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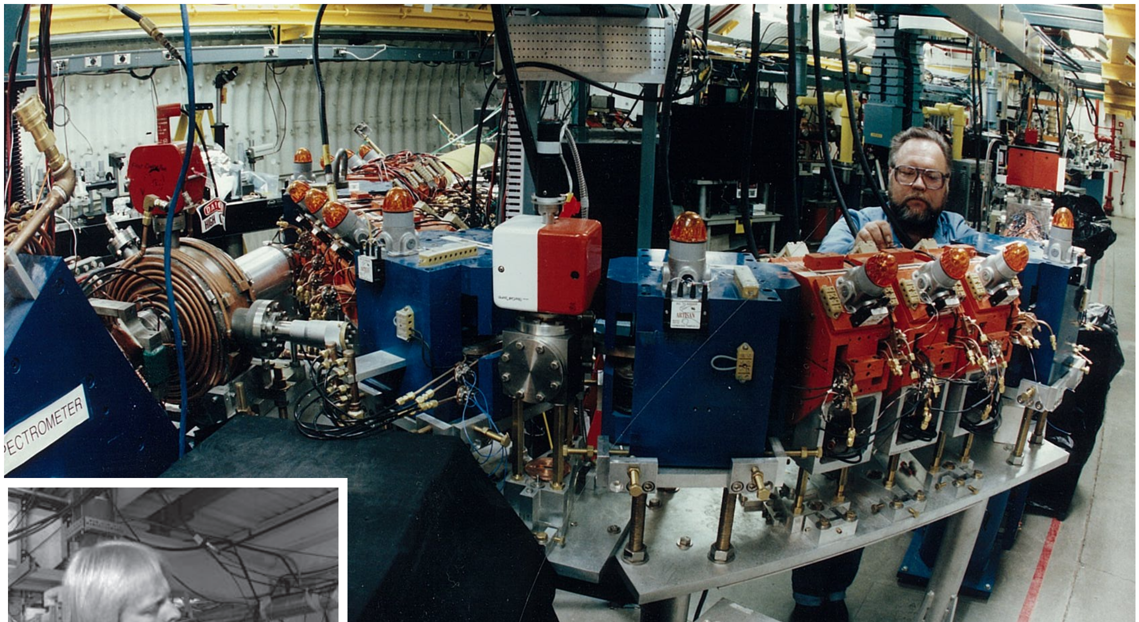
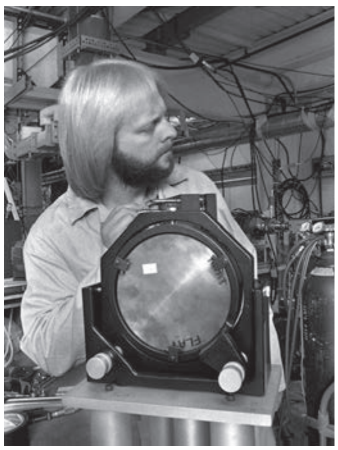
Roadmap to MaRIE

Inside

Los Alamos NATIONAL LABORATORY EST.1943





Key technologies originally developed at Los Alamos in the 1980s and 1990s enabled the present XFEL facilities currently in use worldwide.

In this early-1980s photo (above left) Michael Whitehead works on FEL optics as part of the AT-1 free electron laser experiment. Above right, a technician preps equipment in the 180 degree bend of the Energy Recovery Experiment.

MaRIE's next-generation XFEL builds on decades of Los Alamos R&D

Los Alamos National Laboratory's proposed MaRIE facility is slated to introduce the world's highest energy hard x-ray free electron laser (XFEL).

As the light source for the Matter-Radiation Interactions in Extremes experimental facility (MaRIE), the 42-keV XFEL, with bursts of x-ray pulses at gigahertz repetition for studying fast dynamical processes, will help accelerate discovery and design of the advanced materials needed to meet 21st-century national security and energy security challenges.

