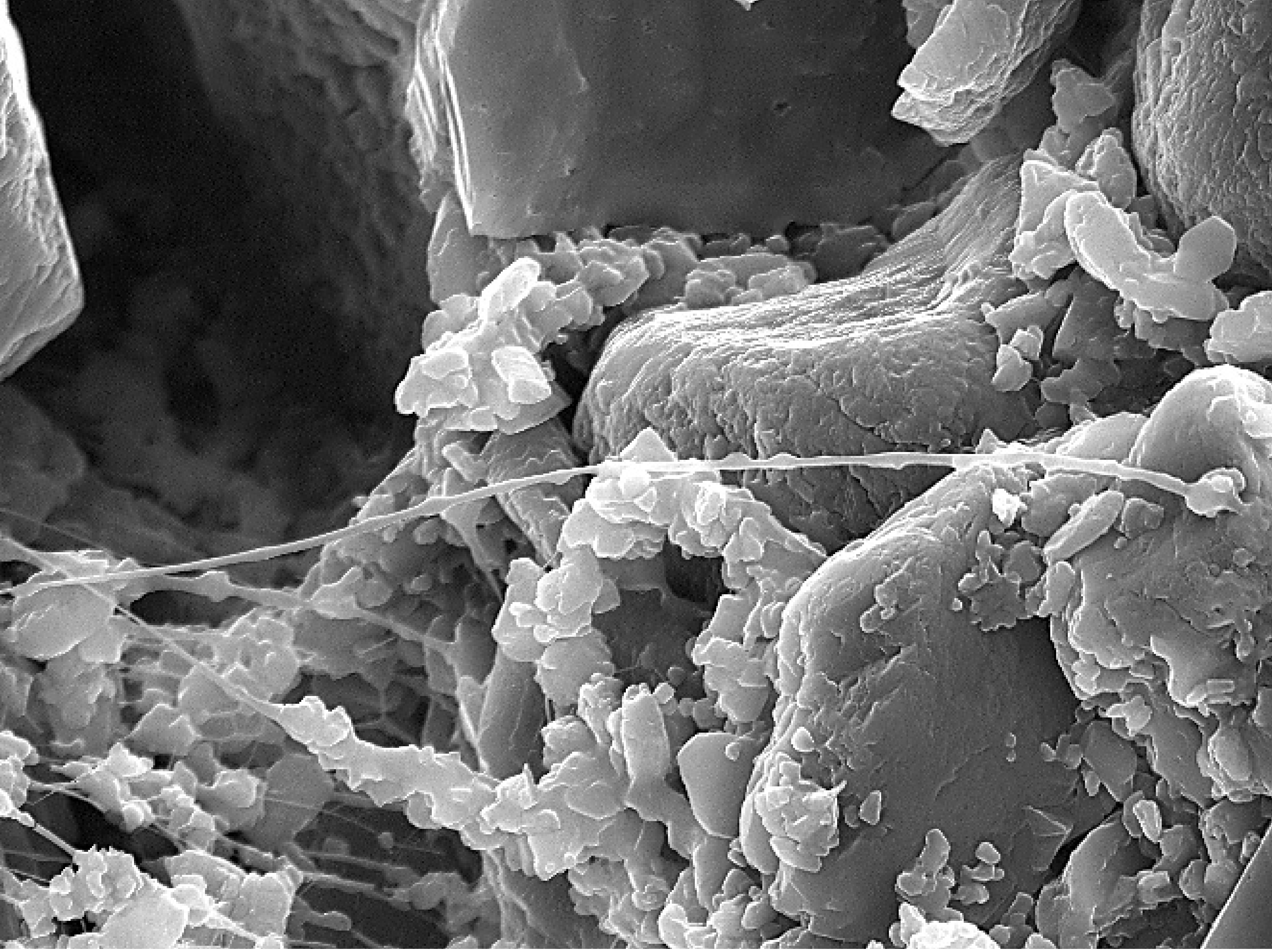
To achieve materials with controlled, predictable functionality, Los Alamos must measure weapon materials and component behaviors under conditions truly representative of stockpile conditions, and beyond the boundaries of those temperature, pressure, vibration, shock, and high mechanical loading conditions—a challenge in and of itself. The resultant data can then inform and validate predictive material and component computer models to increase our confidence in weapon system performance. The models will need to incorporate firm understandings of the most basic material properties at very small scales under these stressing environments.

Tools, capabilities, and expertise

- Unique experimental synthesis and data gathering facilities, including
    - Plutonium Facility
    - Radiological Laboratory/Utility/Office Building
    - Dual-Axis Radiographic Hydrodynamic Test Facility
    - Los Alamos Neutron Science Center
    - Materials Science Laboratory
    - Target Fabrication Facility
    - Sigma Complex
    - Weapons Engineering Tritium Facility
    - High-performance supercomputing
- High explosives, polymer, ceramics, and metallic characterization facilities/equipment/techniques
    - plutonium, uranium, beryllium, and tritium
    - weapons materials processing in support of development activities at production plants
    - permitted intentional detonation of high explosives coupled with radioactive components
    - fabrication and assembly of unique, prototype components
- High energy x-ray, proton, and neutron radiography (dynamic and computed tomography)
- Environmental testing, including thermal, shock, vibration, centrifuge (high g loads), blast tube (hostile environments)
- Process-structure-properties-performance relationship studies of nuclear weapon materials with capabilities in
    - corrosion, interfaces, and electrochemistry; casting/rolling, forming/machining; powder metallurgy; welding and joining
    - polymer and aging R&D; high-energy-density target design and fabrication; materials characterization and forensics; surface science and coatings
    - multiscale materials modeling; science of defects in materials; crystal growth and material preparation; dynamic materials properties
    - dynamic testing; metallography and microscopy; surface science
    - materials chemistry including high explosives, advanced separation technologies, actinides
    - hazardous and radiological materials, air sensitive materials
    - nanomaterials synthesis
    - integrated process modeling
    - high-performance computing



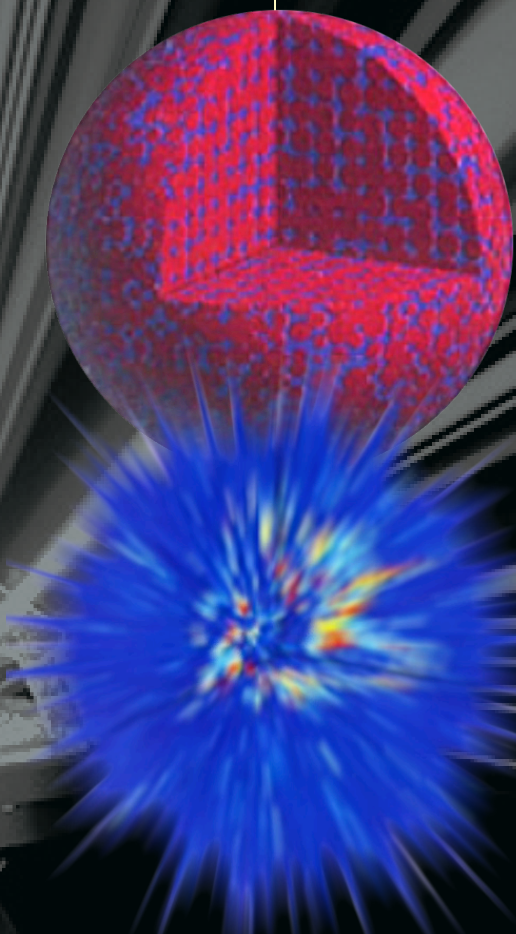
Fibrils of binder extend across a crack in PBX 9501 (a highly filled composite material).



