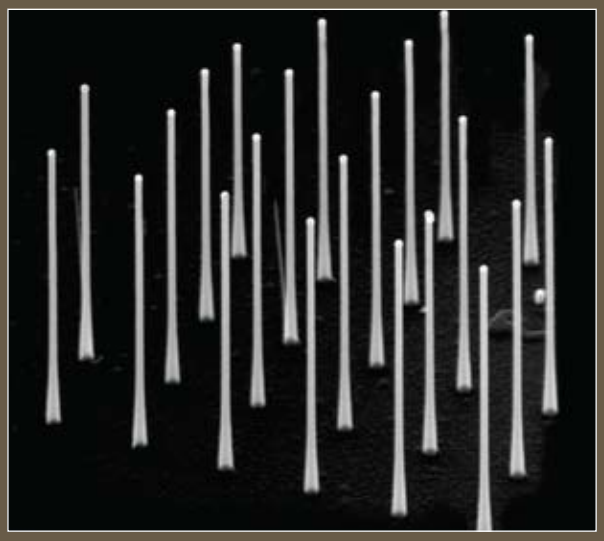
Experimental Physical Sciences

VISTAS

LOS ALAMOS MATERIALS STRATEGY



Los Alamos
NATIONAL LABORATORY
EST. 1943

WINTER 2010

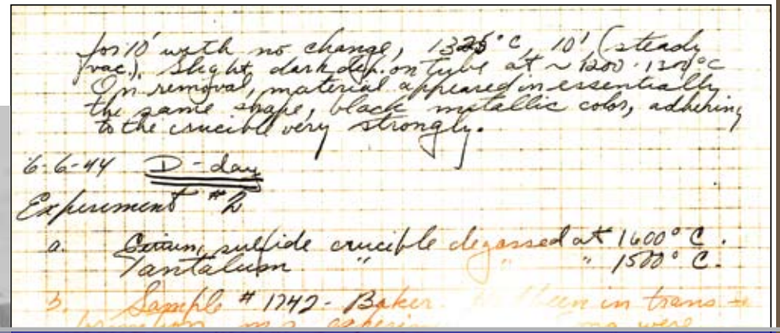
Micrograph of a plutonium alloy containing 0.6% (by weight) gallium cooled to -150°C that went through a partial martensitic transformation from delta to the alpha prime phase. The alpha prime platelets (white) formed in the leaner gallium regions and along crystallographic orientations.

Contents

ON THE COVER:

Open meadow near Valles Caldera; images represent the three strategic themes of the materials strategy and are described in this issue.

Page from Lawrence Litz's notebook, D-Day, 1944



Materials at Los Alamos, past to present

Susan J. Seestrom,
Associate Director
Experimental Physical Sciences

Exploring the physics, chemistry, and metallurgy of materials has been a primary focus of Los Alamos National Laboratory since its inception. In the early 1940s little was known or understood about plutonium, uranium, or their alloys. In addition, several new ionic, polymeric, and energetic materials with unique properties were needed in the development of nuclear weapons. Our Laboratory's proud and distinguished history of advancing the science and technology of materials includes the discovery in 1943 that plutonium forms multiple phases of differing density, followed quickly by the idea of using minor alloying elements to stabilize the phase of interest. We pioneered the development of insensitive high explosives, as demonstrated by the Puye event at the Nevada Test Site in 1974, as well as materials for fusion reactions, radiation casings, and neutron sources. These advances have enabled modern nuclear weapons design concepts and a safe, reliable deterrent.

Today, our materials scientists are continuing the tradition of leading-edge materials research providing national security solutions. For example, building upon our discovery of superconductivity in plutonium-cobalt-pentagallium ($PuCoGa_5$) in 2002, we continue a breadth of collaborative theoretical and experimental research on this material that is opening a new avenue for detailing the electronic structure of plutonium materials as well as advancing our understanding and application of superconductivity.

As the Laboratory has evolved, and as missions in threat reduction, defense, energy, and meeting other emerging national challenges have been added, the role of materials science has expanded with the need for continued improvement in our understanding of the structure and properties of materials and in our ability to synthesize and process materials with unique characteristics. Materials science and engineering continues to be central to this Laboratory's success, and Los Alamos recently identified *Materials for the Future* as one of three *Science that Matters* priorities essential to maintaining and evolving a vital Laboratory.

> "As an integral component in the Laboratory's most ambitious scientific and technical research, materials science and engineering will remain key to the Laboratory's future."

The materials strategy enables Los Alamos to provide national security solutions through controlled functionality of materials. Our strategy maintains a dynamic balance of advancing the science in our three theme areas with supporting the applications in the Laboratory's three mission areas.

Breadth and impact of the materials capability

Materials science and engineering has been at the core of Los Alamos science since the early days of the Manhattan Project and it remains a core capability. It is a $300 million per year enterprise and involves 15 divisions across 8 scientific research directorates and involves 30-40% of the Laboratory's technical staff. The works spans the full range from basic science to applied development and production. Applied work in materials supports all the Laboratory's missions uniformly. Our productivity—approximately 1,600 manuscripts and presentations released annually from the two materials-centric divisions alone—demonstrates our extensive and active external professional participation. These range from conference proceedings to archival publications, for example, approximately 100 *Physical Review Letters* since 2005.

In this, our second issue of *Experimental Physical Sciences Vistas*, we outline our materials strategy. The vision is one of controlled functionality of materials, referring to the ability to create novel materials that are tailored for the unique demands of specific applications. Control is an extremely ambitious vision, requiring both a quantitative understanding of the relationship across composition, microstructure, and properties as well as the prediction and control of synthesis and process variables necessary to fabricate the material.

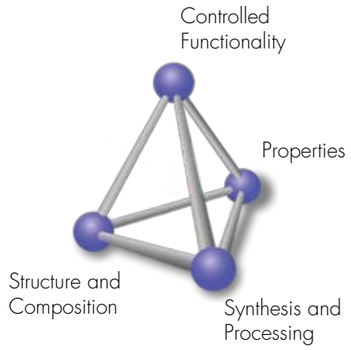
This strategy is fulfilled by an assemblage of world-class scientists, engineers, and technicians who employ their skills in one-of-a-kind facilities such as the Los Alamos Neutron Science Center (LANSCE), the National High Magnetic Field Laboratory (NHMFL), the Center for Integrated Nanotechnologies (CINT), the Materials Science Laboratory, the Sigma metallurgical processing facility, and the plutonium facility.

We are actively shaping the materials complex of the future with new tools and new facilities. In this issue you will read about how Los Alamos is home to two new U.S. Department of Energy (DOE) Energy Frontier Research Centers: the Center for Materials at Irradiation and Mechanical Extremes (see page 6) and the Center for Advanced Solar Photophysics (see page 28). These centers concentrate scientific expertise in an effort to overcome the scientific and technical challenges to U.S. energy security. Taken altogether, our established and emerging capabilities provide the foundation for MaRIE (Matter-Radiation Interactions in Extremes), the Laboratory's next signature facility and tomorrow's cornerstone for this transformational science of prediction and control.

As an integral component in the Laboratory's most ambitious scientific and technical research, materials science and engineering will remain key to the Laboratory's future. And it will continue to call upon the expertise of world-class scientists, engineers, and technicians, both residents and visitors, who discover at Los Alamos the facilities, tools, and network allowing them to fulfill their potential.

Susan J. Seestrom

Science that matters: Materials for the future



We anticipate the advent of a new era in materials science, when we will transition from observing and exploiting the properties of materials to a science-based capability to create materials with properties optimized for specific functions. Performance is the traditional terminology to describe how a material fulfills the defined requirements. We use the term functionality to describe the actual design and tailoring of a material to perform beyond the traditional requirements and sometimes in new ways beyond the basic properties. This concept is the central vision of our strategy: *Controlled Functionality.*

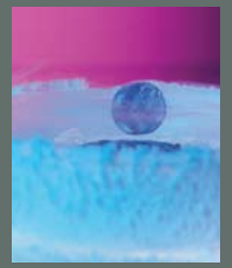
Mission

The materials capability mission derives from our vision together with the Laboratory's national security mission drivers:

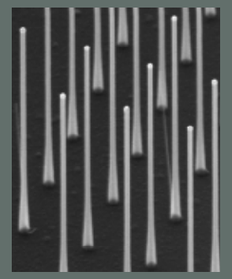
We pursue the discovery science and engineering required to establish design principles, synthesis pathways, and manufacturing processes for advanced and new materials to control intentionally that functionality relevant to ensuring the U.S. nuclear deterrent, reducing global threats, and solving energy security challenges.

Accurate description of materials often involves the characterization of many variables that can only be captured in a statistical sense, e.g., chemical composition, defect concentration, texture, or grain size. These parameters and their linking across temporal and spatial scales determine a material's behavior and performance in a given environment. In other circumstances, describing a material requires that we explore the fundamental quantum nature of matter to understand behavior exhibited either as intrinsic emergent phenomena such as superconductivity or extrinsic emergent phenomena in fabricated nanostructures. In all cases, if we are to control functionality, we need an intelligent system for tailoring a material's performance. Thus, the central scientific goal of our materials strategy is to understand the link between the functional properties of materials and their structure and composition, as realized through synthesis, fabrication, and manufacturing. We further seek to discover functionality that has not yet been observed. These goals require process-aware models that relate materials performance to their properties during and after manufacturing. This can only be achieved through the intimate coupling of experiment with theory and simulation to link the spectrum of materials length and time scales—from the electronic through the continuum and to the application or integrated system level. Such insights will not only transform our ability to achieve controlled functionality, but also allow us to predict and create new materials functionality in previously inaccessible extremes.

Defects and Interfaces:
The mechanistic understanding and control of inhomogeneities, intrinsic and engineered, across all appropriate length and time scales that govern materials functionality.



Extreme Environments:
The underlying principles enabling the understanding of the interactions of materials with extreme conditions in order to create environmentally tolerant properties and the ability to exploit extreme environments to tune materials functionality.



Emergent Phenomena:
The science required to discover and control complex and collective forms of matter that exhibit novel properties and respond in new ways to environmental conditions, enabling the creation of materials with innate functionality.

Strategic themes

We predict and control functionality through forefront science and engineering that crosscuts three themes: *Defects and Interfaces*, *Extreme Environments*, and *Emergent Phenomena.*

Leadership in controlling functionality across these three challenging themes will differentiate our materials capability. We have chosen forward-looking themes that complement one another and build upon our established scientific strengths. Our differentiation comes through 1) the quality and breakthrough nature of the research in each theme; 2) integration across themes; 3) applicability to and impact on our national security needs; and 4) curious and creative people. In combining these, the materials capability will enable the achievement of Los Alamos's applications goals and, in turn, the Laboratory's needs will drive advancement of our science capability. The results will be key solutions to national security challenges, as conceptualized in the materials strategy diagram on the preceding page. A key objective is to anticipate a mission need for specific materials performance and to position materials research to be capable of deploying materials meeting that mission need.

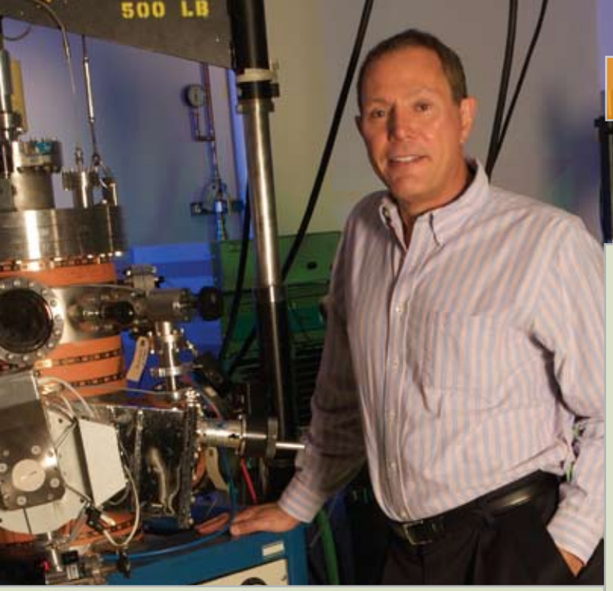
Scientific challenges

Each strategic theme is bounded by key science challenges that demand discovery science and, if successful, will have high impact on mission success. We choose classes of behavior within each theme to focus our research on those materials and functionality of strategic importance to Los Alamos. These concepts are introduced below and then expanded throughout this *Vistas* publication.

Defects and interfaces are the ultimate features that control materials performance, whether to limit it or to enhance it. This perspective shifts the focus of materials inquiry from homogeneous composition and idealized crystallography to understanding and exploiting deviation from that perfect structure to achieve functionality in the specific classes of structural integrity, chemical/corrosion resistance, or electronic/photonic conductance. These demands inspire scientific challenges, including: When is materials functionality deterministic (controllable and predictable) and when is it stochastic? How can we develop a multiscale understanding linking the knowledge of inhomogeneities to a bulk response? Knowing a desired functionality, how do we predict and process the microstructure to achieve it?

Extreme environments require materials to function as designed when subjected to radiation, thermomechanical, electromagnetic, and chemical/electrochemical extremes. In addition, extreme environments can be used to extract information on fundamental properties of materials and to induce new states of matter. Our objective is to exploit the use of extreme environments and novel diagnostics for the characterization of materials with the ultimate goal of predicting and controlling behavior of materials as well as opening up previously inaccessible regimes of materials performance. We include the need to extrapolate the materials properties we can measure to the performance of materials in mission-relevant extreme environments. Science challenges again address the necessity to connect the range of scales from quantum mechanical to observable and attosecond to geologic. We further ask, what are the essential physics and chemistry concepts that must be captured in predictive models? Can we access and exploit phenomena that are uniquely stable at extreme conditions?

Emergent phenomena derive from the unique physical, chemical, and biological response of materials and the coupling of these behaviors to generate new collective behaviors. These new forms of matter are complex materials that exhibit novel functionality and often respond in surprising ways to environmental conditions, enabling the controlled design and creation of materials with specified characteristics. We classify emergent phenomena of interest as intrinsic, extrinsic, and adaptive response. The scientific challenges for this theme explore issues around understanding and control, selectively tuning competing interactions, adaptive functionality, time and length scales, and the development of new synthesis/processing approaches and diagnostics.



Controlling functionality

Director of the Center for Materials at Irradiation and Mechanical Extremes Mike Nastasi, in the physical synthesis lab where nanostructured materials with tailored interfaces are made.