Yet the science of free-electron lasers has a long and distinguished history at Los Alamos National Laboratory (LANL), where for nearly four decades Los Alamos scientists have been performing research, design, development, and collaboration work in FEL science. The work at Los Alamos has evolved from low-gain amplifier and oscillator FEL development to high-brightness photoinjector development, and later, self-amplified spontaneous emission (SASE) and high-gain amplifier FEL development.

Advancing FEL physics

Early FEL research at Los Alamos, beginning as far back as 1977, saw the achievement of experimental demonstrations and theoretical understanding of the high-power FEL oscillators—in particular the FEL oscillation with side bands, the first demonstration of an FEL with energy recovery, the first high-

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MaRIE's next-generation ... cont.

efficiency FEL with a tapered wiggler, and the first harmonic lasing in the ultraviolet realm.

The main driving force for this early work came from Strategic Defense Initiative Office funding to support a high-power FEL prototype design at Boeing with an ultimate goal of building a multi-megawatt FEL facility at White Sands Missile Range in New Mexico.

Intensifying the science

By 1985, with the invention of the radio frequency (RF) photoinjector at Los Alamos, LANL scientists began to characterize, understand, and design a new class of electron injectors that deliver electron beams with very high phase-space density—or high brightness.

Simulations of the first photoinjector experiments and early photoinjector designs at Los Alamos National Laboratory showed an unexpected increase in the beam brightness if a specific electron-focusing scheme was used. Los Alamos was the first to identify, explain, and use this approach for the next generation of very high-brightness electron sources.

These inventions led to the worldwide development of high-brightness electron injectors that are being used as the front end of today's XFEL.

Recently, a continuous-wave normal-conducting RF photoinjector has been tested at LANL that would have produced the high-average-current electron beams to drive the U.S. Navy's high-power FEL.

Richard Sheffield (right) and Dinh Nguyen at the Advanced Free Electron Laser Facility, around 1993.

Demonstrating success

In late 1990s, Los Alamos collaborated with the University of California, Los Angeles (UCLA) to demonstrate the principle of SASE experiments in the infrared wavelength. The key to SASE success was the high-brightness electron beams that were available from the Advanced FEL photoinjector at Los Alamos. The LANL team executed two high-gain SASE experiments: one with an undulator designed and built by LANL; the other with a longer undulator designed and built