Experimental preparation for blast tube and device catch system.

Above: foam target for an OMEGA experiment. The capsule diameter is approximately 1.7 mm.

Background: using multiplexed photonic Doppler velocimetry, the Laboratory measures the shock physics properties of metal in unprecedented detail and resolution, gaining deeper insights as it reports on the condition of the nuclear deterrent and considers reusing older systems without nuclear testing. The technique also can be used for the vibrational analysis of auto and aircraft systems.



Above: three-dimensional simulation of a National Ignition Facility experimental capsule.

Tools, capabilities, and expertise

- High-energy-density physics research
- Nuclear diagnostics
- Advanced physics codes
- Designing burning plasma devices
- High-energy-density physics databases
- Mixing and turbulence research
- Nuclear instrumentation (neutron imaging, gamma rays to measure time of peak neutron production, yield, density of capsule material)
- Target fabrication
- National Ignition Facility

High-energy-density physics research

Observing materials in extremes to improve weapons models

High-energy-density physics studies the behavior of matter at extreme conditions with pressures above 1 million atmospheres, temperatures above 1 million degrees, and densities that can be many times solid density of a normal solid material. Lasting only billionths of a second, high-energy-density experiments give Los Alamos scientists an opportunity to glean insights into the science of nuclear weapons not possible without nuclear testing.

Since the 1970s, Los Alamos's experimental capabilities, diagnostics, and analytical tools have addressed fundamental high-energy-density physics questions and helped develop and improve weapons models. The Lab's technical expertise in target fabrication, assembly, and characterization; precision machining; and foam development for experiments is instrumental in executing experiments at Lawrence Livermore National Laboratory's National Ignition Facility (NIF) and the University of Rochester's OMEGA Laser Facility designed to support validation and improvements of Advanced Simulation and Computing codes, which Los Alamos uses to predict the behavior of the stockpile.

The grand science challenge is to achieve ignition (producing more energy than what was put in to initiate the fusion reaction) and thermonuclear fusion in the lab, akin to recreating all the phenomena at the core of a nuclear device. The resulting high-energy-density experiments are producing valuable weapons stewardship information. All attempts at ignition have been unsuccessful to date.

Burning plasma research

At NIF and OMEGA, Los Alamos researchers are creating plasma both hot and dense enough to cause deuterium-tritium (the fuel source) to "burn"—that is, undergo thermonuclear fusion—inside a compressed capsule, spawning a neutron and an alpha particle that heat the plasma and set off a runaway reaction that liberates the nuclear energy in the fuel. The work draws on the Lab's vast experience in the design of burning plasma devices, advanced physics codes, and experimental techniques.

High-energy-density physics experiments

Another class of experiments is intended to guide development and validation of stockpile stewardship-science computer codes, to validate those codes, and explore new physics. Such high-energy-density experiments seek to understand specific physics in a more fundamental, rather than integrated, manner. Los Alamos designed an experiment at OMEGA to study radiation propagation through matter by directing a radiation wave down a foam-filled tube. By tailoring the foam density and the radiation temperature, the radiation wave can be faster or slower than the speed of sound, or about the same speed as sound. The physical laws governing each regime are different, and so test the researchers' models and codes.

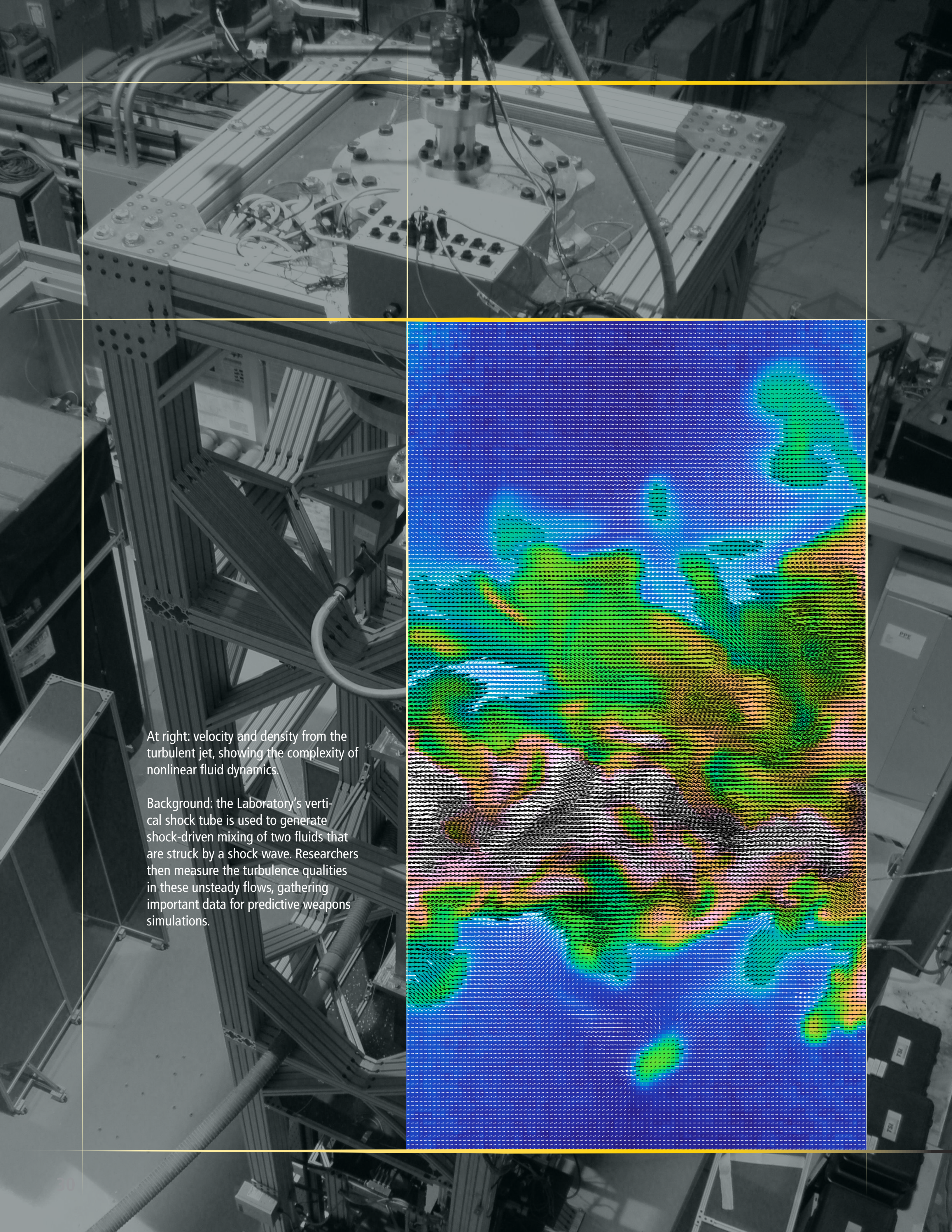
Turbulent mixing is a complication in inertial confinement fusion because bumps or flaws that develop during the implosion will expand and cause metal to mix with fuel, impeding the heating process and perhaps snuffing out the fusion burn. To study thermonuclear burn in heterogeneously mixed materials, Los Alamos is experimenting with foam-filled capsules containing pure tritium gas to measure the effect in a more controlled fashion than high-yield platforms allow. In another, more fundamental, mixing experiment researchers are creating extreme shear flows in the high-energy-density regime, beyond conditions—such as temperature, density, shock speeds, and plasma conditions—studied in previous turbulence research.