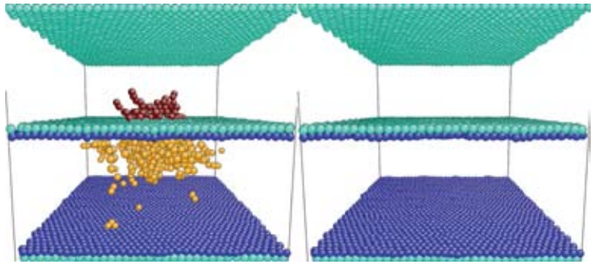
The Center for Materials at Irradiation and Mechanical Extremes (CMIME), a new Energy Frontier Research Center, strongly bridges two theme areas of the Laboratory's materials strategy—defects and interfaces and extreme environments—while also exhibiting emergence in self-healing phenomena. This work of fundamental scientific exploration and discovery is a quest toward tomorrow's revolutionary materials for nuclear reactors.

Focusing on the design of new materials with predictive behavior at thermomechanical extremes, center scientists will research how atomic structure and energetics of interfaces contribute to defect and damage evolution in order to design metal- and ceramic-based nanocomposite materials with tailored response at irradiation and mechanical extremes. By eliminating radiation-induced defects or controlling micro-cracking at interfaces to dissipate shock energy, these ultrahigh-strength, damage-tolerant nanocomposites will have potential applications as structural materials, fuel cladding, and waste forms in the next generation of nuclear power reactors as well as structural materials in transportation, energy, and defense.

According to Center Director and Laboratory Fellow Michael Nastasi, the center's scientific foundation comes from recent Los Alamos work on nanocomposite materials. These materials, designed from the "bottom-up" with quasi-optimized length scale, morphology, and interface structure and energetics, can exhibit vast improvements in strength and resistance to damage from particle irradiation and shock deformation. The research in this center will test hypotheses about the interface geometry, atomic structure, and energetics leading to the development characteristics for identifying "super-sink" interfaces at irradiation and mechanical extremes. The center will explore unit processes of point or line defect interactions with interfaces and develop understanding of how the correlated behavior of many such atomic-scale interactions across multi-length and time scales leads to an emergent phenomenon of damage tolerance in nanocomposites.

CMIME features two thrust areas—irradiation extremes, led by Nastasi, and mechanical extremes, led by Center Co-director Amit Misra—and draws expertise throughout the Laboratory's materials capability, from synthesis of nanocomposite oxides, deformation processing, physical vapor deposition, solidification processing, laser shock, and ultrafast laser spectroscopy, to ion beam analysis and irradiation, electron microscopy, and atomistic modeling. External collaborators include the Massachusetts Institute of Technology, the University of Illinois at Urbana-Champaign, and Lawrence Livermore National Laboratory.

Funded by the DOE's Office of Science, Basic Energy Sciences, CMIME leverages existing facilities at Los Alamos, including CINT, the Ion Beam Materials Laboratory, the Electron Microscopy Laboratory, and high performance computing resources. The research in this center will provide a significant part of the scientific foundation for MaRIE, the Laboratory's planned signature experimental facility.

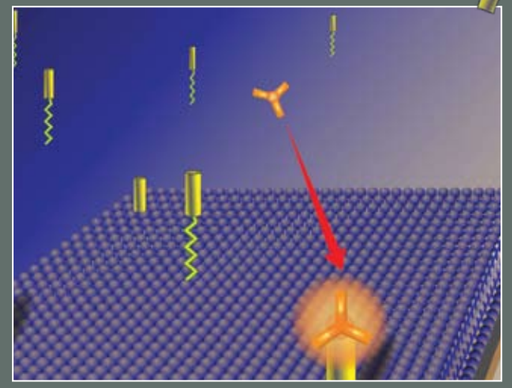


Molecular dynamics simulations showing the time sequence of a collision cascade at the interface between nanolayers of copper (Cu) and niobium (Nb). The left figure shows the initiation of the collision cascade and the Cu (gold) and Nb (red) atoms displaced from their lattice sites. The right figure is several picoseconds later and shows that a perfect lattice was recovered through the absorption of displaced atoms at the Cu-Nb interface.

Los Alamos National Laboratory's national security missions

In conducting forefront science, Los Alamos National Laboratory must ensure it is enabling national security solutions. The Laboratory's three programmatic themes—nuclear deterrence, global threat reduction, and energy security—encompass huge national need. Our use-inspired science must constantly have these missions in mind, and the balance of investing in capabilities that will realize the materials vision with meeting challenging mission deliverables is the core strategic challenge for a science and technology organization. Meeting that challenge is how the Laboratory makes a difference for the nation.

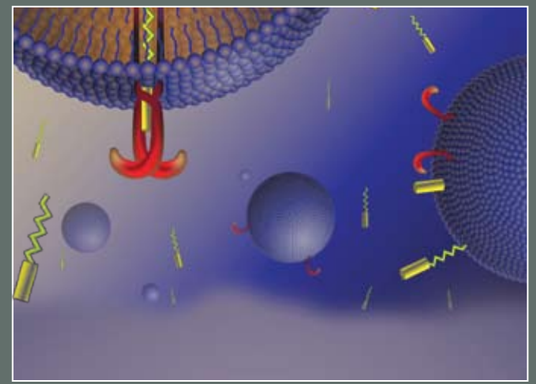
As demonstrated by the following examples of research for detecting and mitigating emerging infectious diseases, advancing nuclear energy, and ensuring our nuclear deterrent, Los Alamos National Laboratory relies on materials research to underpin its contributions in all of our national security mission areas. The materials strategy reflects our responsibility to anticipate future national security needs and steward our science base to be ready to meet those challenges. The remainder of this *Vistas* issue describes our three materials research themes and provides examples of the science that enables Los Alamos to provide national security science-based solutions to the nation.■



Schematic of cell membrane mimetic architecture (lipid bilayer) at the interface between the inorganic transducer (optical waveguide) and the biological sample (e.g., serum) to be measured. The lipid bilayer serves the same function as the host cell membrane in capturing the pathogen biomolecule. Once the pathogen-secreted biomolecule partitions into the lipid bilayer, a reporter antibody binds to the exposed portion of the biomolecule initiating signal transduction (fluorescence).

Diagnosing and managing emergent diseases

Infectious diseases that have evolved to evade the immune system or developed resistance to drug intervention are rapidly becoming the face of the global health threat. Examples include the H1N1 influenza strain and drug resistant tuberculosis. All pathogens produce characteristic biomolecules (disease markers) early in an infection. Detecting the patterns of expression exhibited by the disease markers provides an important means of not only diagnosing infection, but also tracking the emergence of drug resistance and immune escape.

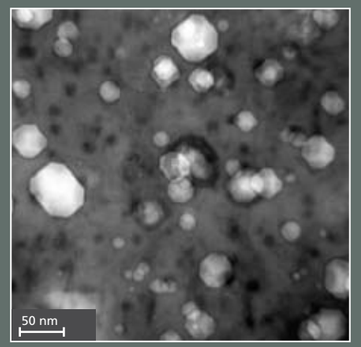


Schematic of the toll-like receptor mechanism for the innate immune response to infection from bacterial pathogens. Biomolecules (in yellow) shed by a pathogen early in infection first insert into the cell membrane of the host dendritic cells. They then bind monomeric units of toll-like receptors (TLRs, in red), forcing the TLRs into close proximity, thereby initiating a signaling cascade that results in expression of cytokines (in green). The roles of the cell membrane are to bind and concentrate the pathogenic biomolecules, mediate TLR-biomolecule recognition and down-stream signaling.

Los Alamos is addressing this problem through the development of sensitive, specific, and quantitative assays for the detection of disease markers. A critical aspect of this work is the interface between complex biological samples and the sensing transducer that converts a highly specific biomolecular recognition event into a measurable signal. The complexity of the samples places extreme requirements on sensing films. The biosensor team has developed two distinct sensing films for the detection of disease markers. The first is robust self-assembled monolayer sensing films that permit detection of biomarkers in complex fluids. The second is a fluid lipid bilayer system that faithfully mimics the surface of a cell membrane. As depicted in the figures above and at left, these lipid bilayers have been used to mimic the role that the cell membrane play in the early innate immune response, thereby providing an early diagnosis of infection.

Solving energy security challenges

Los Alamos's expertise and facilities for studies of irradiation damage and special nuclear materials position us uniquely for advancing nuclear energy technologies. In an ongoing study funded by the DOE's Advanced Fuel Cycle Initiative, we have a unique opportunity to characterize material that had been irradiated in the Fast Flux Test Facility at DOE's Hanford Site in Washington to a maximum dose of 155 displacements per atom, the highest dose ever achieved on a fast reactor irradiated fuel duct. Working in hot cells, we remotely cut the 12-foot-long duct into smaller sections for analysis. The first compression tests, on conventional size samples, were performed in the hot cells. We used electro-discharge machining to fabricate custom tensile, compact tension, and Charpy specimens for more detailed characterization of the changes in mechanical properties with irradiation dose and temperature. In addition to the mechanical property studies, additional samples are being cut from this valuable component to investigate the microstructure using small-angle neutron scattering and transmission electron microscopy. One of these images is shown in the figure of void growth (0.3%) in a sample taken from the high dose location in the duct. The understanding of materials degradation gained through this study and others is enabling us to improve today's structural materials and lifetime predictions to enable more reliable, economical, and longer operating life for nuclear reactors.



Bright field transmission electron micrograph showing voids imaged from a section taken from the ACO-3 duct, which was sent to Idaho National Laboratory for analysis of the microstructure. Temperature of irradiation was 444°C and total dose was 155 displacements per atom. Image: Idaho National Laboratory.

An interdisciplinary facility dedicated to research on current materials and those of future interest, the Materials Science Laboratory has been the cornerstone of Los Alamos National Laboratory's materials science complex since its dedication in 1994.

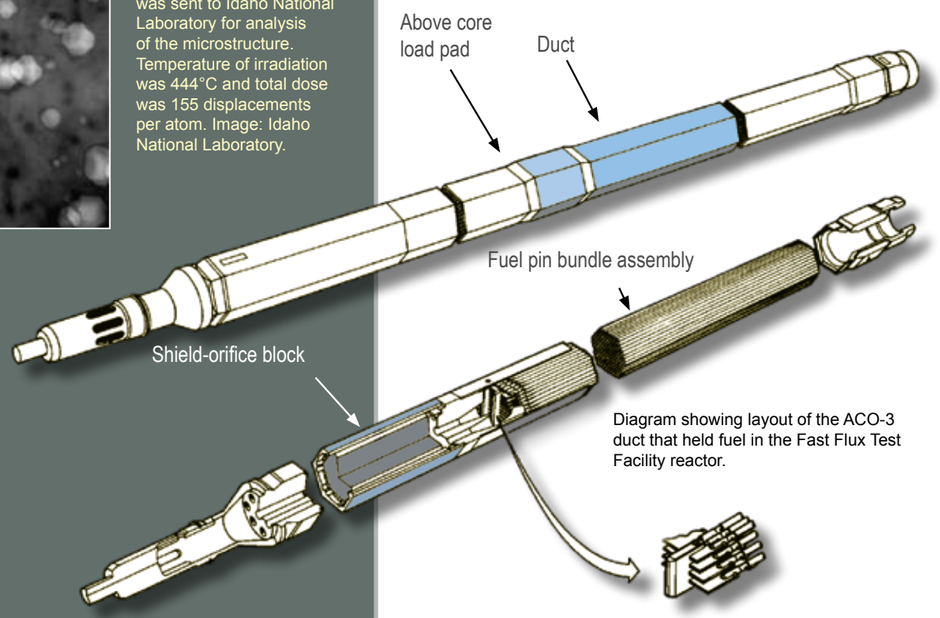


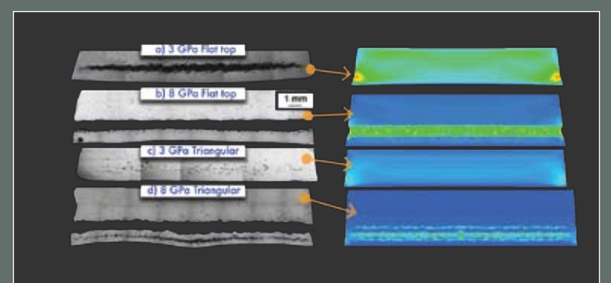
Diagram showing layout of the ACO-3 duct that held fuel in the Fast Flux Test Facility reactor.

Left: Ellen Cerreta views samples in the optical microscope.

Ensuring the safety, security, and reliability of the U.S. nuclear deterrent

Damage evolution under dynamic loading continues to be a key area of materials research for the nuclear weapons program. Through coupled modeling and experiments, we are starting to predict reliability and performance, under limited conditions, for structural metals. An example of our current dynamic damage prediction capability is shown in the figure below. Both experimental and simulation results for copper shocked in a gas gun with two different peak shock pressures and using two different shock wave shapes (flat top and triangle) are shown. Total failure (the 8 gigapascals [GPa]), flat top shock wave case b) is captured quite well in the simulation. However, the details of evolving plasticity and damage in the incipient cases (a and c) and the more complex 8 GPa triangular shock wave (d) are not represented well in our current models.

Advances in continuum predictive capabilities rely upon computational models that accurately capture relevant deformation processes at the mesoscale. Modern, statistically relevant diagnostic tools such as electron backscattered diffraction and x-ray diffraction techniques that permit a microstructure to be interrogated in three dimensions allow deterministic relationships that describe seemingly stochastic processes to be established. Through carefully controlled, small-scale, dynamic experiments and multiscale materials characterization, microstructural features (both heterogeneous and homogenous in nature) can be linked to damage evolution and failure of materials. Then these linkages can be physically represented in our constantly advancing damage models.



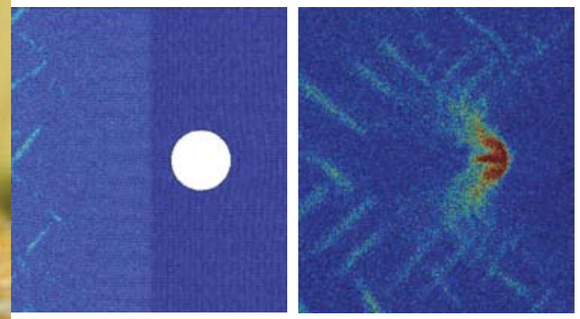
Above: Optical images of the damage in copper shocked at 3 and 8 GPa with a flat top and triangular shock wave and the corresponding simulation results of the damage in these specimens.

Defects and interfaces

Most solid substances consist of crystallites containing near-perfect, periodic arrangements of atoms. Normally, however, the imperfections in these arrays control the properties of the materials, typically either by providing limiting pathways for performance of the bulk material, or by inducing functionality that would otherwise be absent in the bulk. At their base level, these irregularities in atomic patterns come in three dimensionalities: point defects (such as interstitials or substitutions); line defects (dislocation loops, edge dislocations); and planar defects (twin planes, interfaces). At higher levels, more macroscopic features (such as voids, polycrystalline morphology) are larger expressions and/or complex combinations of these fundamental quantities. For noncrystalline materials, such as polymers and glasses, analogies are drawn to fluctuations in the material distribution (such as cross-links or unusual coordination sites) constituting "abnormal" regions. Surfaces or interfaces between materials in composite structures are the most obvious macroscopic realization of defect structures.