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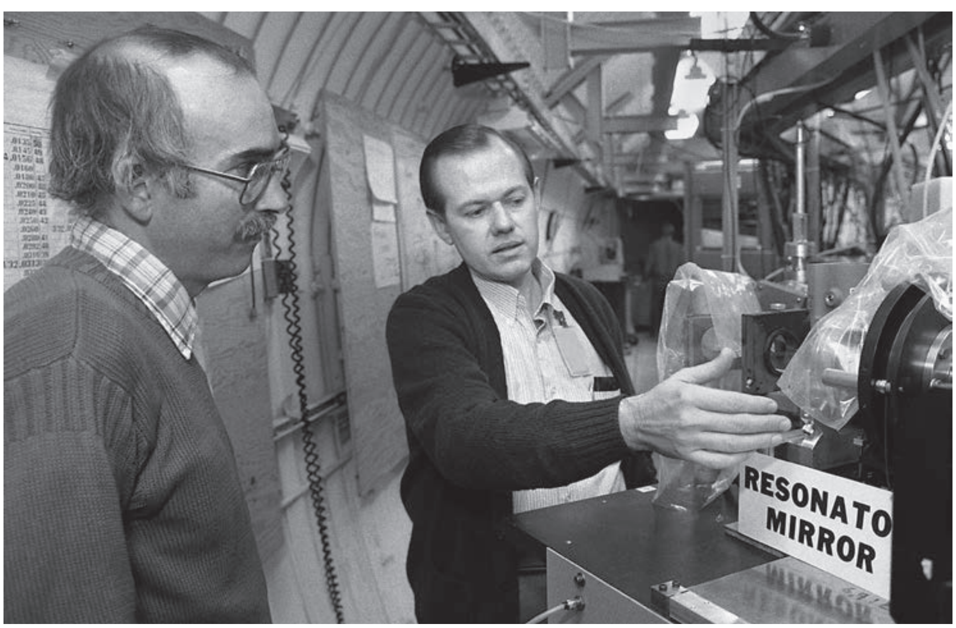
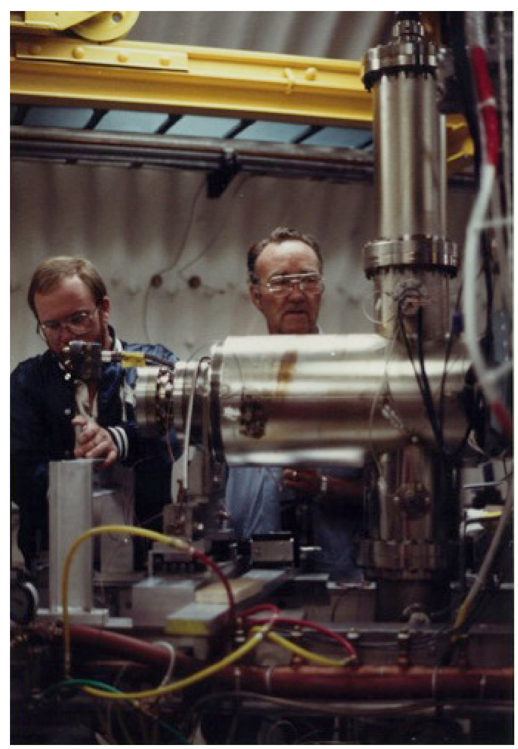


Above: Jerry Watson (right) and Tom Wangler inspect an optical resonator mirror during the 1983 free electron laser dedication. Right: Scott Volz and Boyd Sherwood construct the APEX photoinjector.



MaRIE's next-generation ... cont.

by a UCLA/LANL/Kurchatov Research Center collaboration and brought to Los Alamos for experiments. The LANL/UCLA team was the first to show large SASE gains in free space. These experiments demonstrated the necessity of using the high-brightness electron beams from the RF photoinjectors for the high-gain FEL amplifiers.

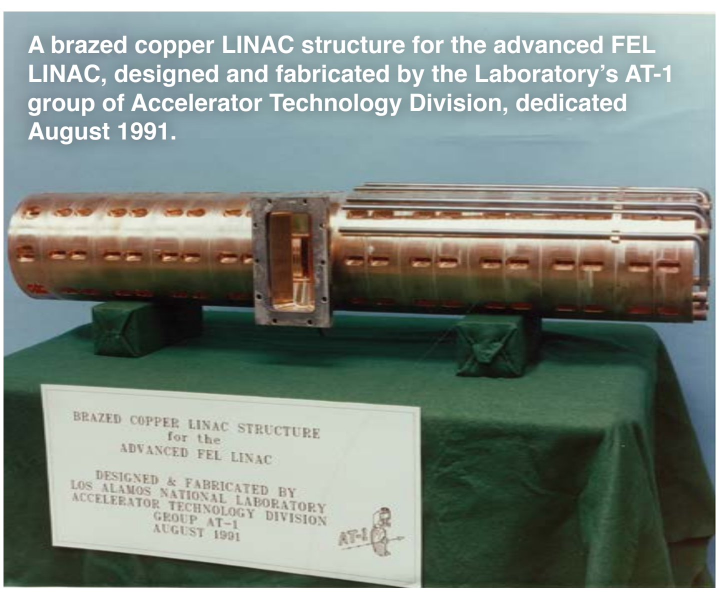
Following the initial success of the pioneering infrared SASE experiments at LANL, other laboratories successfully demonstrated SASE lasing in the visible, ultraviolet, and, finally, x-ray wavelengths. A multi-laboratory collaboration that included LANL was formed to design and build an x-ray SASE FEL called the Linac Coherent Light Source (LCLS) at SLAC. In 2008, SLAC successfully demonstrated SASE lasing with the LCLS at angstrom wavelength, claiming the title of the world's first hard XFEL.