Nuclear diagnostics

A strength of Los Alamos National Laboratory is its breadth of nuclear instrumentation and knowledge and its flexibility in applying these techniques to new problems. For example, Los Alamos developed two powerful technologies in the 1970s and 1980s for underground nuclear tests. The Laboratory is now successfully collecting data on every neutron-producing experiment at the National Ignition Facility using these techniques.

In one instrument, two images of neutrons inside an inertial confinement fusion capsule are taken using an array of pinholes machined into a piece of tungsten and a scintillator that converts neutrons to light, which is then captured by a high-resolution camera. The first image shows neutrons emitted directly by the fusing deuterium-tritium fuel, known as the hot spot. The second image shows neutrons scattered by the colder, denser fuel surrounding the hot spot. By superimposing the two images, scientists get a three-dimensional view from which the size and shape of a burning plasma can be measured and compared with code simulations of the experiment.

The second instrument employs gamma rays, either created from neutrons colliding with atoms near the hot spot or from the deuterium-tritium reaction itself, to measure quantities needed to constrain computer simulations of the capsule implosion. Scientists obtain data about the time of peak neutron production, the total neutron yield, and the density of the capsule material after the capsule is imploded.



At right: velocity and density from the turbulent jet, showing the complexity of nonlinear fluid dynamics.

Background: the Laboratory's vertical shock tube is used to generate shock-driven mixing of two fluids that are struck by a shock wave. Researchers then measure the turbulence qualities in these unsteady flows, gathering important data for predictive weapons simulations.

Turbulence and mixing

Advancing physics for predictive weapons simulations

Anyone who has seen clouds resembling crashing waves has caught a glimpse of large-scale fluid instabilities. Known as Kelvin-Helmholtz clouds, they form from the instability produced when air layers of differing densities and speeds drift past each other.

When two fluids−liquid or gas−mix, similar wave structures appear. If the mixing occurs slowly, the physics is fairly easy to explain.

Scientists know less about turbulent mixing—those chaotic property changes arising spontaneously as two fluids mix in extreme conditions, such as the high-speed, high-energy environment of nuclear weapons.

As a result, Los Alamos is one of the few places in the world where scientists study mixing and turbulence in extreme environments—from the smallest scales in inertial confinement fusion capsules to the largest scales of supernova explosions—in an interdisciplinary combination of experiments, theory, modeling, and numerical simulations. The need to simulate and predict the performance of the nation's nuclear weapons stockpile drives the science. Predicting the performance is a multi-physics challenge, requiring a full understanding of each underlying physical process, including turbulent mixing.

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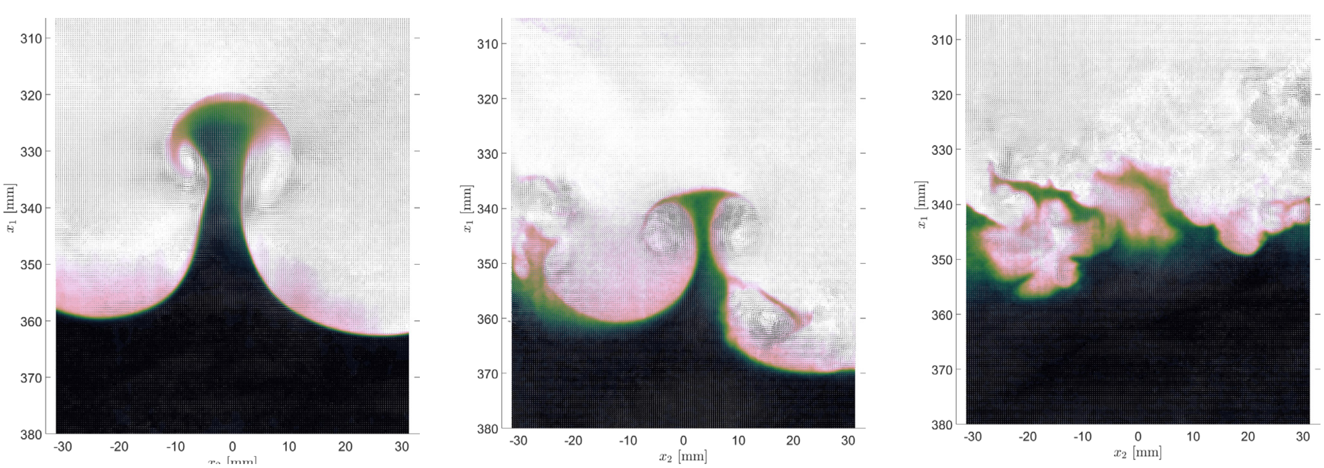
Results from turbulence and mix experiments at Los Alamos are improving the Lab's understanding, modeling, and simulation of variable-density mixing, shocked flows, and flows in extreme regimes. With these data, Los Alamos is able to modify turbulence models and include the important physics necessary for predictive weapons simulations.

"Our comparisons between experiments and simulations have become very sophisticated," said Kathy Prestridge, Physics Division Extreme Fluids team leader. Weapons codes also must take into account the effect of initial conditions—those factors driving mixing and persisting throughout the flow. Prevailing theory held that mixing materials could not possibly store memories about their initial conditions, "but our turbulence happens so fast that it doesn't have time to forget its initial conditions," Prestridge said.



Turbulent mixing from the Laboratory's vertical shock tube experiment at Mach 1.3, 3.4 ms after the shock wave passes three different types of initial conditions. The initial interface increases in complexity from left to right. Air is in white, and sulfur hexafluoride in black, and the shock passed from top to bottom. The colors represent density, and the field is overlaid with velocity vectors.