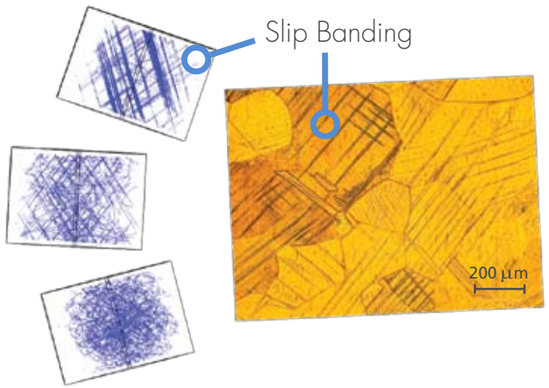
The imperfections in these otherwise homogenous materials create gradients in local properties affecting how the material and an applied field interact with one another. Here, fields are defined quite generally, including mechanical strains, temperature and chemical gradients, and electromagnetic fields. Depending on the physical arrangement and concentration of the defects and the result of the interaction, the net effect could be either diffusive scattering of the impinging field or controlled focusing resulting in a transformative event. This outcome may then be either highly beneficial or detrimental to the material's desired functionality. The quantitative understanding of how defects and interfaces interact with fields, and how they can then be arranged or manipulated for an optimal effect, is then a core challenge to quantitative materials science and attaining predictive design capabilities.

In general terms, the desired functionality can be grouped into three classes: mechanical response; chemical transformation; and electronic/photonic interactions. The first class includes structural deformation spanning static through shock loadings and



Temperature distribution calculated from a molecular dynamics simulation of 10-nanometer void collapse in the explosive RDX (red is 1000 Kelvin, blue 300 Kelvin). At left, a shock wave (lighter blue) is approaching the void, and at right, the shock has collapsed the void. Shear bands that spontaneously arise in the compressed perfect crystal also give rise to temperature increases.

its dependence on morphology and texture as well as changes resulting from aging and environment. The second includes both desired chemical transitions, such as catalysis or electrochemical changes, and corrosion processes or their prevention. The third category includes aspects of superconductivity, electronic devices, photovoltaic applications, and detector development. These classes of materials functionality all require a common set of crosscutting tools for their understanding: characterization and diagnostic capabilities; theoretical analysis and modeling tools; synthesis, fabrication and processing capabilities; and the ability to apply a range of external environments. The examples accompanying this article address each class of functionality and many of the applicable tools.



Complex interactions of slip banding superimposed on polycrystalline structure in a strained copper sample are revealed by micrography (at right). Simulations show the effect of orientation of the crystal with respect to the applied strain on the resulting slip band structure (blue lines).

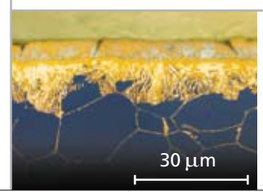
Material functionalities to fulfill Los Alamos National Laboratory's mission challenges span requirements in nuclear weapons stockpile stewardship (e.g., materials aging and replacement), threat assessment and reduction (e.g., material evaluation and detector development), and energy security (e.g., robust energy sources, transmission and energy-efficient devices). Functionality for these applications depends on the limitations/benefits arising from defects and interfaces, and these pose three scientific questions cutting across these seemingly diverse areas.

- Can we characterize or determine how the defect/interface interacts with an applied field, and partition this response into deterministic (controllable) vs. stochastic (random) contributions?
- Can we develop a multiscale understanding for how response originating from these centers (likely captured at the atomistic level) coalesces into a bulk response, and define the criteria for the evolution of the response, be it stable or unstable?
- Knowing a desired level of functionality or tolerance, how do we predict and process the microstructure to achieve and maintain it?

We consider each of these questions in turn in the following sections of this article.

Characterization techniques

The first fundamental challenge raised here is identifying and characterizing defect structures and how they interact with applied fields of interest. Los Alamos maintains a strong complement of state-of-the-art characterization tools utilized for these purposes, including scanning probe microscopies for capturing atomistic level of detail, orientation image mapping for characterizing polycrystalline morphology, and diffraction techniques for strain mapping. CINT and its partnership with Sandia National Laboratories is a principal focal point for characterization tools at the atomistic/nanoscale level. Neutron scattering probes at the Lujan Neutron Scattering Center at LANSCE exploit the unparalleled penetrating power of neutrons to directly probe the internal structure and strain of materials rather than relying on the near-surface characterization provided by most other techniques (see "Discovering deformation mechanisms," page 14). Facilities for applying extreme environments (shock loading, magnetic fields, radiation) enable researchers to probe the interactions of defects at low concentrations with strong fields and still generate detectable signals. Extensive laser facilities complete

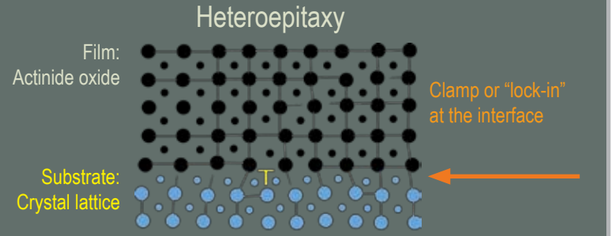


Cross-sectional view of the surface of a tantalum sample containing carbides (yellow) decorating the surface and grain boundaries as a result of heat-treatment in a carburizing environment.

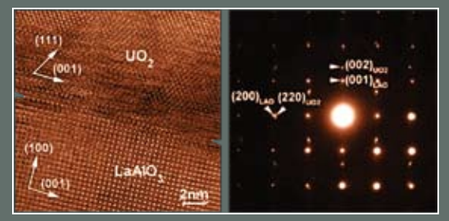
"Locking in" actinide oxides

Electronic functionality

Actinide oxides are of great interest to the DOE as processing materials for nuclear weapons and nuclear energy applications. However, because the actinides exist in multiple oxidation states of varying crystal structure and physical properties, the preparation of single-crystal-like material is necessary for a better understanding of the intrinsic properties of the materials. Standard preparation techniques can produce only limited single-crystal-like samples of these variants required for accurate determination of properties. Los Alamos scientists have been successful in growing thin epitaxial films on a variety of substrates to achieve single-crystal-like actinide oxides with specified oxidation states. This is accomplished because the substrate crystal "locks in" the crystallographic dimensions of the oxides being deposited on its surface. This epitaxy stabilization makes it possible to create crystal structures that might not otherwise be stable in a pure form. This growth technique provides an alternative way to grow single-crystal-like films of various actinide oxides that have not been previously prepared. Characterization of those samples reveals important information needed to fully understand the "real-world" materials, especially where strain and interface may also play significant roles. This methodology is also utilized to tune the electronic and physical properties of the deposited materials in order to achieve new functionality.



A schematic drawing of heteroepitaxy to "lock in" the oxidation-states of the actinide-oxides. The crystal lattice can be pinned by taking advantage of the strong bonding across the interface between the substrate and the film in heteroepitaxy. Different oxidation-states of actinide-oxides can be formed if the right substrate or epitaxial template is used.



Epitaxial (100) UO_2 films deposited on a single crystal (100) $LaAlO_3$. a) a cross-sectional high-resolution electron microscopy (HRTEM) image taken along the [100] $LaAlO_3$ zone axis; b) the selected area electron diffraction pattern. The HRTEM image shows a sharp interface between the UO_2 film and the $LaAlO_3$ substrate. There are no detectable second phases and no voids in the film. The well-defined and sharp diffraction dots on the diffraction patterns further confirm that the UO_2 film is of high-quality epitaxy.

the set of tools available to create and characterize defect centers with exquisite spatial (nanometer) and temporal (femtosecond) resolution.

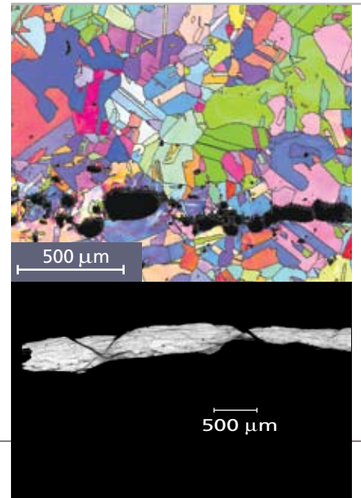
A closely related issue is understanding how much of a material's functionality is stochastic versus deterministic. The explicit answer to this question depends on what the material and phenomena are, where all interactions will have some level of intrinsic stochastic response arising from thermal fluctuations. Beyond this, there will arise effectively stochastic behavior from the details of the material structure that are unknown for the particular sample being studied. One approach to separating these factors is synthesizing well-controlled high-purity samples. For example, the Laboratory has the premier capability in producing high-quality crystals of high explosive materials critical in understanding the roles played by various types of defects. Similarly, molecular beam epitaxy is utilized to synthesize high-purity nanocrystals and composite structures with controlled interfaces. And, the recently developed method of polymer-assisted deposition is providing access to previously inaccessible relatively large single crystals. Such efforts are critical to quantitatively understanding the fundamental structure-property relations.

In this context, it is worth noting that computer simulations always model perfectly controlled samples, either a truly perfect material or one particular realization of a random structure. Integrating over many such realizations provides a means to characterize the average, deterministic response of materials and the stochastic distributions about that mean. These tools for the quantification of uncertainty, initially developed for complex integrated simulations for the nuclear weapons program, are now extended to all aspects of our materials programs and are critical in developing confidence bounds and enhancing predictive capability.

Multiscale understanding and response

The next challenge in this area is quantifying the growth processes of either the defects themselves or the fields generated by them and developing an integrated multiscale framework mapping from the fundamental processes to the bulk response. Capturing these cascading events spans a broad range of length and time scales and presents significant challenges of integration. One example of this is the creation and coalescence of voids leading to material failure, where the voids could be created either through radiation damage or tensile strain. Researchers have conducted experiments to impart systematically controlled levels of tensile strain, followed by imaging the samples using three-dimensional tomography or two-dimensional slices of the material. Sequential experiments are then combined into effective "videos" of the evolving damage at the mesoscale that can be integrated with numerical simulations to infer the location and nature of initiating events. For slower strain rates, the deformation processes can be followed during the experiment using the penetrating power of neutrons, supplemented by traditional surface observations. For high strain-rate studies, Los Alamos has pioneered the development of both the Dual-Axis Radiographic Hydrodynamic Test (DARHT; for x-rays) and Proton Radiography (pRad; for protons) facilities for capturing two-dimensional and three-dimensional time-resolved information of shock dynamics experiments. These techniques have provided us with significant new insights and more quantitative information than previously available for many problems of strategic national interest. (For example, see "Proton radiography," page 22).

Still, most of these dynamic characterization techniques can sample only limited length scales and, therefore, require modeling and numerical simulations to provide the integration through to bulk performance. Particularly through the Nuclear Weapons Advanced Simulation and Computing program, Los Alamos has extensive multiscale modeling capability utilizing our leading high performance computing (HPC) resources. These tools include quantum chemistry (electronic structure) calculations, molecular dynamics simulations, dislocation dynamics, and phase field models for the mesoscale, along with a broad selection of codes for simulating polycrystalline and continuum response. HPC can handle millions to trillions of fundamental cells or particles enabling both high-resolution simulations and the direct leapfrogging of length scales. Examples are explicit atomistic simulations of micron-size samples or continuum simulations having micron resolution. Tim Germann and co-workers have demonstrated the power of this capability in both elucidating and predicting experimental results (see "Shock value," page 15). Even so, there remains a large amount of effectively stochastic structure (e.g., polycrystalline morphology) that cannot be represented adequately in these simulations, such that a truly quantitative understanding of the response is currently unattainable. Such gaps drive the design of experimental facilities that include multiple diagnostics of the same event, particularly where they



The high strain-rate failure of tantalum (top) appears to nucleate with voids that grow and coalesce along grain boundaries. The crystals are identified by orientation image mapping and are colored by their orientations. The large deformation/high-rate ductile failure of a uranium-niobium alloy (bottom) proceeds by localization of shear bands that cross grain boundaries.

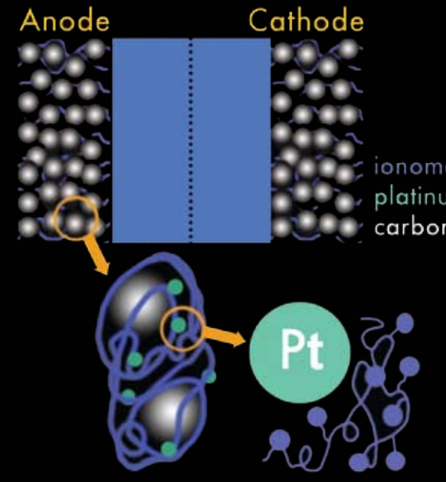
Fuel cell longevity

Chemical functionality

The cost and durability of platinum-based electrodes remain two major barriers to the commercialization of polymer electrolyte fuel cells. With improved electrode structures (see the figure below) that are essentially three-dimensional networks of catalyst-polymer interfaces, the amount of required platinum could be reduced and the durability of the electrode to electrochemical, thermal, and water-content fluctuations could be increased.

Fuel cell electrodes are prepared by dispersing an ionically conducting polymer (ionomer) with carbon-supported platinum nanoparticles in a solvent. Interpenetrating networks of catalyst, ionomer, and pores are simultaneously formed during solvent evaporation and the organization of the materials at many length scales is important. This interfacial structure must carry out three types of transport effectively: (1) electronic; (2) ionic; and (3) mass (gases and water). The resulting structure must also be durable to thousands of hours of operation.

Our approach is to study the evolution of the electrode structure from the dispersion state to the final electrode, using multiple techniques to probe different length scales of interest and to provide both averaged and local spatial information. Ionomer mobility (nuclear magnetic resonance), particle size and internal structure (neutron scattering), phase-segregation tendencies (atomic force microscopy), and platinum-carbon size and spatial distributions (x-ray diffraction and transmission electron microscopy) are examples of information contributing to our optimization efforts at Los Alamos.



Efficient fuel-cell operation requires maintaining a complex hierarchical structure to enable balanced electronic, ionic, and mass transport across the interfaces. As shown here, platinum nanoparticles are dispersed on carbon substrates, which are interspersed with the conducting ionomer, all in close contact with the electrodes.

supply information at differing length scales. This concept defines the path to our MaRIE signature facility to greatly enhance our dynamic characterization capability of materials, especially under the extreme conditions defined by the Laboratory's mission space.