Los Alamos National Laboratory has continued to actively engage in developing state-of-the-art RF photoinjectors, superconducting accelerators, advanced beam manipulation, and x-ray self-seeding techniques geared toward the next-generation XFEL.

MaRIE will build upon this rich history in FELs by enabling LANL's strategic planning goal that includes next-generation facilities. Los Alamos researchers are designing a 42-keV XFEL that specifically addresses the application of coherent x-rays to LANL's national security missions. This MaRIE XFEL will facilitate delivery of nuclear and global security solutions, enable innovative science and engineering excellence, and attract and retain a vital future workforce.

Los Alamos National Laboratory is proud to be the host of the International FEL Conference, scheduled for 2017 in Santa Fe, New Mexico.

Technical contacts: Dinh Nguyen, Bruce Carlsten, and Richard Sheffield



A brazed copper LINAC structure for the advanced FEL LINAC, designed and fabricated by the Laboratory's AT-1 group of Accelerator Technology Division, dedicated August 1991.

A researcher adjusts instruments as part of free-electron laser development studies conducted at Los Alamos in the early 1980s.

Probing the unseen

Free-electron lasers defined

Free-electron lasers (FELs) are powerful sources of tunable coherent radiation. An FEL light pulse can put out millijoules of energy in less than 100 femtoseconds (10 trillion in a second). The wavelength of the light is adjustable from millimeters to fractions of nanometers by changing the electron energy and the magnetic system. Peak power arises when a multi-gigawatt electron beam traverses a series of alternating magnets known as a wiggler, interacts with the radiation, and in the process bunches electrons spaced one wavelength apart. The bunched electron beam emits radiation coherently, that is, the emitted radiation waves are in step with one another. The FEL is tunable by adjusting how fast the electron beam travels by increasing or decreasing its kinetic energy, or by adjusting the period or the magnetic field of the wiggler.

MaRIE's x-ray free-electron laser

Multiple radiographs and coherent x-ray diffraction patterns collected at time steps through the evolution of dynamic processes can deliver critical information on the dynamic response to various impulsive loading conditions, such as shock waves or radiation interactions. Los Alamos has pioneered the science and technology of flash radiography since the earliest days of the Laboratory. For example, in the late 1990s Los Alamos scientists invented the technique of charged particle radiography, using the 800-MeV proton beam at the Los Alamos Neutron Science Center to generate multiple "stop-action" radiographs of dynamic systems during a single event.

MaRIE will have the capability to provide a series of images, a movie, over time scales of microseconds through thick samples of material undergoing a dynamic event. Current brilliant x-ray FEL sources focus their beams on small (1-micron or so) size spots with few atoms, and the inelastic scattering deposits enough energy to turn the sample into a plasma.Illumination with higher energy x-rays and a larger spot size and sample volume can reduce the intensity of deposited energy from the x-ray probe, albeit while accepting spatial resolution that is larger. This is exactly the mesoscale on which MaRIE is focused.

Left: Peter Kenesei (Advanced Photon Source, APS), Ali Mashayekhi (APS), Amanda Wu (Lawrence Livermore National Laboratory), Kenneth Evans-Lutterodt (Brookhaven National Laboratory) staging additively manufactured U6Nb measurements using kinoform lens at the APS 1-ID beamline.

Science and technology on the roadmap to MaRIE

Progress on the path optics required for high-energy x-ray light sources

In a promising step toward the development of the wide range of optics needed by MaRIE (Matter Radiation Interactions in Extremes) and other high-energy x-ray light sources, Los Alamos researchers, in collaboration with Brookhaven National Laboratory (BNL) and the Advanced Photon Source (APS) at Argonne National Laboratory, successfully explored the possibility that new diffractive optics can efficiently focus high-energy photons (E > 50 keV).