Tools, capabilities, and expertise

- Mixing and turbulence research
- Los Alamos's Turbulence Laboratory, including the vertical shock tube and turbulent mixing tunnel
- Direct numerical simulations
- University of Rochester's OMEGA Laser Facility
- Supercomputers at Los Alamos such as Trinity, which makes complex three-dimensional simulations of nuclear detonations
- Particle image velocimetry and planar laser induced fluorescence

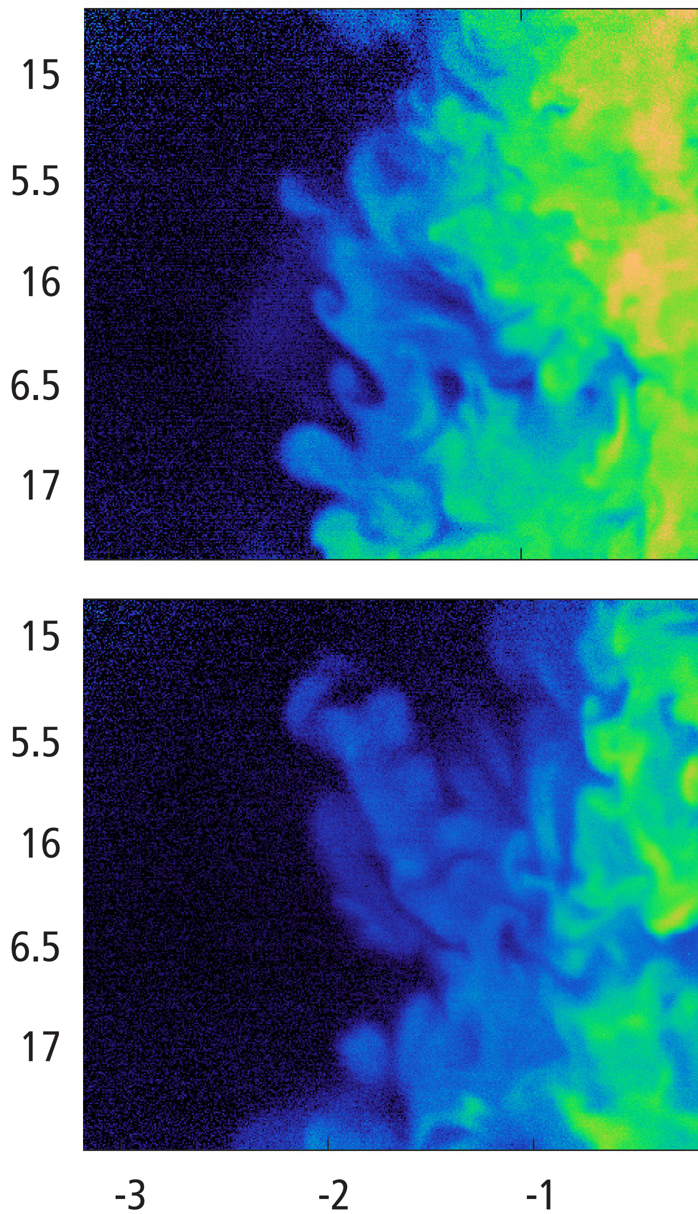
To imitate the starting conditions, Los Alamos researchers built the Vertical Shock Tube Facility, which mixes two fluids using a shock wave to study how initial conditions affect the mixing of the flow. Sudden turbulent flows caused by shock waves, or other strong forces, behave differently than steady turbulent flows. Scientists plan to scale up the experiments to Mach 10 to study similar flows in more extreme conditions.

The vertical shock tube can simultaneously measure the density and velocity of a high-speed flow, in unparalleled resolution at some of the smallest mixing length scales. "Nobody in the world has measured these quantities," Prestridge said.

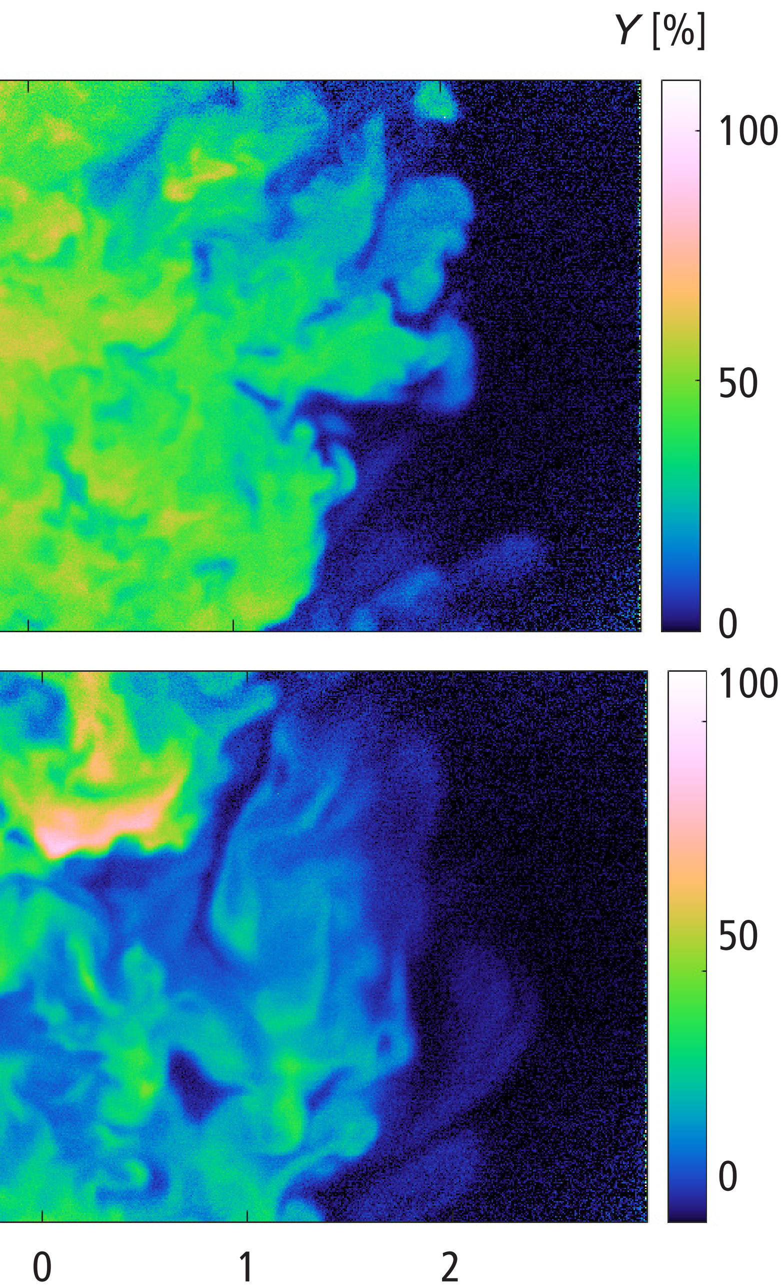
Over the years, researchers have learned that the more complex and high energy the flow is, the more difficult it is to measure mixing quantities. A National Ignition Facility capsule provides some information, and miniature shock tube experiments at the University of Rochester's OMEGA laser provide a bit more, however, the vertical shock tube and other experimental facilities at Los Alamos National Laboratory provide the most information about hydrodynamic mixing.