Achieving functionality

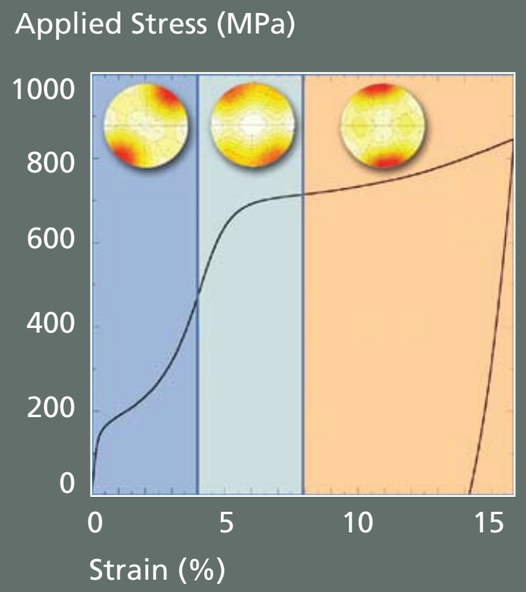
Finally, given some desired functionality and the knowledge of the defects needed to achieve it, how do we design and process the microstructure in order to produce it? Currently, this is typically an empirical process that includes some knowledge of crystal morphology and processing steps. An example here is the formulation of plastic-bonded high explosives, where these typically have 1-2% void fraction. These voids are critical for reliable and controlled initiation and propagation characteristics, but their distribution tends to be an empirical function of crystal morphology, binder choice, and processing sequence. Fundamental studies of the functions of these voids are ongoing and will enable the development of improved formulations. Similarly, oxide-dispersion strengthened steels resist radiation-induced damage by virtue of the oxide particle content, yet predicting an optimal dispersion of these particles and how to achieve it remains challenging. We observe the performance of fuel cells over extended operating cycles (>10,000) degrading due to coarsening of the platinum catalyst particles. Progress is being made in stabilizing the desired structure by varying the chemical methods used in formulating the complex platinum/carbon support/polymer system (see "Fuel cell longevity," page 13).

Most recently, the development of layered copper/niobium materials (~5 nanometer/layer) showing remarkable strength and resistance to radiation damage is a magnificent demonstration of the utilization of interfaces for controlled properties (described on page 6). Our current challenge is replicating this type of exquisite control using a variety of techniques to fabricate larger volumes or different morphologies. Techniques we are exploring include molecular beam epitaxy, severe plastic deformation, and exploitation of self-organization phenomena. For the particular arrangement desired, we must understand the scale of the forces between the defect structures and determine how to achieve a stable and long-lived morphology. The grand challenge inherent in developing novel materials for demanding applications is understanding the physics behind defects and interfaces controlling functionality, and then exploiting that physics to discover and optimize new materials.■

Discovering deformation mechanisms

Mechanical functionality

Neutron diffraction provides an unmatched ability to probe bulk materials, particularly those of high atomic number, such as uranium. This is a material that cannot be readily probed by x-rays or other particles that is of high relevance to the weapons program. The stress-strain curve of martensitic uranium – 6% niobium alloy can be broken into three distinct regions: an initial easy plastic deformation, followed by significant hardening, and then transitioning back to a facile deformation process. By monitoring the evolution of the crystallographic texture during deformation as a function of temperature and stress, researchers at LANSCE were recently able to unambiguously identify the micromechanical deformation mechanism active in each regime. As shown below, the inverse pole figures representing the preferred crystallographic texture shown in each segment manifest distinct signatures of the deformation modes. To 4% strain, the material deforms through the motion of twin boundaries to grow preferred martensitic variants. From 4% to 8% strain, the enforced strain is accommodated by a hitherto unobserved mechanical twin. Finally, beyond 12% strain, the material deforms by traditional slip modes that are active in pure alpha-uranium. These micromechanical data are critical for the development of physics-based constitutive models that can be used in predictive computational codes.



Pole figures generated from neutron diffraction data identify the crystallographic transitions that dominate in each of the three regimes of deformation of uranium-6% niobium, as described above.

Tim Germann describes the results of a molecular dynamics simulation analyzing the effects of grain boundaries on void nucleation.

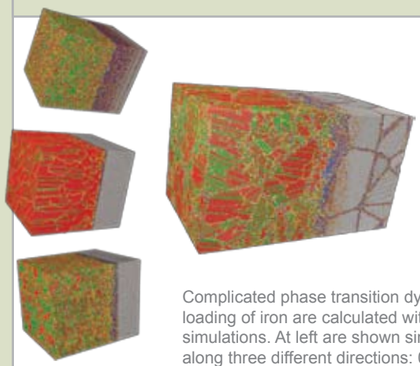
Shock value

The deformation of materials fundamentally depends upon atoms sliding past one another. Tim Germann's passion is developing large-scale molecular dynamics modeling tools to analyze, visualize, and ultimately better understand these atomistic-scale interactions. He came to Los Alamos to help develop the SPaSM (scalable parallel short-range molecular dynamics) code for the CM-5, the 1024 processor "massively parallel" supercomputer of the day. SPaSM enabled simulation of ion implantation cascades in silicon, which were the first multimillion atom simulations of physical processes. Continued improvements now allow simulations on a trillion (10^{12}) atoms using the petaflop Roadrunner system. This directly represents several cubic microns of material, fully described in atomistic detail. These enormous simulations are able to connect physical responses across several orders of magnitude. Such advances are key to predicting dynamic materials performance for both nuclear weapons and conventional defense technologies.

Germann and co-workers applied these tools to advance our understanding of the pathways and kinetics for the phase changes in iron that occur under shock loading. Starting with single crystal samples, they found the response depends upon the crystal orientation, shown on the left side of the figure at right. When the shock is aligned with the 001 direction of the crystal (middle panel) there is a fairly clean and rapid phase transition from the initial body-centered cubic (bcc) structure (grey) to the final hexagonal close-packed (hcp) structure (red). There is some level of polycrystal formation from the initial single crystal (yellow boundaries) and a small amount of twinning (green lines). Comparatively, the phase transition process for shocks aligned with either the 011 or 111 directions (top and bottom) appears to be much more chaotic, continues to evolve over more extended times, and involves a large amount of the metastable face-centered cubic (fcc) phase (green). Along these latter orientations, there are apparently no readily accessible transformation pathways or nucleation seeds, so the transformations likely originate from local thermal fluctuations in the compressed material.

Simulations were then performed on polycrystalline samples with randomly ordered ideal crystals and disordered grain boundaries. The predicted behavior, shown on the right side of the figure, appears to be mostly similar to the 001 direction: a fairly prompt and reasonably clean transition process to predominantly hcp product. There is an identifiable zone of uniaxially compressed bcc material (blue). Clearly, the response of the bulk material is a complex function of the morphology and not a simple average of the individual crystals. The imperfections at the grain boundaries likely help facilitate the phase transition, though several pockets of highly twinned material remain. Further studies are being pursued to deconvolute the controlling factors.

This establishes a general theme that precisely controlled numerical samples containing a prescribed level of imperfections can be used to elucidate the role of those imperfections in the dynamic evolution of the materials. Similar studies are underway to elucidate the mechanisms controlling material failure and surface ejecta under shock loading.



Complicated phase transition dynamics for the shock-loading of iron are calculated with molecular dynamics simulations. At left are shown single crystals shocked along three different directions: 011 (top), 001 (middle), and 111 (bottom). At right is shown a simulation of a polycrystalline sample. Connections between these simulations depend strongly on the polycrystalline morphology.

Extreme environments

The theme of extreme environments refers to materials behavior at extremes of radiation/irradiation, temperature, pressure, shock, detonation/deflagration, harsh chemicals (pH, salts, oxidizing, reducing), magnetic field, and warm, dense plasmas. Many of Los Alamos National Laboratory's national security mission areas require materials to function as designed in such extreme environments, particularly those associated with nuclear weapons and fission or fusion energy. In addition, extreme environments can be utilized to extract information regarding fundamental properties of materials, as well as to induce new states of matter. Such endeavors often require novel diagnostics. A future objective is to characterize and understand the response of materials in extreme environments with the ultimate goal of predicting and controlling functionality of materials in these extremes. Furthermore, we anticipate that such an understanding will open previously inaccessible regimes of materials performance. We include the need to extrapolate the materials properties we can measure to the performance of materials in mission-relevant extreme environments.

Given our objective to control and tailor synthesis routes, processes, and materials response in extreme environments, we define three key scientific challenges critical to this theme area:

- How do we connect the range of scales from quantum mechanical to bulk and attosecond to geologic?
- What is the essential physics and chemistry that must be captured in predictive models?
- Can we access and exploit phenomena that are uniquely stable under extreme conditions?

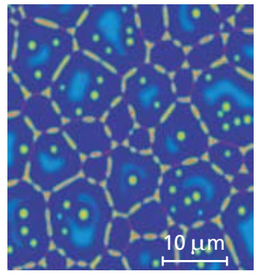
Materials respond to conventional and extreme conditions through time-dependent transformations such as defect formation, defect migration and aggregation, phase transformations, or twinning, resulting in structural and property changes over broad length and time scales. This response is highly dependent on the initial conditions, including those that are process- or manufacturing-induced and/or as generated in nature (weather, environment). The response and resulting dynamic processes are usually initiated at the nanoscale and along interfaces, and evolve as a function of pressure, temperature, deformation, and chemical environment. Understanding the response is essential for developing predictive models of long-term behavior (e.g., nuclear materials, natural hazards), and will impact next generation materials for nuclear energy, transportation (lightweight vehicles, collision response), national security, geothermal energy, and fossil energy. We briefly review and highlight the importance of materials response in four classes of environments important to our missions:

- Radiation extremes
- Thermomechanical extremes
- Chemical and electrochemical extremes
- Electromagnetic fields

Radiation extremes

For Los Alamos to lead the scientific frontiers associated with nuclear energy, we must take advantage of our unique capabilities and diversity to study and control key aspects of the fuel cycle. For example, we understand that interfaces act as obstacles to slip and sinks for radiation-induced defects. Hence, nanolayered composites provide orders of magnitude increase in strength and enhanced radiation damage tolerance compared to conventional materials. Such nanostructured composites have potential applications as structural materials and coatings in nuclear power reactors and other energy and transportation applications, if they could be produced at the necessary volume and cost. Thus, we ultimately desire to control the microstructure of irradiated materials for nuclear energy applications, both fission and fusion, since the microstructure determines critical properties such as thermal conductivity (heat transport) and radiation-induced swelling. Microstructural control will allow for technological advances in support of nuclear energy such as an acceleration of fuel certification from the current 20-year process to a much more reasonable time scale of several years.

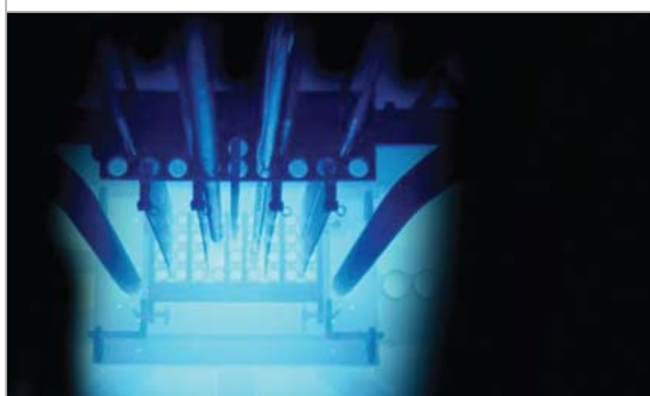
To achieve these goals, the pursuit of the optimal material will require a departure from the historical approach, which traditionally has been of a "cook and look" mentality, with little in the way of detailed modeling or real understanding of the processes that dominate the material response. In the future, we will rely on the integration of multiscale modeling and simulation with experiment to guide material development. Detailed understanding will start with the event origin, i.e., the birth of an energetic fragment or particle through fission/fusion or activated product decay. Next, we must understand the cascade that results from the particle's interaction with the fuel (in the case of fission reactors) or first wall (in the case of fusion reactors), and finally understand the processes that lead



Phase-field simulation of gas bubble nucleation and evolution (helium, yellow) in a polycrystalline material (uranium oxide, blue) showing nearly continuous coverage of the grain boundaries plus scattered interior sites.

to persistent effects such as fuel swelling and/or embrittlement. Achieving this goal will require an investment in new tools for in situ microstructural characterization (e.g., x-ray diagnostics for looking at defect generation and concentrations and its evolution with time), advanced modeling capabilities (e.g., investment in time-dependent formalisms that do not invoke the Born-Oppenheimer approximation), and the development of guiding principles that will enable rapid development of optimal materials. As an example, the figure above shows a state-of-the-art simulation of damage in nuclear fuel caused by fission product migration and associated gas bubble formation. This simulation is one of the current generation of calculations and models that are beginning to capture the essential features of the radiation damage process. Ultimately, a predictive capability will guide the development of new materials, providing game-changing technologies for the fuels and structural components for nuclear energy technologies, and is one reason why a robust predictive capability is key to our materials strategy.

The core of the Omega West Reactor, which was used at Los Alamos from 1956 until 1992 for a variety of research projects. The reactor's fuel rods were immersed in water, which provided cooling, moderation, and radiation shielding. The blue glow—called Cherenkov radiation—is light emitted by electrons from the reactor that travel faster than the speed of light in water.

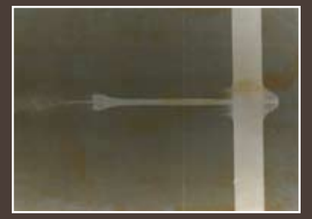


Thermomechanical extremes

The design, synthesis, and manufacture of new materials with increased functionality and performance in the thermomechanical extremes associated with nuclear weapons, homeland security, and energy technologies requires an increase in our fundamental understanding of matter over the broadest range of thermomechanical conditions. Scientific progress in our understanding of a material's response in these regimes will produce models that enable performance predictions and allow us to develop a foundation for functional material control that will ultimately replace process-based qualification with product-based specification. In particular, our current quality and certification methodology for the nuclear weapons complex is, of necessity, more focused on adherence to a detailed process recipe and materials pedigree than on true requirements, because we cannot confidently predict materials performance. Achieving a focus on real requirements—properties—will open the door for manufacturing innovation, modernization, and processing options that will lead to a responsive infrastructure.

The realization of this goal requires an increase in our understanding at all length scales that influence dynamic behavior. As an example, we consider the strength of a material under dynamic loading conditions (see "Proton radiography," page 22). Note the comparison of annealed copper subject to dynamic loading with that of pre-strained copper. This demonstrates how the initial microstructure and its properties (strength) influence dynamic response and will contribute to an understanding of the influence of the microstructure on the performance of materials in extreme environments.