MaRIE, the Laboratory's proposed facility for time-dependent materials science at the mesoscale, will ultimately provide a bright source of high energy x-ray photons; but without focusing elements, the size of the beam on the sample will not allow the full potential of the source to be exploited. The researchers fabricated two types of refractive optics—the familiar solid refractive lens in an unconventional material (diamond), and the less familiar kinoform shape in silicon. Their work, in preparation for MaRIE, demonstrated the use of silicon kinoform lenses and diamond solid refractive lenses to successfully focus beams of high-energy x-ray photons with energies between 50-100 keV, producing focal spots as small as 230 nm.

Many materials relevant to national security are high-density materials, and these materials are relatively opaque to low energy (E < 30 keV) x-ray photons. To study and understand these materials, researchers would like to deeply probe these materials with sub-millimeter x-ray beams, enabling micron-scale characterization. This characterization in combination with modeling, will give better insight into materials behavior in the extreme environments of interest. Higher energy photons interact less strongly with matter, can penetrate more deeply into material, and deposit less energy—result-

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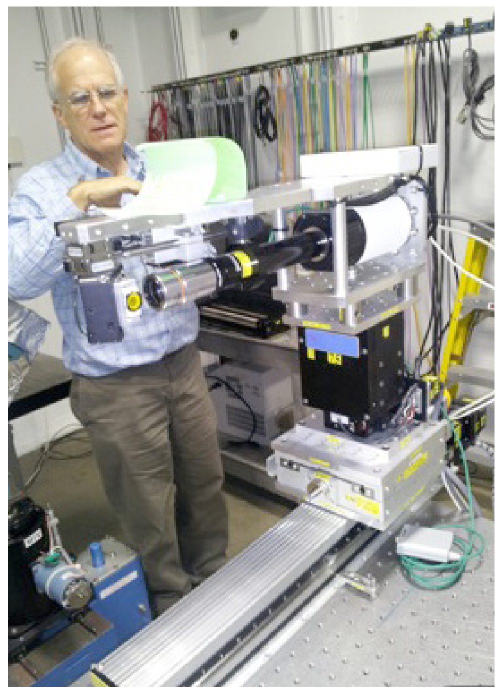
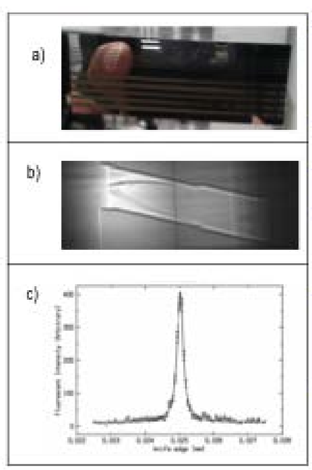


Above: Main collaborator Sarjivt Shastri (APS).

At left, Richard Sheffield checks distances for lens focal length and efficiency measurements at APS 1-ID beamline.



a) Optical image of silicon wafer of size = 1 by 3 cm, showing 10 kinoform lenses. Designed focal lengths were 0.25 m, 1 m, 2 m, 12 m and 17 m. Design energies were 51.2 KeV and 62.5 KeV.

b) X-ray "shadow image" of the f=1m, E=51.2 KeV, (absorption contrast)

c) Results at APS beamline 1-ID, at 51.2 KeV with F=0.25 m: Spot size: 230nm, 1D gain: 87±4, with an efficiency of 17%. Also used same lens to obtain a 1.5 micron spot size at 102.4 KeV

Progress on ... cont.

ing in less probe heating. This weaker interaction with matter is exactly what makes conventional focusing optics such as mirrors or zone plates either ineffective, inefficient, or expensive.