To isolate the effects of strong density gradients in turbulent flows, the turbulent mixing tunnel was developed at Los Alamos. Operating in a subsonic environment, it provides thousands of dynamic measurements of density and velocity fields scientists use to understand both mean and instantaneous mixing behavior. Jet mixing experiments show the fluid mixing and are able to resolve the smallest scales of mixing. With this information, researchers can understand how strong density gradients, like those pictured in the sulphur hexafluoride jet experiment (below), impact the turbulent velocities in the flow and the dissipation of kinetic energy into thermal energy.

With MaRIE, the Lab's proposed facility for studying matter-radiation interactions in extremes, scientists will probe turbulent mixing, tracking flows at the smallest scales relevant to this field. "MaRIE can help us understand mixing in more extreme length scales at high fidelity than we can do today," Prestridge said.



Below: experiments at the Laboratory's turbulent mixing tunnel of air (top) and sulphur hexafluoride (bottom) jets. Analysis of the density and velocity fields like these enable researchers to quantify differences in the turbulent mixing caused by density gradients and buoyancy effects.

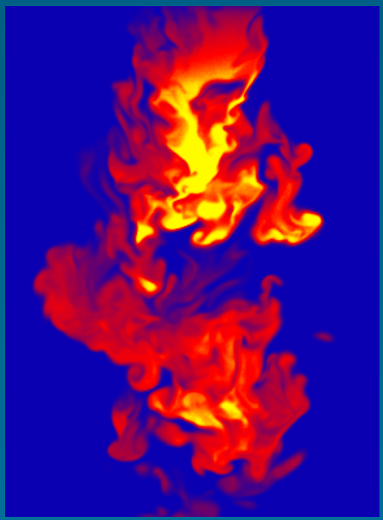


Why turbulence matters

Understanding the behavior of fluids under extreme conditions is fundamental to being able to predict the performance of nuclear weapons. Under the extreme pressures and temperatures produced inside a nuclear weapon, all materials become fluids. These fluids flow violently, exhibiting complex behavior such as turbulence, and mix with each other in complicated patterns. The details of these effects can make a difference in how the weapon performs.

Los Alamos researchers use large supercomputers to track the behavior of fluids in a nuclear explosion in complex simulations. These calculations can follow the motion for multiple fluid elements as they are driven by the heat and pressure of the explosion. However, even the Lab's largest computers are incapable of tracking fluid behavior on the smallest scales. Because fluids behave chaotically, even effects on the scale of a millionth of a meter or smaller can matter to the outcome in principle. To capture the influence of these fine scales, researchers rely on computer models that capture the important features of what is happening in the real world, without requiring tracking of every tiny change along the way.

Accurately creating these computer models requires calibrating them with experiments performed on real fluids. In laboratories throughout Los Alamos and at other facilities such as the National Ignition Facility at Lawrence Livermore National Laboratory, researchers study the behavior of fluids under extreme conditions. They can observe metals turning into liquids, fluids of different densities flowing past each other, and the whorls and eddies created in violently flowing fluids. Taken together, these data are used to improve computer simulations of nuclear explosions, and increase our understanding of the nuclear weapons in the nation's stockpile.



Experiments bring clarity to the chaos of turbulence.

At right: the polycrystalline structure of as-annealed zirconium.

Experiments in materials and nuclear science provide critical data for the nuclear weapons program.

At left: a researcher makes measurements of fission cross sections on the Time Projection Chamber at the Los Alamos Neutron Science Center.

Background: the Chi-Nu detector.

Data to design

Improving weapons design through experimental data

The path from experimental discovery science and data generation to programmatic impact is a long and complex one. The path begins with the experimental community, where hypotheses are tested and data are generated. The path continues through the modeling and simulation community, where physical processes are translated to mathematical models, which subsequently are implemented in coupled physics simulation tools. The path ends with the design community, where critical assessments of the nation's stockpile are made. Motivating factors for establishing experimental plans and priorities include the broader program's need to validate physics hypotheses, to generate data for testing and calibrating new physics models and databases, and to inform the broader weapons program's requests for more accurate and predictive modeling and simulation capabilities. No matter the motivation, it all points to the underlying necessity for integration across the Science Campaigns, the Advanced Simulation and Computing Program (ASC), and the design community.

The portion of this path between the experimental community and the modeling community most definitely travels two ways. These two communities are largely comprised of the Science Campaigns and the ASC Program's physics and engineering models (PEM) program element. Together, these two communities maintain the bulk of the nuclear weapons program discovery science, physics theory, and physics modeling capabilities. The Science Campaigns produce the data necessary to develop, test, and validate physics models. PEM assists in designing and interpreting Science Campaign experiments. And both programs work together to develop a better, more complete, and more accurate understanding of physical processes relevant to the weapons program. It is with this better understanding that the PEM program can move forward in the development of relevant physics models with increased fidelity and predictive capability.

A new physics modeling capability, backed by the soundest experimental data, is only of use to a designer if it is suitable for implementation and functions robustly within our integrated codes. Thus, the path from data to design continues through the algorithm and code development community. Indeed, future modeling and simulation capabilities may require algorithm development (e.g., scale-bridging or adaptive physics), as researchers move from purely continuum-scale representations of relevant physics to multiscale representations. Therefore, it is imperative that before modeling capabilities are developed, Science Campaign and PEM scientists work with the ASC integrated codes (IC) to ensure model development plans are consistent with IC codes and algorithms.

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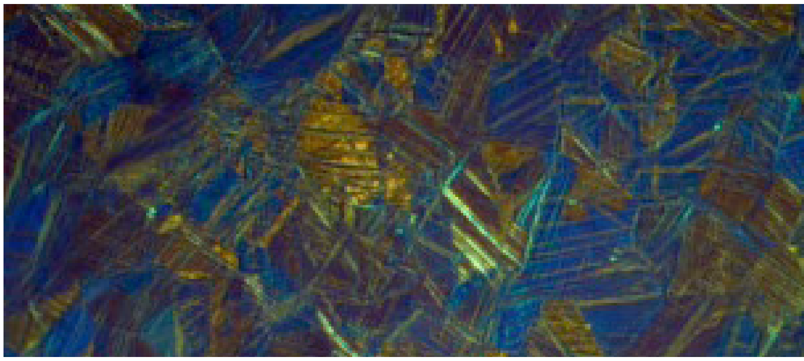
Before being passed to the design community for production use, the final stop for new physics data and models is the ASC Verification and Validation community. Within the codes, this community ensures that data and models have been implemented properly and are providing accurate representations of physics response.

Materials

In addition to the equation-of-state and nuclear physics modeling activities mentioned herein, the ASC PEM program element is responsible for developing models to account for the performance of high explosive (HE) materials, models for the yield strength and damage of polycrystalline metals, and models for ejecta source, fluid turbulence, and mixing. The PEM modeling community must work closely with the Science Campaign's experimental community to design and



Zirconium shocked to 8.0 GPa, demonstrating the changed polycrystalline structure with retained high-pressure solid phases.