Our ability to make these connections is further complicated for materials that undergo phase transformations, such as tin and cerium, where the material can pass through multiple phases prior to reaching a final solid state with a strength we wish to understand. The ability to predict response and control material properties under dynamic loading is a definable goal of our materials strategy. Thus, to fully understand the details that drive performance will require: a) careful sample characterization (e.g., chemical composition, grain structure, texture, defect concentrations and distributions); b) diagnostics capable of resolving defect mobility, microstructural changes (e.g., grain reorientation growth and temporal evolution; phase), elucidation of the stress field and strain response, and measurement of the dissipative processes (temperature); c) large-scale simulations of these same events to validate our modeling and understanding; and finally, d) how the synthesis and processing affect the end product leading to these microstructural characteristics and their effect on continuum performance. The potential of new facilities such as the proposed beamline for the Dynamic Compression-Collaborative Access Team at the Advanced Photon Source (tunable x-rays coupled to dynamic drivers); the LCLS (LINAC Coherent Light Source) at the SLAC National Accelerator Laboratory (8-24 kiloelectronvolt [keV] x-rays coupled to laser drive); and the possibility of a hard photon source (50-150 keV x-ray free-electron laser coupled to dynamic drivers) at MaRIE, to provide unprecedented characterization of dynamic material processes is fantastic. These types of characterization, in concert with supercomputing capabilities such as Roadrunner and Sequoia (and ultimately, the next generation of exaflop computers), will provide the foundation and validation of accurate physical models that will enable us to move from an era of observation to one of control.

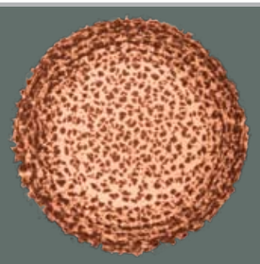


Top: Radiographic image of an explosively formed jet penetrating armor.

Middle: Proton radiography showing shock waves generated from a flyer target impact.

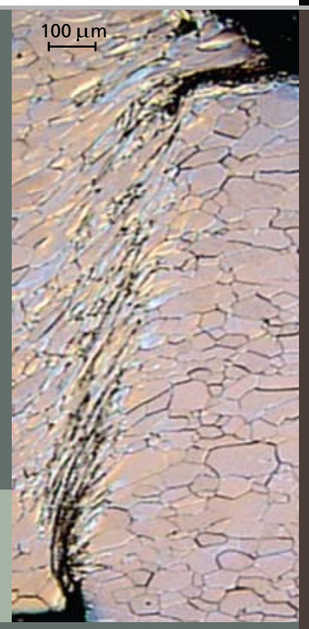
Bottom: Metal interstitial composites (MICs) deflagrating. MICs typically have higher energy density than most high explosive materials and provide opportunities for creating and using the high temperatures for transient experiments and applications.

Thermomechanical extremes can be generated by a variety of methods, including gas guns and explosives. Above: An explosive device is used to defeat a target of interest. In this test, the extremes of pressure and temperature are used to mitigate a potential security threat.



Understanding the influence of microstructure on the response of materials to dynamic loading.

Above: Fragmentation field generated through explosive drive.



Right: Response of a metal to shear.

Finally, access to thermomechanical extreme states of matter results in a rich array of physical and chemical changes that requires a broad range of science, from quantum physics to the collective continuum response, to interpret. The DOE Office of Basic Energy Sciences 2007 workshop report, "Basic Research Needs for Materials under Extreme Environments" offers specific examples, including: "Compression induces changes in bonding properties, giving rise to altogether new compounds and causing otherwise inert atoms or molecules to combine. … When combined with changes in temperature, altogether new forms of matter may be produced." Recently, there has been progress in the generating of new forms of nitrogen (polymeric nitrogen) through the use of "temperature jumps" coupled to diamond anvil cell technologies. To exploit such forms of matter, we must isolate them and verify that they are stable, meaning, the transformation has a large enough kinetic barrier (i.e., analogous to the diamond to graphite transition). Once proven, they will provide new materials that could potentially be used as green, low-signature propellants (e.g., a polymeric nitrogen driven rocket), for low-profile high-energy energetic devices (energy densities approaching 10 times conventional explosives), and in energy storage applications.

Chemical and electrochemical extremes

The concept of chemical or electrochemical extremes is highly material dependent. In general, moderate temperatures and pressures, coupled with extremely reactive materials (oxides, fluorides) create an environment of "reactivity" that is in itself extreme. For example, modern, efficient fuel cell (e.g., molten carbonate) and nuclear reactor (e.g., molten salt reactor) concepts suffer from materials limitations, particularly with respect to corrosion, or their survivability in the chemical extremes created by their operating conditions. Furthermore, some weapon components are found in chemically extreme environments, principally due to their reactivity with other nearby materials, yet need to survive in this environment.

Often, we passivate materials to set up a quasi-equilibrium boundary layer separating the corrosive and the structural material. However, not all materials can be passivated. If we could learn to create atomic or molecular layers that are impermeable and chemically resistant to the corrosive, we could design materials that would meet long-term operational needs in corrosive environments. Therefore, understanding how to cap structures and/or make sites chemically inactive is a long-term goal of our materials strategy. The same argument can be applied to electrochemical corrosion, where in this case, the "cap" may be the development of an insulating layer that prevents the transfer of electrons and thereby eliminates the chemical potential. Thus, when we consider designing materials, we must, in addition to considering bulk material properties such as strength, consider the surface reactivity in the operating environment, which may often place the materials in chemical extremes, and is critical to controlling material functionality.

Chemical and electrochemical extremes also offer opportunities for the destruction of unwanted or undesirable chemical species (e.g., high explosives or nerve gases neutralized in supercritical water), and developing a detailed mechanistic understanding of the destruction process will allow rapid optimization to ideal conditions. These environments may also be useful for synthesis, in "forcing" reactions to take place, when at more modest concentrations, the reactions would never take place. Finally, chemical extremes could potentially be used for the defeat of homemade explosives and terrorist devices, as well as for use in reactive munitions.

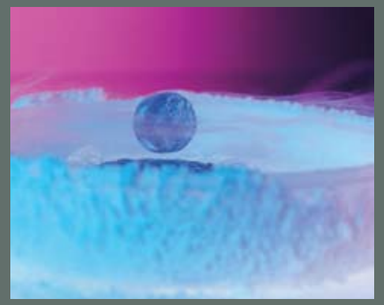
Electromagnetic extremes

The use and application of electromagnetic extremes provides opportunities for answering some of the most challenging intellectual puzzles that remain for solid-state physicists. In addition to pulsed magnetic fields such as those used at the NHMFL (see “In extreme conditions,” *Vistas*, Spring 2009, pp. 28-35), the advent of lasers enabled us to create electromagnetic fields on the order of those in atoms and molecules. Today, magnetic field intensities in the laboratory can approach the coupling energies of correlation effects in electronic materials, with pressures approaching 100 GPa. By using such fields, along with complementary techniques, we are gaining an understanding of fundamental phenomena such as superconductivity. This requires using high magnetic fields in conjunction with electrical conductivity, magnetic susceptibility, optical characterization, and magneto-restrictive response, as well as complementary techniques such as nuclear magnetic resonance and electron paramagnetic resonance. Ultimately, it is our belief that the application of high fields will provide mechanistic insight into the physics of high-temperature superconductors and other devices. This will offer new concepts that could lead to even higher temperature materials, revolutionizing our energy transmission grid and facilitating lossless power transfer across our nation.

As an example, we consider plutonium and its inherent radioactive decay, which means that plutonium will always have some level of impurities. High-field studies enable us to shrink the orbit of electrons and explore intrinsic properties of plutonium and other materials that might otherwise be dominated by such imperfections. This also enables exploration of intrinsic properties of nanoscale materials and effects, since such dimensions correspond to magnetic fields on order of 100 tesla, and of field-polarized states. For these states, probing short time scales also drives one to utilize ultrafast spectroscopy. Recent experiments on cerium doped with lanthanum and thorium demonstrated that magnetic fields induce a phase transition from the alpha to gamma phase in the same way as pressure, providing direct evidence that the dramatic crystallographic change is driven by changes in electronic structure.

Other important applications requiring enhanced and designed magnetic and dielectric materials include pulsed power, semiconductors, accelerators for medical imaging and particle physics, and even synthesis and processing (e.g., the use of fields to develop controlled anisotropies during materials fabrication). One example would be the ability to make compact accelerators. For example, at DARHT, we accomplished a magnetic saturation level with the Axis II induction cells that is 30 times greater than the Axis I induction cells for a size increase of only approximately 6 times larger—a five-fold improvement. This resulted from the use of modern materials, specifically an amorphous metal known as Metglas with magnetic strength five times greater than the standard ferrite cores.

Whether our interest is in coherent control of spin for spintronics, geometric magnetic frustration for novel electromagnetic materials, nuclear magnetic resonance measurements of biological or biomimetic materials, novel superconductors, or weapons materials—extreme conditions of electromagnetic fields provide unique capabilities to measure and control materials and are an essential part of our Laboratory’s materials strategy.■



A magnet levitating above a high-temperature superconductor, cooled with liquid nitrogen. A persistent electric current flows on the surface of the superconductor, effectively forming an electromagnet that repels the magnet. The expulsion of a magnetic field from a superconductor is known as the Meissner effect.

The Single-turn Magnet, capable of producing field in excess of 300 tesla, is proven to leave the sample probe intact in fields up to 240 tesla.

By using modern magnetic materials, DARHT Axis II induction cells achieve 30 times the performance of the Axis I induction cells while being only 6 times larger. As we develop the ability to design functionality into materials, future accelerators will be even smaller, yet have greater pulse length and energies.

Dana Dattelbaum on the edge of the catch tank of her two-stage gas gun holding a diamond anvil cell. The gun and anvil are used separately to create the extreme environments for her materials studies.

Hot spot physics

Hot spots, regions of localized high pressure and temperature in a shocked heterogeneous material, are responsible for the initiation and detonation properties of solid high explosives. However, modern high explosive models treat hot spots empirically, and as a result, scientists have poor predictive capability. Dana Dattelbaum leads a multidisciplinary team working to understand new aspects about the physics of hot spots and their relation to the initiation of explosives.

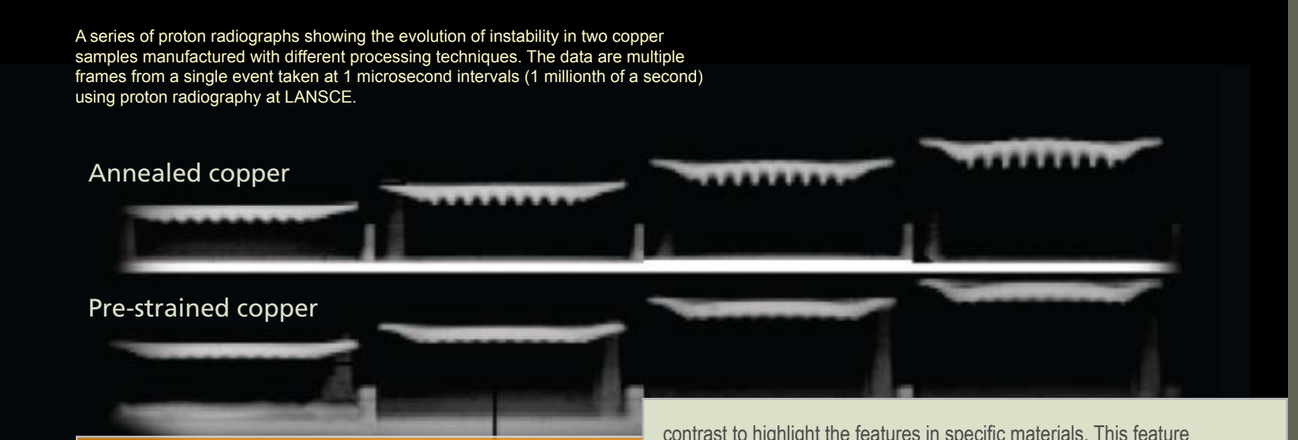
The ignition of hot spots, and their subsequent growth, influences the initiation thresholds, initiation mechanisms, and detonation properties of most condensed phase high explosives, whether conventional, insensitive, or non-ideal. Despite decades of research into the physics of high explosives, at present, researchers have only a basic understanding of the broad mechanisms underlying shock-induced hot spot generation, hot spot ignition, hot spot interactions and reactive wave spread leading to initiation and detonation. A detailed understanding of these processes is absent—precisely why a Los Alamos cross-divisional team is tackling this problem.

The driving methodology of the research is to introduce well-defined hot spot features into energetic materials on the micron scale and understand their influence on shock initiation. For example, gas gun-driven plate impact experiments at Los Alamos National Laboratory have been performed on gelled nitromethane explosive containing particles as hot spot centers. The experiments reveal new insights into the influence of hot spot size and number density on initiation mechanisms and the temporal characteristics of energy release with respect to the shock front and its magnitude.

The large-bore, two-stage gas gun used by Dattelbaum’s team provides well-controlled shock inputs for initiation experiments on energetic materials. Facilities and expertise for the fabrication and characterization of explosive samples essential to interpreting hot spot effects are drawn from across the Laboratory.

Using solid glass beads as well-defined hot spot sources, Dattelbaum’s team has discovered that while large (40 micron) beads at a number density in which they are approximately 2 diameters apart have little effect on the reactive flow at high input shock pressures, smaller (~1 micron) beads, spaced closer together have a measurable effect. Other members of the team have introduced controlled void features into explosive crystals, using femtosecond laser and mechanical micromachining methods, as another type of hot spot seed. Current efforts are working to probe the influence of void features on the hydrodynamic and reactive flows.

Dattelbaum’s research into dynamic properties is supported by static high pressure measurements, focused on improving equations of state for the energetic materials and state-of-the-art reactive and non-reactive simulations aimed at quantifying features of hot spot formation through a collaboration of experimentalists and theoreticians. The work supports the development of next-generation reactive burn models and the improvement of equations of state for numerous weapons-relevant materials.



A series of proton radiographs showing the evolution of instability in two copper samples manufactured with different processing techniques. The data are multiple frames from a single event taken at 1 microsecond intervals (1 millionth of a second) using proton radiography at LANSCE.