Tools, capabilities, and expertise

- Small-scale experiments
- OMEGA, Z, and NIF experimental platforms
- Physics theory and modeling
- Advanced coupled-physics algorithms
- Next-generation integrated physics codes
- Exascale computing platforms
- MaRIE (Matter-Radiation Interactions in Extremes) proposed experimental facility
- DANCE (Detector for Advanced Neutron Capture Experiments)
- Neutron output studies with the Chi-Nu array
- High precision fission cross sections with the TPC (Time Projection Chamber)
- Fission product yield measurements with SPIDER (Spectrometer for Ion Determination in Fission Research)
- Neutron radiography and radiation effects

interpret experiments so that appropriate data sets are generated for model testing and calibration, as well as for future validation and verification activities.

HE models set the "initial conditions" for the remainder of the physics problems of interest. A proper accounting of HE performance will include models for detonation reaction, along with equations of state for HE reactants and products. Weapons safety considerations require additional thermo-chemo-mechanical models and models for slower-rate, non-detonation HE reactions. All of these models must be compatible with the computational schemes available within ASC's integrated physics codes. The ASC PEM HE community works closely with the Science Campaigns to better understand the physics and chemistry of HE performance, and to incorporate a more sophisticated representation of the relevant material behavior into our models and databases.

Models for strength and damage focus on the needs of the design community with respect to polycrystalline metal components. The associated models provide representations of a material's behavior under stress, and when coupled with appropriate equations of state, provide a complete continuum description of solid material response. The full spectrum of capabilities required includes models for plasticity, phase transformations, both ductile and brittle damage, and ultimate material failure. The associated continuum descriptions of material physics often depend on guidance from physics experiments or other modeling activities focused on lower length scales (e.g., molecular dynamics, single crystal models, phase transition kinetics, etc.). And as with all other modeling activities, the models slated for use within the design community must be compatible with ASC's integrated physics codes. The ASC PEM materials community works closely with the Science Campaigns to better understand the consequences of materials processing and aging on materials microstructure, the physics of materials performance across all relevant length scales, and to bring a higher fidelity of physics representation of relevant material behavior into our continuum-scale material strength, damage, and failure models for use by the broader weapons community within our integrated physics codes.

Nuclear physics experiments

A considerable amount of work continues to be devoted to quantify the uncertainties in fundamental measurements. Laboratory researchers have developed empirical models and advanced nuclear theories that underpin understanding of these data. Yet, in the absence of underground nuclear testing, a more accurate understanding of each aspect of the physics involved is required.

During studies of performance during the 2000s, a need for better fission data was established. The process by which a nucleus fissions is the most complicated of nuclear reactions. The probability of such an event is known as the fission cross section. The probability of each of more than 1000 potential fragment pairs is known as the fission fragment yields. Each fragment emits a different set of prompt neutrons and gamma rays. The residual debris subsequently decays over a much longer time—emitting additional neutrons, beta particles, and gamma rays. This process cannot be experimentally observed as a whole. Instead, a suite of measurement techniques to examine individual components is required.

The study of neutron reactions requires three components: neutron sources, targets, and detectors. The Los Alamos Neutron Science Center (LANSCE) provides one of the brightest neutron sources in the world. LANSCE covers all neutron energies relevant for weapons studies, ranging from the high MeV energy (Target 4) to the lower eV and keV energies (Target 1) and provides multiple beamlines for different detectors at each. Los Alamos's Science Campaigns have, in close collaboration with Lawrence Livermore National Laboratory, developed the next-generation fission detectors for use at LANSCE. The Chi-Nu detectors (led by Los Alamos) are measuring the energies of the neutrons emitted from fission. The fission Time Projection Chamber (TPC), led by Livermore, is measuring fission cross sections.

Ionization chambers have existed since radiation was discovered and played a key role in confirming the existence of fission. The massive energy pulse delivered by the fragments is a unique, easily measured signature. Most chambers, however, are limited to providing a simple time trace of this energy deposition. In these measurements, simplified assumptions are the only way to estimate many of the systematic errors.

The TPC, in essence, is a giant three-dimensional camera providing a movie of each ionization event. A revolutionary redesign of the historic ionization chamber, it measures beam uniformity in real time. As these are radioactive targets, their emissions provide an autoradiograph to assess target uniformity. With these two quantities, researchers can accurately correct for these conditions and quantify the potential impact on past measurements.

Chi-Nu takes a traditional approach to measuring the distribution of neutron energies from fission and modernizes the analysis approach. Time of flight is often used to infer neutron energies—by knowing the timing and flight length, the energy is easily derived. Here a double time of flight—neutron production to fission to detectors—allows the measurement of the distribution of emission energies as a function of incident energy.

The problem is that the experiment's surroundings scatter neutrons, changing their flight length. Modern computing allows researchers to "see" inside an experiment in ways impossible outside a simulation. By following individual particles, researchers can see where events occur that cause their paths to deviate. The observation is also important to derive an effective flight path and make many other corrections to the data. Recent studies have shown some of these corrections to be 20-40%.

While the TPC and Chi-Nu techniques are now reaching maturity, each additional measurement will take one to two years to complete. These new data, along with improved understanding of previous data, will be used to create new evaluated data libraries. These in turn will be processed into application code libraries to support a wide variety of stockpile stewardship, global security, and even nuclear energy, and other missions.

One step closer to understanding detonation

Scientists at Los Alamos National Laboratory are preparing to conduct a series of first-ever neutron-diagnosed subcritical experiments that promise to yield new data about nuclear weapons. The work could settle questions about the effectiveness of both aging plutonium pits, which trigger nuclear detonation, and new designs if required in the future. These proof-of-concept experiments are also planned to corroborate and refine existing supercomputer simulations of nuclear explosions.

Since the United States stopped testing nuclear weapons in 1992, second-generation nuclear weapons designers have never participated in an actual nuclear test. Instead they rely on simulations and limited subcritical experiments. These experiments use actual nuclear materials in very small amounts to gather new data on how plutonium reacts under extreme conditions, validate the simulations, and refine scientists' understanding of nuclear detonation. But these data have some gaps.

The neutron-diagnosed subcritical experiments will employ a novel gamma-ray detector developed at the Laboratory to go one step farther into the physics of nuclear detonation. Starting with a pit identical to those in the stockpile, Los Alamos researchers will alter the pit to behave much like it would in implosion leading to fission, but without the ultimate detonation. In the experiment, a device called a dense plasma focus will bombard the plutonium with neutrons, which will generate a stream of gamma particles measured by the detector. The results will shed new light on the behavior of plutonium as it approaches criticality, which sustains nuclear fission in a weapon.

This research leverages the Laboratory's decades of world-class research into nuclear theory and experimentation by its senior scientists, plus innovative contributions by current postdoctoral researchers. Recent breakthroughs at Los Alamos with dense plasma focus, which lie at the forefront of plasma physics, combined with developments in high-speed electronics make these new experiments possible. The work is funded under the Laboratory Directed Research and Development program at Los Alamos, a competitive program funding innovative research.

Neutron-diagnosed subcritical experiments give younger physicists a chance to design nuclear experiments under the guidance of senior mentors. Perhaps more importantly, the neutron experiments will test researchers' judgment and validate the credibility of their predictions about pit performance.

Los Alamos National User Facilities

Los Alamos Neutron Science Center (LANSCE)

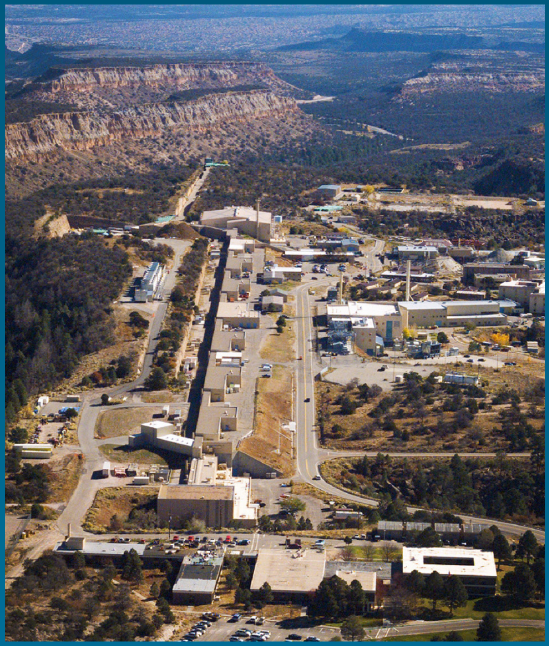
Providing intense sources of neutrons and protons for experiments supporting civilian and national security research

- Five major experimental facilities operate simultaneously. These facilities contribute to the Stockpile Stewardship Program, produce radionuclides for medical testing, and provide a venue for industrial users to irradiate and test electronics. In addition, they perform fundamental research in nuclear physics, nuclear astrophysics, materials science, and many other areas.

- The LANSCE User Program plays a key role in training the next generation of top scientists—attracting the best graduate students, postdoctoral researchers, and early-career scientists.

- The U.S. Department of Energy, National Nuclear Security Administration—the principal sponsor of LANSCE—works with the Office of Science and the Office of Nuclear Energy, which have synergistic long-term needs for the linear accelerator and the neutron science that is the heart of LANSCE.

lansce.lanl.gov



Center for Integrated Nanotechnologies (CINT)

Exploring the continuum from scientific discovery to the integration of nanostructured materials into the micro- and macro- world

- Integration is the key to fully utilizing the novel properties of nanoscale materials and creating new nanotechnologies to benefit society.
- World-class expertise and facilities available at CINT focus on the experimental and theoretical exploration of behavior, the development of synthesis and processing approaches, and an understanding of new performance regimes, testing design, and integration of nanoscale materials and structures.
- A U.S. Department of Energy/Office of Science Nanoscale Science Research Center.

cint.lanl.gov

National High Magnetic Field Laboratory-Pulsed Field Facility (NHMFL-PFF)

Probing and characterizing thermodynamic properties of new materials to understand the basic underpinning of their behavior and discover new states of matter

- The only place in the world where researchers can design experiments using the highest magnetic fields ever nondestructively produced on a repetitive basis.
- Allows researchers access to a wide variety of experimental capabilities in pulsed magnetic fields and assistance from some of the world's leading experts in condensed matter physics and pulsed magnet science.
- Sponsored primarily by the National Science Foundation, Division of Materials Research, with additional support from the State of Florida and U.S. Department of Energy.

nhmfl.lanl.gov

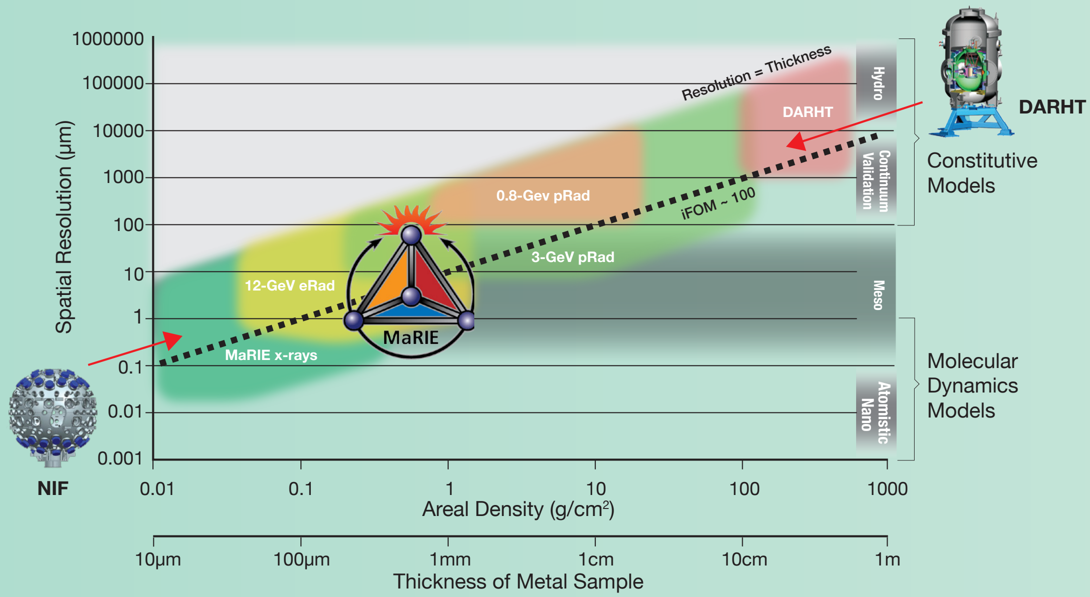
MaRIE: Matter-Radiation Interactions in Extremes

Supporting key National Nuclear Security Administration goals

The nation's stockpile stewardship is designed to provide predictive capabilities for weapons performance in the absence of nuclear testing. To date there is a "knowledge gap" for science tools for stockpile stewardship between the atomic scale of materials—addressed by facilities such as the National Ignition Facility at Lawrence Livermore National Laboratory and the Z Pulsed Power Facility operated by Sandia National Laboratories—and the integral scale addressed by the Dual-Axis Radiographic Hydrodynamic Test Facility at Los Alamos and the U1a complex at the Nevada National Security Site.

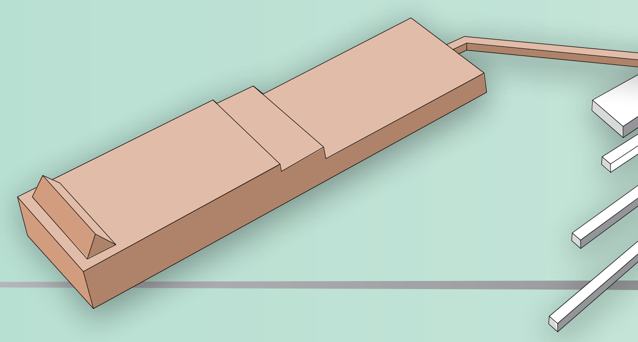
MaRIE will deliver the ability to offer time-dependent control of material processes, structures, and properties during manufacture and production. Experimental characterization will be complemented by capabilities in synthesis and fabrication and will be integrated with advanced theory, modeling, and computational tools.