Proton radiography

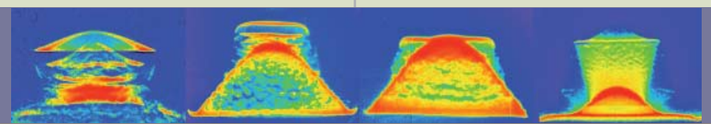
A tool in progressing materials dynamics from observation to control

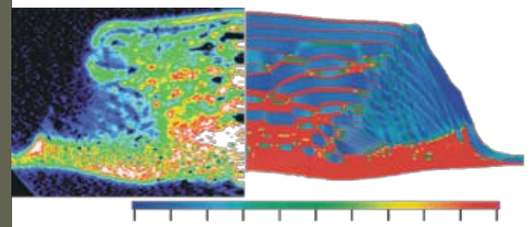
With the cessation of U.S. nuclear testing in 1992, the need to develop predictive models and new experimental probes of the dynamic behavior of materials when driven by high explosives has grown substantially. To quote the DOE Office of Basic Energy Sciences 2007 workshop report, "Basic Research Needs for Materials under Extreme Environments:" "... this knowledge will only be gained by innovative basic research that will unlock the fundamentals of how extreme environments interact with materials and how these interactions can be controlled to reach the intrinsic limits of materials performance and to develop revolutionary new materials." Over the last decade, we have developed a new imaging technique that uses high-energy protons, rather than x-rays, to radiograph materials during dynamic experiments. Proton radiography (pRad) allows researchers to make movies and obtain much more detailed information on the motions and densities of materials when driven by shock compression than was ever before possible. High-energy proton beams serve as an almost ideal radiographic probe for studying the physics of nuclear weapons because their mean free path can be tailored to see inside almost any experiment. Protons are charged particles that bend as they move through magnetic fields, so they can be focused by magnetic lenses. For each experiment, different collimators can optimize the contrast to highlight the features in specific materials. This feature enables the pRad program at LANSCE to address many different physics problems with the same proton beam energy, and thus opens up new opportunities for quantitative experiments, accurate model development, and designer training that will revolutionize how the U.S. nuclear stockpile is stewarded in the future.

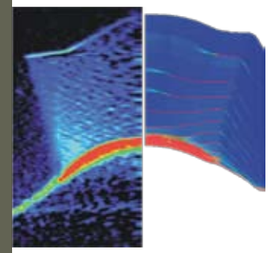
There have been more than 400 dynamic experiments performed since the pRad effort began. Currently, about 40 dynamic experiments are performed each year. Two-thirds of these experiments are related to weapons physics and the other third is designed to study specific weapons engineering issues or to enhance the measurement capabilities at LANSCE. Proton radiography at Los Alamos is being used to perform classified and unclassified experiments relating to equation of state for high explosives and materials, damage and fracture, material properties of explosives, and hydrodynamics. We provide three examples illustrating the impact of pRad on materials research.

For example, proton radiography provides an ideal probe to diagnose dynamic materials under extreme pressures, strains, and strain rates. The series of experiments in the figure above studies the strength of materials at very high strain rates using the detonation products from high explosives (HE) to rapidly accelerate a metal coupon without a shock. On the coupon surface facing the HE, a sinusoidal (ripple) pattern has been machined. This sinusoid acts as a seed for the onset of Raleigh-Taylor (RT) instability growth as the coupon accelerates. The growth of the RT fingers depends sensitively on the initial conditions of the material, which vary with processing. Thus, the slower-growing fingers in the pre-strained (stronger) sample reveal that it resists high strain-rate deformation better than the annealed (softer) sample. These experiments provide data to validate the calculations that model such behaviors under extreme conditions. This technique has been used to investigate the high strain-rate strength of different metals manufactured under various processing techniques.

A series of proton radiographs of disks (left to right: aluminum, copper, tantalum, and tin) that have been explosively shocked from below. The radiographs reveal the internal structure of the materials in these extreme conditions. For example, the aluminum sample shows the formation of layers of spall while the tin sample displays characteristics of melting.







Above: Experiment and simulation of the failure of a tin disk due to spall (unmelted). Left: Tin that has melted upon spall. Each set of results displays experimental data on the left and simulations on the right. The shots had different metal thickness, which led to different metal pressures and the difference in spall and melt behavior.

Along with fracture, materials can fail due to spall, where high strain inside the metal causes it to rupture internally. Proton radiography provides a time evolution of the internal material failure mechanisms that characterize spall damage. In the past, models have only been tested by matching the velocity of the outer surface of the failing material. This limited experimental information is not sufficient to constrain the models. A series of pRad experiments examined failure in aluminum, copper, tantalum, tin, and other materials. The figure (below left) shows proton radiographs of the spall failure in these materials at late times. Each material clearly exhibits distinct properties under spall conditions that test both the equation of state and failure models for the materials. It is challenging to use the same computational code to capture the stiff spall layers of tantalum while also capturing the melting of tin.

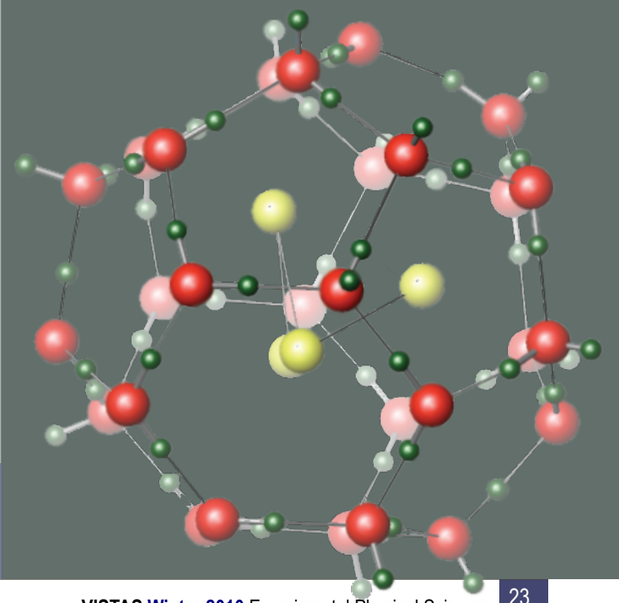
While the preceding showed tin melting, in this final example we explore how changing conditions can result in spall without melting. Proton radiography can capture the different properties of tin under both of these conditions and provide data needed to validate the modeling of these failure modes. The figure above shows comparisons between calculation and experiment for two types of tin experiments; the first, where the tin does not melt, and the second, where the tin does. The shots had varying metal thicknesses, which led to different metal pressures and different melt and spall behavior. Such melt behavior under high-explosive loading is a crucial prediction capability, but it is difficult to find experimental data that reveal enough physics to truly exercise any model. The pRad tin data proved uniquely capable to allow the comparison and give the intuitive understanding of the evolving physical process and the performance of the computational model.

High pressure and neutrons

Optimizing materials for energy needs

HIPPO (high pressure–preferred orientation) was designed with the goal of doing world-class science by making neutron powder diffractometry an accessible tool to the national user community. Located at LANSCE, HIPPO achieves very high neutron count rates, i.e., refinable data in less than 1 minute in some cases. In addition to general purpose neutron powder diffraction, e.g., for crystal structure refinement, HIPPO supports studies of crystal orientation distribution (texture), amorphous solids, liquids, magnetic diffraction, small crystalline samples, and samples subjected to non-ambient environments such as temperature, pressure, or uniaxial stress. HIPPO has unique high-pressure anvil cells capable of achieving pressures of 15 GPa at ambient and high (2000 Kelvin) temperatures. A unique application of HIPPO is research in the field of hydrogen containing materials such as clathrates or hydrogen storage materials. Clathrate hydrates have great potential in energy and environmental applications as a clean energy resource, a CO_2 capture/storage medium, a hydrogen storage material, and a toxic gas separator. The figure below illustrates the crystal structure of hydrogen clathrate hydrate as determined by HIPPO under conditions relevant to energy applications.

HIPPO studies have determined the crystal structure of hydrogen clathrate hydrate at high-pressure low-temperature conditions. Water molecules (oxygen atom–red spheres, hydrogen atom–green spheres) form three-dimensional ice-like frameworks, while hydrogen molecules (hydrogen molecule–yellow spheres) are encapsulated in the cages. Note that the four hydrogen molecules in a large cage are arranged in a tetrahedral geometry and are oriented toward the centers of the hexagons formed by the framework water molecules.



Emergent phenomena

In materials, emergent phenomena can be described as the unique expression of complex behavior and functionality arising from interactions among physical, chemical, and biological properties. These complex materials also respond in interesting ways to environmental conditions. Hence, a predictive understanding of emergent phenomena will enable the controlled design and creation of materials with desirable electronic, photonic, chemical, and energy transduction characteristics. Included in this theme is the discovery science required to generate new materials and the creation of materials tailored for defense and energy security applications.

Emergent phenomena are revealed when the properties of a material cannot be predicted or understood in terms of the properties of the constituents comprising the material. This is often stated as the "whole is more than the sum of the parts," just as the phenomenon of superconductivity cannot be simply predicted from the band structure of a material, but rather results from quantum mechanical phenomena exhibited on a macroscopic scale. The discovery and optimization of emergent behavior in materials with multiple, competing interactions provides an important opportunity in realizing controlled functionality. Emergence is a unifying theme across disciplines ranging from biology to condensed matter physics to nanotechnology. Examples of emergent behavior abound, from the biological function of membranes to the itinerant behavior in the electronic structure of actinide compounds.

Our challenge is to develop sufficient understanding to be able to design and assemble materials with a desired set of emergent properties and resultant functionality. Simply, we aspire to control energy and information transduction in complex materials, and hence their functionality, through manipulation of the charge, spin, and lattice degrees of freedom of a complex material.

Critical questions include the following:

- How can we selectively tune competing interactions to achieve specific emergent properties?
- Can we realize adaptive functionality through emergent phenomena?
- How can we control functionality with novel architectures that result from new synthesis, fabrication, and processing strategies involving hybrid physical/molecular/biomimetic fabrication and assembly concepts?
- On what (materials-specific) time and length scales is emergence revealed? What new tools (experimental and theoretical) are required to discover, characterize, understand, and control emergent phenomena?

Discovery science is required to establish design principles, synthesis pathways, manufacturing processes, theory, and modeling and characterization techniques to realize materials exhibiting new emergent phenomena. The fulfillment of this vision involves discovering the key length and time scales on which emergence is revealed to enable the control of materials structure, dynamics, and function on the appropriate scales. Our vision for future research and development in emergent phenomena requires fundamental studies across a wide range of materials in the three classes of emergent phenomena described as follows.

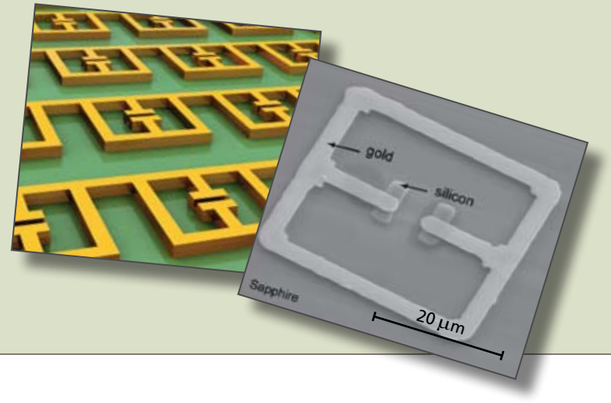
Intrinsic control of emergent phenomena

Intrinsic emergent phenomena derive from the fundamental quantum nature of correlated systems, as revealed by the spin, charge, and lattice degrees of freedom. Controlling the interactions that lead to magnetic, superconducting, and other emergent states of matter requires new knowledge in arenas such as the following:

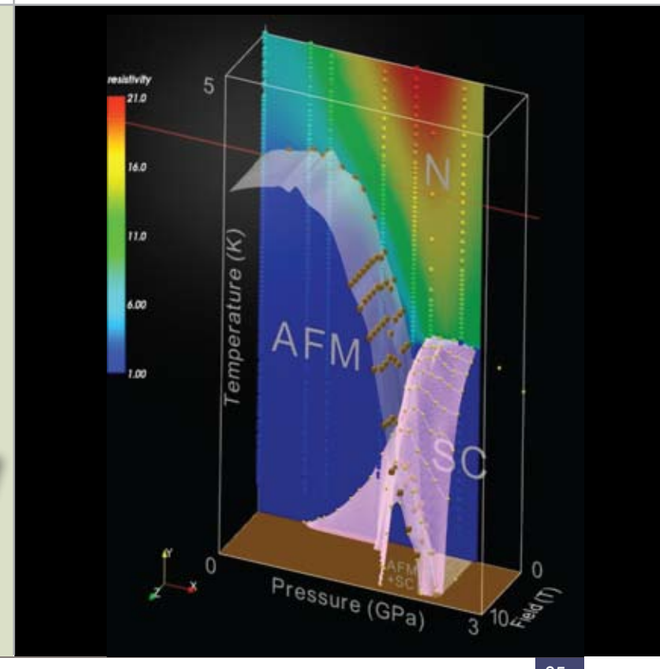
- Understanding equilibrium and non-equilibrium behavior in complex materials
- Controlling properties of plutonium and other actinides through the manipulation of electronic correlations and/or mixed valency
- Designing and optimizing (multi-)functionality in emergent phenomena

Below left: Array of split ring resonators (SRR) that comprise a metamaterial with an electric-only response. Each SRR acts an RLC (resistor inductor capacitor) circuit whose resonance frequency is determined by the dimensions and geometry of the unit cell. An electric field at that frequency applied across the gap induces a resonance that dramatically enhances the interaction of the electric field with the cell. If the wavelength of the light is much longer than the unit cell size, the metamaterial can be considered an effective medium so that the electric response of the material is determined by its extrinsic structure.

Below right: Scanning electron microscopy image of the unit cell of a frequency tunable metamaterial.



Temperature-pressure-magnetic field phase diagram for the strongly correlated material $CeRhIn_5$. At atmospheric pressure, $CeRhIn_5$ orders antiferromagnetically at 3.8 Kelvin. Applying pressure to $CeRhIn_5$ induces a phase of coexisting magnetic order and unconventional superconductivity, and at pressures above 1.7 GPa magnetic order disappears once its ordering temperature becomes equal to the superconducting transition temperature. Applying a magnetic field at these high pressures, however, induces magnetic order inside the unconventional superconducting phase. These results on $CeRhIn_5$ have become a prime example of the remarkable tunability of complex emergent states in strongly correlated matter.



A fundamental type of emergence deriving from intrinsic materials properties involves correlations between electrons in solids, yielding a range of phenomena from magnetism to superconductivity to ferroelectricity. Strongly correlated matter (SCM) refers to classes of such materials that display emergent behavior, resulting from strong electronic correlations leading to a coupling of competing degrees of freedom. A hallmark of SCM is the existence of multiple, nearly degenerate, potentially frustrated, ground states that, in turn, yield a strong sensitivity to small perturbations, a potentially useful feature enabling controlled functionality. (Frustration results from the presence of competing interactions that cannot be simultaneously optimized.) Indeed, plutonium, a material central to the Laboratory's mission, falls in this category, displaying a range of unexpected emergent properties such as the dramatic change from the ductile behavior of delta–plutonium to the brittle behavior of alpha-plutonium via electronic tuning.

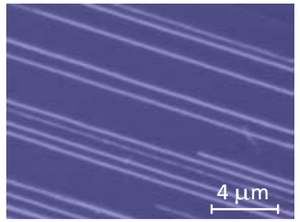
The experimental discovery of new SCM materials and phenomena that drives the formulation of new theoretical concepts and organizing principles will allow an understanding of the fundamental connections between correlations, competing interactions, and emergence in SCM, ultimately enabling their control. For example, the development of an understanding of the role of anisotropy in unconventional superconductivity, ultimately enabling control of the mechanism through the growth of specific crystal structures, is a challenge relevant to emergence in SCM. The full range of state-of-the-art synthesis, experimental, computational, and theoretical techniques at Los Alamos National Laboratory (including large-scale facility infrastructure at LANSCE, NHMFL, CINT, and ultimately MaRIE) enabling measurement under extreme conditions of pressure, temperature, and magnetic fields coupled to crystal growth capabilities will be required to achieve this goal.

Extrinsic control of emergent phenomena

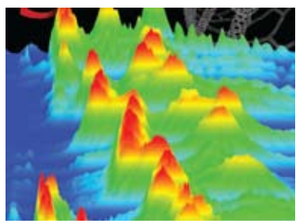
Novel collective and/or emergent phenomena and new functionality in designed materials are produced through discovery, control, and exploitation of nanostructures, quantum confinement, and nanoscale interfaces and defects, such as the following:

- Exploitation of nanostructures to create materials with optimized (multi-) functionality
- Development of hybrid material approaches (e.g., organic-inorganic, bio-mimetic/bio-inspired materials, metamaterials) to achieve desired materials properties
- Understanding of the role of interfaces and defects in controlling emergent functionality

Emergence is particularly important in the design and extrinsic control of functionality in nanoscale materials. Nanoscale architectures may be integrated to produce material systems where the coupling between structures can lead to new behavior. The ability to synthesize and understand novel complex condensed matter systems, combined with the growing ability to engineer various materials components into novel nanoscale structures is allowing a new expansion of our ability to create systems that can perform unique or complex functions based on their emergent behavior. An important feature of both complex systems and nanoscale integrated and composite systems is the existence of active nanoscale interfaces—that is, interfaces that introduce new features that are not intrinsic to either constituent. A key goal is to establish the scientific principles needed to design, synthesize, and integrate materials into nanocomposite architectures and systems such that the collective behavior of these coupled nanomaterials will yield unprecedented emergent functionality. A relevant example of emergence in nanophotonics structures is the development of tunable electromagnetic metamaterials whose linear and nonlinear electromagnetic properties depend on the nanostructure and can be actively tuned, enabling applications ranging from tunable amplitude, phase and polarization modulators, "perfect" absorbers, electromagnetic cloaks, and nanoscale force engineering.



Scanning electron micrograph of ultralong highly aligned single-walled carbon nanotubes grown by chemical vapor deposition technique.



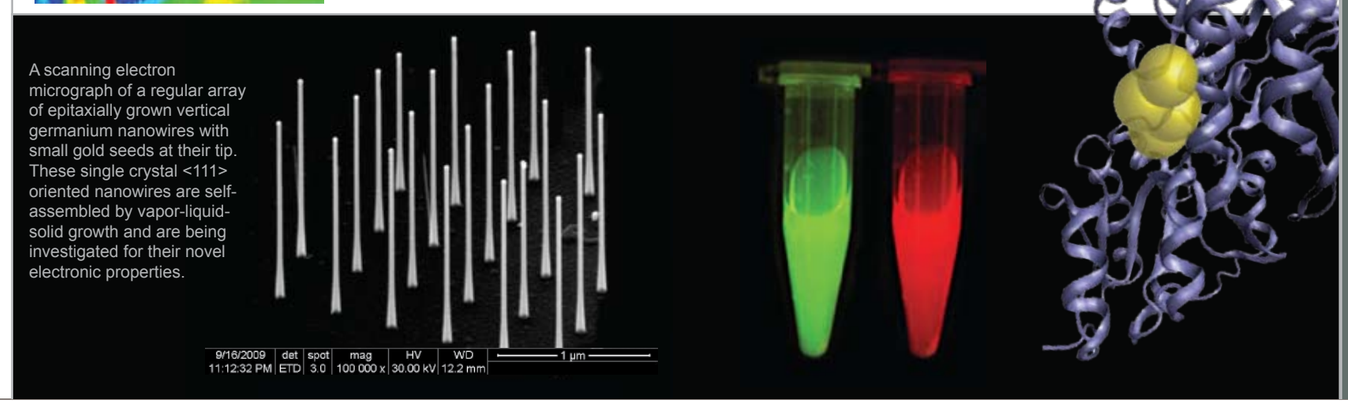
Resonance Raman spectroscopic characterization of a single-walled carbon nanotube ensemble. Each peak in the image represents the optical and vibrational behavior of a specific structure of nanotube and demonstrates the wide range of optical and electronic behaviors accessible with this unique material.

Adaptive control of emergent phenomena

By adaptive materials, we mean materials that respond to environmental stimuli by changes in properties, either intrinsically or in combination with extrinsic control mechanisms, so that the functionality of the material adapts to the environment. This includes the exploration of adaptive materials by developing innovative tools, techniques, and synthesis approaches to develop the ability to controllably vary material properties and thus lead to design principles, as well as the use of adaptive materials and control techniques as innovative tools to reveal hidden characteristics. Examples include the following:

- Exploitation of nanostructures to create materials with optimized (multi-) functionality
- Discovery of new approaches for self-assembly across multiple length and time scales and the control of multicomponent assembly (including classical defects-like dislocations)
- Creation of novel phases and functionality in complex materials using external, adaptive methods including ultrafast coherent control, magnetic fields, and pressure
- Development of new tools to characterize and adaptively manipulate function and mechanism on atomic through micron scales
- Combination of ultrafast and nanoscale diagnostic techniques to dynamically explore functionality, the limits of length and time scales on functionality, and the use of feedback from the system to evolve functionality to a desired state
- Combination of natural (intrinsic) biological phenomena with engineered biological (extrinsic) phenomenon, and its adaptation to or application in imposed environments

Demonstrating the emergent property of wavelength tunable luminescence, small clusters of noble metal atoms synthesized using biological molecules as templates can be used for applications in areas such as biological imaging and sensing.



A scanning electron micrograph of a regular array of epitaxially grown vertical germanium nanowires with small gold seeds at their tip. These single crystal <111> oriented nanowires are self-assembled by vapor-liquid-solid growth and are being investigated for their novel electronic properties.

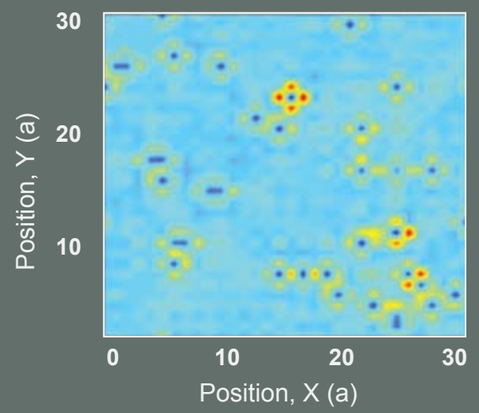
Scanning tunneling microscope

Revealing the wonders of correlated materials

The scanning tunneling microscope (STM) is a tool that utilizes quantum mechanical tunneling of electrons from the tip into a substrate. With its simple mechanism and extreme spatial resolution, STM allows visualization and investigation of the details of lattice forming atoms, magnetic properties of materials, and local electronic and optical properties of materials. STM is only one example of a growing suite of techniques that can be called "scanning probes" that are all focused on characterizing materials with extreme spatial resolution.

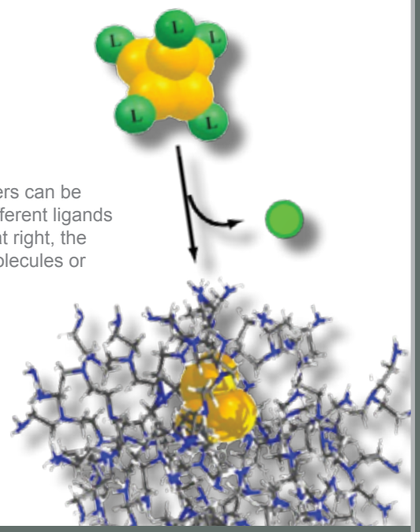
At Los Alamos, scanning probe experiments are connected to theory and modeling efforts through cross-disciplinary collaborations. Theory is focused on modeling and simulation of the mechanisms for STM tunneling, details of the electronic states in materials with strong correlations, and the nanoscale inhomogeneity.

Key questions asked by theorists include how competing interactions lead to the variety of ground states seen in materials, like oxide films, high T_c superconductors and heavy fermion materials, and what controls inhomogeneity and short time-scale properties of materials. Modeling of defects often leads to nanoscale modifications of properties, as seen in the figure below.

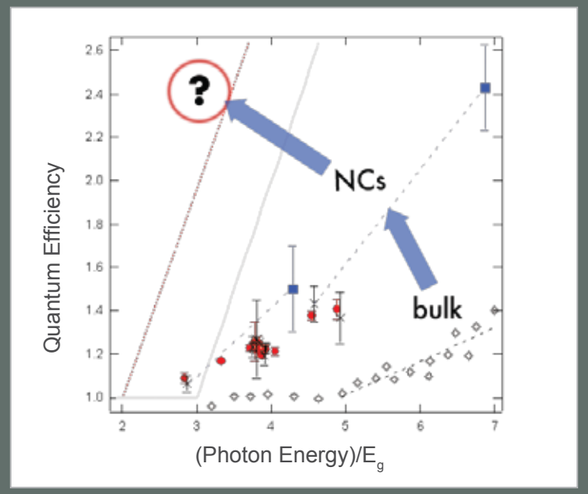


Calculated atomically resolved density of electronic states in d-wave superconductor with static potential impurities, seen as bright spots. Local density of states is the main observable in scanning tunneling microscopy. X and Y units are in angstroms.

The organization and function of a cell is a beautiful example of how molecular and nanoscale components can be assembled into a unit with adaptive emergent properties. The understanding of how to reproduce such emergence in synthetic materials is a central theme in the area of soft materials, involving the direction of self-assembly across multiple length and time scales, the integration of self-assembled systems with templates, and the control of multicomponent assembly. Direct inspiration is provided by biology, and exploring the fundamentals of material assemblies that incorporate biological components or integrate biological and non-biological components is a key area of future research where functions of assemblies will be targeted toward the understanding of emergent properties in complex assemblies. A relevant example of such an inspiration is the development of artificial photosynthetic materials for energy harvesting.■



Fluorescent gold clusters can be created using many different ligands or templates. Shown at right, the templates are small molecules or proteins.



Center for Advanced Solar Photophysics

The Center for Advanced Solar Photophysics, a new Energy Frontier Research Center, cuts across all three focus areas of Los Alamos National Laboratory's materials strategy in its aim to discover solutions to global energy challenges through exploration of novel approaches for high-efficiency conversion of solar energy into electrical power or chemical fuels.

According to Center Director and Laboratory Fellow Victor Klimov, previous advances in this area have mostly relied on iterative, incremental improvements in materials quality and/or device engineering aspects. "However, it is widely recognized that the growing demands of our society for clean, sustainable energy can only be met through disruptive technologies that utilize new physical principles and new materials for approaching thermodynamic efficiency limits in solar-energy conversion," he said. "This represents one of the biggest fundamental challenges of modern science."

The center will explore and exploit the unique physics of nanostructured materials to boost the efficiency of solar energy conversion through novel light-matter interactions, controlled excited-state dynamics, and engineered carrier-carrier coupling. Examples of phenomena studied in the center include: 1) field enhancement in metal nanostructures for improved light-harvesting and high-efficiency coupling schemes; 2) quantum confinement in semiconductors for tailoring absorption spectra and directional transport in energy-gradient assemblies; and 3) strong electron–electron interactions in quantum confined materials for increased photogeneration rates via carrier multiplication. The expected outcome of this research is novel approaches for harvesting solar light and converting it into electrical charge with dramatically increased efficiencies using materials and architectures fabricated via inexpensive, scalable chemical methods.

The DOE-funded center combines the world-leading efforts of both Los Alamos and the National Renewable Energy Laboratory in addition to seven prominent researchers from five academic institutions nationwide.

Left: Developing the concept of carrier multiplication, as first demonstrated at Los Alamos National Laboratory, is a central goal of the Center for Advanced Solar Photophysics. The measured quantum efficiency of electron-hole pair formation per absorbed photon in semiconductor nanocrystals (red and blue symbols) as a function of photon energy normalized to the nanocrystal energy gap (E_g) reveals that nanocrystals exhibit a lower energetic threshold of carrier multiplication than the bulk phase semiconductor (black symbol). Goals in carrier multiplication research include elucidation of its mechanism, reduction of the energetic onset to the energy conservation limit of 2 E_g, and improvement of the spectral efficiency to one electron-hole pair per E_g of photon energy.

Superconductors by design

Filip Ronning (left), Jian-Xin Zhu (center), and Eric Bauer (right) discuss design principles during the growth of a new superconductor in a project aimed at understanding anisotropy to develop superconductors by design.

Condensed matter physics is entering an exciting age where the emerging ability to control materials functionality offers tremendous promise for addressing the world's most basic energy needs.

Key to fulfilling this potential is superconductivity, the perfect flow of electricity resulting from quantum mechanics on a macroscopic scale that may be harnessed for energy storage or efficient power transmission. The specific class of unconventional superconductors uses inherent strong electronic correlations of d- or f-electrons to enable control of superconductivity, allowing the flow of current without loss at temperatures nearly half that of room temperature, and thus providing the best opportunity for meeting these energy needs.

"But, almost all the known superconductors have been discovered by accident," said Filip Ronning, highlighting the inability of the international scientific community to design superconducting materials from basic principles. Ronning and Eric Bauer lead a world-class team of experts in superconductivity that aims to establish the scientific foundations to develop superconductors by design. The team includes Los Alamos researchers and international collaborators specializing in condensed matter, high magnetic fields, and materials synthesis.

To discover the fundamental atomic-scale, structure-property materials characteristics generating unconventional superconductivity, the team employs an integrated experimental, theoretical, and simulation approach to expand the limits of research and materials synthesis at high magnetic fields and pressure. The research is funded by the Laboratory Directed Research and Development program.

Experimental work identifying which materials-specific anisotropic properties correlate most strongly with superconductivity is combined with theory developing the predictive capabilities to identify the correct atomic building blocks of these correlated electron materials for improving superconducting properties. Out of this, a set of design principles is being developed to optimize the desired anisotropic aspects and ideal crystal structure for unconventional superconductivity.

The ability to perform a systematic exploration to identify and control important anisotropies giving rise to superconductivity is singular to Los Alamos, according to Ronning. "Our focus on f-electron materials at Los Alamos makes us unique. The lower energy scales in these particular materials are highly tunable and allows for their systematic exploration in ways that we simply couldn't do in other strongly correlated electron systems, like the high-T_c cuprates," he said.

In its quest, the team relies on a comprehensive suite of experimental probes and state-of-the-art theoretical tools found only at Los Alamos. This includes the NHMFL and the associated one-of-a-kind transuranic angle-resolved photoemission spectroscopy. State-of-the-art theoretical tools for strongly correlated electrons include the local density approximation coupled with dynamical mean field theory.