Los Alamos proposes to build a coherent, brilliant x-ray source with energy and repetition rate characteristics uniquely matched to address materials performance challenges associated with the National Nuclear Security Administration's mission. This high-energy, 42-keV, x-ray free electron laser accelerator that is brilliant and coherent with the temporal properties to make time-dependent measurements will push temporal scales and provide unprecedented spatial resolution for "thick" multigranular samples.



The MaRIE (for Matter-Radiation Interactions in Extremes) capability is designed to address several aspects of materials behavior under extreme conditions. In particular the proposed capabilities will help characterize the behavior of interfaces, defects, and microstructure between the spatial scales of atomic structures and those of the engineering continuum. The role microstructure plays in affecting material's macroscopic engineering properties, such as strength, stability under heat and pressure, elasticity properties, and durability in use over time, is well recognized.

Artist's rendering of a MaRIE preconceptual design.



marie.lanl.gov

MaRIE will provide researchers with the ability to

- create flexible and reduced-cost stockpile materials options for the nuclear weapons complex through accelerated qualification, certification, and assessment, including advanced/additive manufacturing opportunities;
- probe real-time materials response at length scales providing the linkage between materials defects, interfaces, and nonequilibrium structures and performance (the "mesoscale");
- subject samples to extreme environments and use imaging and diffractive scattering from multiple probes at multiple spatial and time scales to connect models to product performance;
- reduce the uncertainty of physics-based predictions of performance, thus providing sufficient confidence for the material over the life cycle of the system;
- leverage exascale efforts to validate and calibrate reduced-order models used in advanced codes;
- predict and control behavior from materials and devices to manufacturing processes; and
- recruit and retain future generations of nuclear weapons stewards.

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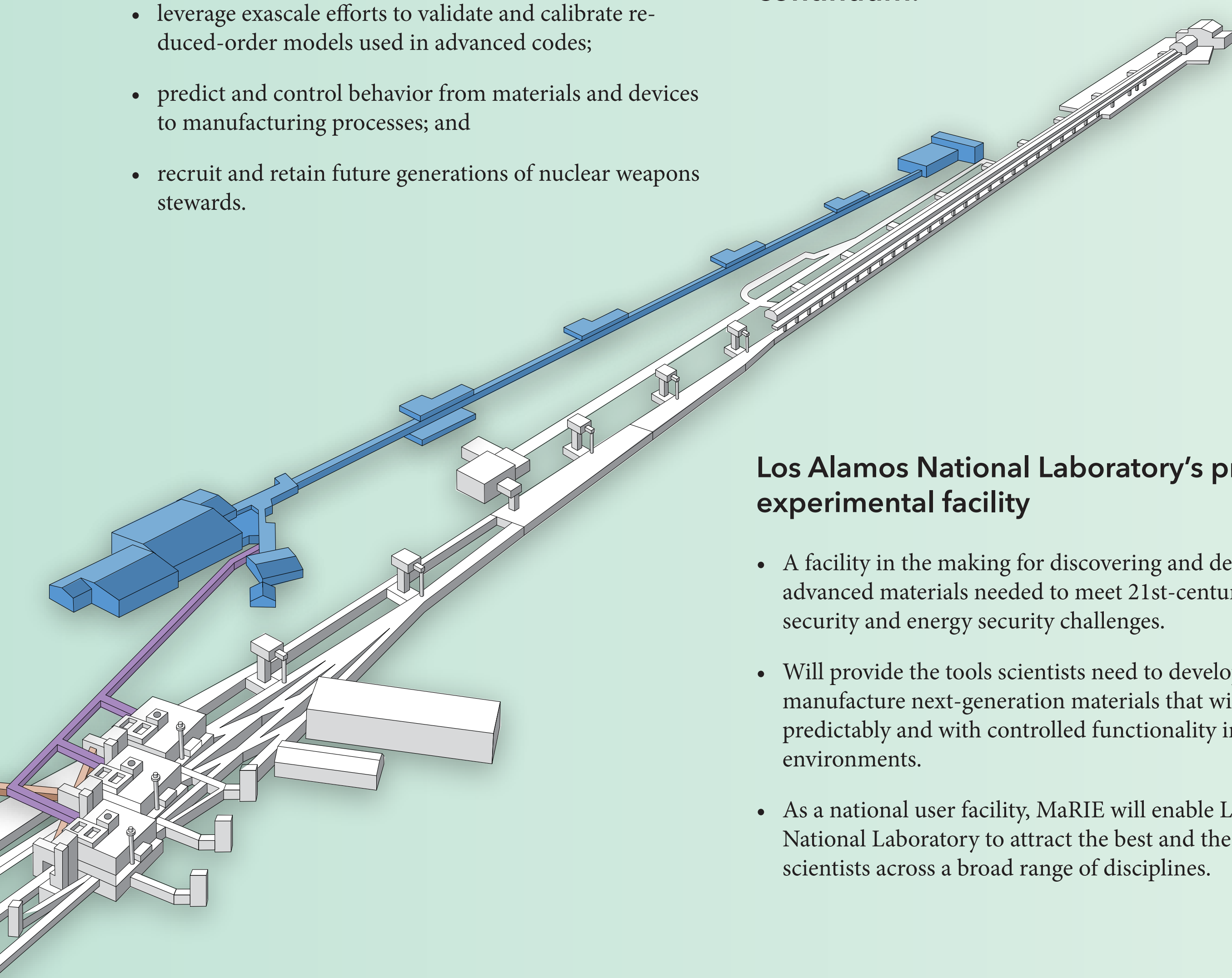

Los Alamos National Laboratory's proposed experimental facility

- A facility in the making for discovering and designing the advanced materials needed to meet 21st-century national security and energy security challenges.
- Will provide the tools scientists need to develop and manufacture next-generation materials that will perform predictably and with controlled functionality in extreme environments.
- As a national user facility, MaRIE will enable Los Alamos National Laboratory to attract the best and the brightest scientists across a broad range of disciplines.

Associate Director Experimental Physical Sciences:
Mary Hockaday
Editor: Karen E. Kippen
Designer, illustrator: Jim Cruz
Copyeditor: Kris Fronzak

Contributors: Steve Batha, Curt Bronkhorst, Eric Brown, Jay Carnes, Diana Del Mauro, Anemarie DeYoung, Franz Freibert, Rusty Gray, Dan Hooks, Rick Martineau, Joe Martz, Albert Migliori, Charles Poling, Kathy Prestridge, Mark Schraad, Mike Stevens, Morgan White

Experimental Physical Sciences Vistas
c/o Karen Kippen, Mail Stop A106
Los Alamos National Laboratory
P.O. Box 1663
Los Alamos, NM 87545

Vistas@lanl.gov

Los Alamos
NATIONAL LABORATORY
EST. 1943

NNSA
National Nuclear Security Administration