"Designing unconventional superconductors is certainly a grand challenge, one that might fit well within the concept of a facility like MaRIE. It has that kind of depth," Bauer said. The research "is definitely something to be excited about," as the team's success will take condensed matter to a new level of understanding in superconductivity and materials research.

Implementation

People, facilities, and capital equipment

In implementing our strategy, we choose to focus on capabilities as embodied in people, capital equipment, and facilities. Our strategic vision, mission, and themes guide us in determining the key capabilities that carry us forward. The process by which we translate those strategic elements into an implementation plan is through analysis of our strengths and weakness, along with the external opportunities and threats. A current status snapshot and gap analysis complete the input data that will result in an implementation plan to be issued in fiscal year 2010.

A vital Laboratory is built upon curious and creative people. Los Alamos scientists, engineers, and technicians exhibit infectious enthusiasm and world-class expertise for scientific discovery and technology development. We are committed to recruiting and supporting tomorrow's exceptional and innovative staff. Our vibrant postdoctoral program, admired as a model by our sister laboratories, is the foundation for our talent pipeline, as well as for growing our network of collaborators worldwide. The integrated teaming that occurs across the Laboratory—an expert in any discipline a scientist might wish to consult is likely only a mesa away—further distinguishes our approach. Last, we seek mid-career hires to fill key leadership roles. We will continue to use these well-established mechanisms to nurture the research endeavors that propel us to make controlled functionality of materials a reality.

Well-equipped, state-of-the-art laboratories are the second key ingredient to successful execution of our materials strategy. Techniques underpinning materials research include, for example, x-ray characterization, spectroscopy, crystal growth, metal casting, forming and joining, ion beam deposition, and, of course, electron microscopy (see accompanying feature). Today's economic realities require that we invest wisely, per our strategic priorities, in order to thoughtfully maintain our laboratories to continue to attract and satiate the curiosity of our researchers.

Our user facilities are a magnet for bringing people, staff as well as collaborators, to the Laboratory. Los Alamos's planning and development efforts toward realizing MaRIE, our future signature experimental facility, are crucial in supporting our materials strategy. The first step on the path to MaRIE is the LANSCE Refurbishment Project, which builds upon the established success of this user facility to enhance its ability to probe even more deeply into materials science unknowns. Together with CINT, the NHMFL, the Materials Science Laboratory, the Sigma metallurgical facility, and the plutonium facility, this suite of specialty facilities enables us to fabricate and characterize materials using any element in the periodic table, and thus showcase our leadership in materials science for national security.

Los Alamos National Laboratory is committed to advancing the frontiers of materials science and engineering and condensed matter physics in order to continue providing innovative solutions to protect the security of our nation. We will do so by advancing our strategic themes in a disciplined and coherent manner. Success is predicated on the differentiation we achieve through our people, tools, and facilities.■

The Electron Microscopy Laboratory at Los Alamos

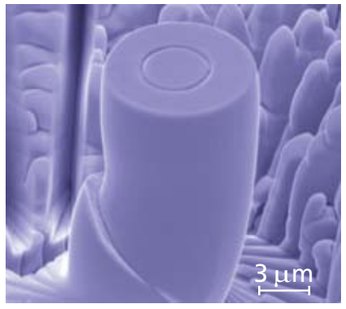
The Electron Microscopy Laboratory (EML) is a user facility dedicated to the support of materials research at Los Alamos National Laboratory through imaging, elemental, and crystallographic analyses of materials microstructures. The EML staff maintains and operates the instruments within the facility for Los Alamos scientists, postdoctoral associates, technicians, graduate students, and visiting researchers.

Since the inception of the EML in the 1980s, the staff and users have developed expertise in materials research that is both broad and deep. Together, they have had an ongoing and significant impact on microstructural characterization for a large variety of materials research programs at Los Alamos, specifically in the study of the effects of variables such as chemical inhomogeneities, processing, stress state, testing temperature, strain rate, and radiation damage on the microstructural constitutive behavior, damage evolution, and electronic and optical behavior of a wide variety of materials. The EML staff and its users maintain an open, collaborative community that, along with a special expertise in unusual materials, makes the facility unique.

Previous microstructural research done by Laboratory researchers affiliated with CINT on the relationships between interfaces and defects in nanomaterials set the stage for the foundation of both of the Los Alamos-based Energy Frontier Research Centers. Similarly, the EML serves as a center for the study of microstructural effects on superconductivity and other phenomena, such as the optical behavior of nanomaterials. An exact knowledge of the material structure and chemistry is essential in interpreting macroscopic behavior and for validating physics models. New state-of-the-art instrumentation being installed in fiscal year 2010 is designed to expand this arena of exploration to the single-atom level, a revolutionary advancement.

Electron microscopy is one technique that serves as a bridge between the present and MaRIE, which will be dedicated to the study of materials in extremes. Currently evolving techniques such as in situ and multidimensional analyses will serve as inroads towards the integrated experiments proposed for MaRIE.

The EML is well positioned to develop novel capabilities for the near and longer term needs of materials research at Los Alamos.



Above: Nathan Mack in the Electron Microscopy Laboratory.

Far left: Pat Dickerson fabricates a micropillar in the Focused Ion Beam Laboratory.

Left: Micropillar after compression testing to failure.

Experimental Physical Sciences contacts

Associate Director
Susan J. Seestrom

Los Alamos Neutron Science Center Facility Director
Kurt F. Schoenberg

Materials Physics and Applications Division Leader
Antoinette J. Taylor

Materials Science and Technology Division Leader
Wendy R. Cieslak

Physics Division Leader
Robert D. Fulton

505-665-4454

ON THE BACK:
The Center for Integrated Nanotechnologies Gateway to Los Alamos Facility, located in the center of Los Alamos National Laboratory's Materials Science Complex, offers users a singular research environment by combining nanoscale materials science and bioscience capabilities under one roof.

Experimental Physical Sciences mission

We develop and apply a broad set of capabilities in materials science and experimental physics to programs and problems of national importance. The success of our science requires world-class research and processing facilities, including our Los Alamos-based national user facilities—the Los Alamos Neutron Science Center, the Center for Integrated Nanotechnologies, and the National High Magnetic Field Laboratory.

Experimental Physical Sciences vision

We cultivate a responsive, high-performance staff that conducts innovative, cross-disciplinary research and development that produces breakthrough solutions to the most pressing national security challenges.

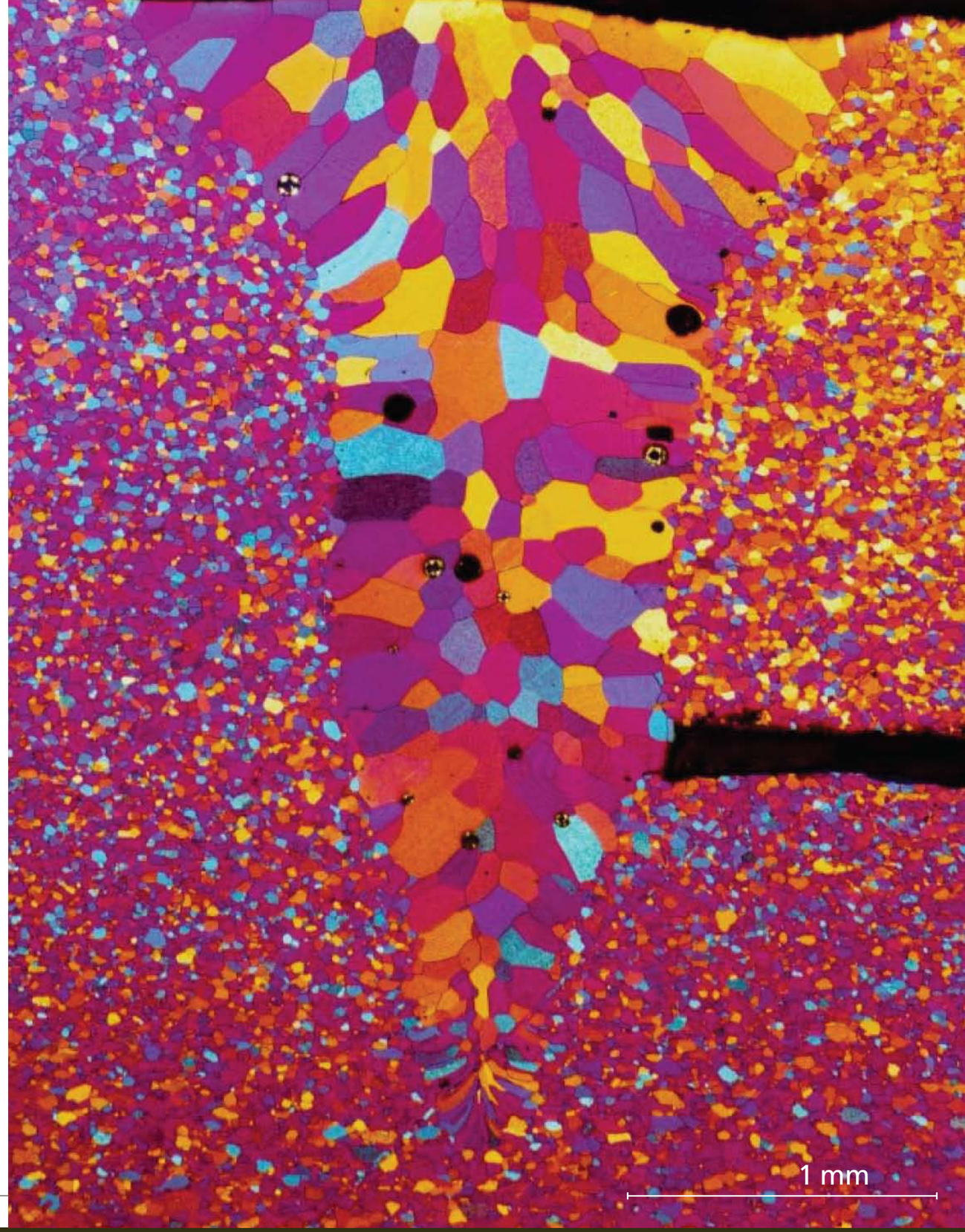
Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by Los Alamos National Security, LLC, for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396

A U.S. Department of Energy Laboratory
LALP-09-036

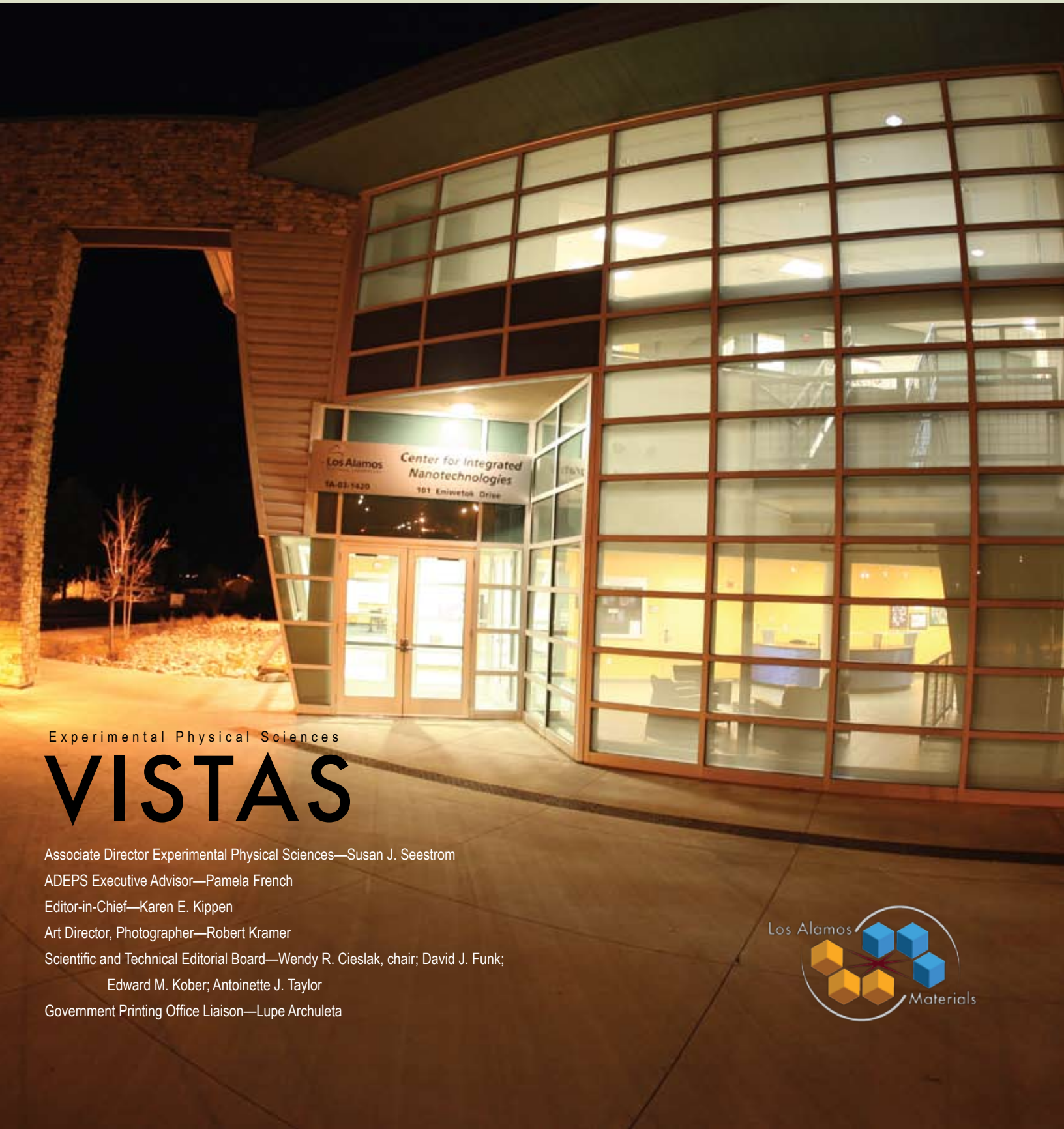
Address Mail to:
Experimental Physical Sciences Vistas
Mail Stop G756
Los Alamos National Laboratory
Los Alamos, NM 87545

Front and back inside covers feature the work of Ramiro Pereyra, who has won top awards in International Metallographic Society competitions, including the prestigious Jacquet-Lucas Award for Excellence in Metallography.

AT RIGHT:
Metallographic evaluations are often done to determine the integrity of welds. Although the depth of penetration was good in this molybdenum weld, porosity (black spots) is revealed in the melted area that will weaken it.



Presorted Standard
U.S. Postage Paid
Albuquerque, NM
Permit No. 532



Experimental Physical Sciences

VISTAS

Los Alamos Materials