The top panel in the figure on the previous page is a visible light image of a silicon wafer of size approximately 1 by 3 cm on which are etched 10 kinoform lenses. The design and fabrication with electron beam lithography and reactive ion etching was performed at the Center for Functional Nanomaterials at BNL and at the Cornell Center for Functional Nanomaterials at Cornell University. The lenses were tested at the Advanced Photon Source at Argonne National Laboratory. Shown in the middle panel is an x-ray transmission image of the lens showing some of the microstructure of the lens. The bottom image shows a knife-edge scan depicting a spot size of 230 ± 20 nm at 51.2 keV.

The gain was 87 ± 4, i.e. the resultant flux density on the sample is equivalent to increasing the light source ring current by a factor of 87. A 1 m and a 2 m lens were also tested. The 2 m lens had a gain of 181 and a spot size of 1.0 ± 0.1 microns. Finally, the researchers made a first attempt at using a solid refractive diamond lens to focus hard x-rays, and focusing functionality was observed, but given that diamond fabrication technology is not as advanced as silicon fabrication technologies, more research is need to improve performance.

Participants include Richard Sheffield (Experimental Physical Sciences, ADEPS), Kenneth Evans-Lutterodt (Brookhaven National Laboratory), Sarjivt Shastri (Advanced Photon Source), Don Brown (LANL), A. Stein, (Cornell University), M. Metzler (Cornell University) and P. Kenesei (Argonne National Laboratory).

The research, which was funded by the MaRIE program (Cris Barnes, capture manager), supports the Laboratory's nuclear deterrence mission and Materials for the Future science pillar.

Reference: "Kinoform Lens Focusing of High-Energy X-Rays (50-100 keV)," *Proc. SPIE*, **9207**, 920704-1-9 (2014).

Technical contact: Richard Sheffield

Dattelbaum, Saxena named 2014 APS Fellows

The American Physical Society (APS) recently elected Dana Dattelbaum (Shock and Detonation Physics, WX-9) and Avadh Saxena (Physics of Condensed Matter and Complex Systems, T-4) 2014 Fellows.

Dattelbaum was cited for "pioneering studies of dynamic properties and excited state behavior of materials using advanced diagnostics techniques and for her leadership and service to the Society and the Shock Physics community." She was nominated by the Topical Group on Shock Compression of Condensed Matter.

Dattelbaum's experiments in shock sensitivity and dynamics of explosives support simulations of nuclear weapons performance and enhance the safety of the nation's nuclear stockpile. Dattelbaum currently probes explosives during dynamic events but is often restricted to examining surface phenomena. Her current research is on the roadmap to MaRIE (Matter Radiation Interactions In Extremes), where she will be able to investigate what is happening in the bulk material. Dattelbaum received a PhD in organic chemistry from the University of North Carolina at Chapel Hill and joined the Laboratory as a Director's Postdoctoral Fellow.

Saxena was nominated for "foundational contributions to phase transitions in functional materials and nonlinear excitations in low-dimensional electronic materials." He was nominated by the Division of Materials Physics.

Phase transitions can be highly transient processes, and Saxena's work has provided a theoretical foundation for understanding these events. With the exquisite temporal and spatial resolution of MaRIE, Saxena's predictions can be tested experimentally. Saxena received a PhD in physics from Temple University and was a visiting scientist at Los Alamos before joining the Lab as a technical staff member.

APS nominations are evaluated by the Fellowship Committee of the appropriate APS division, topical group or forum,

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Dana Dattelbaum

Avadh Saxena

APS Fellows ... cont.

or by the APS General Fellowship committee. After review by the full APS Fellowship Committee, the successful candidates are elected by the APS Council. APS is a non-profit membership organization working to advance and diffuse the knowledge of physics through its outstanding research journals, scientific meetings, and education, outreach, advocacy and international activities. APS represents more than 50,000 members, including physicists in academia, national laboratories and industry in the United States and throughout the world.

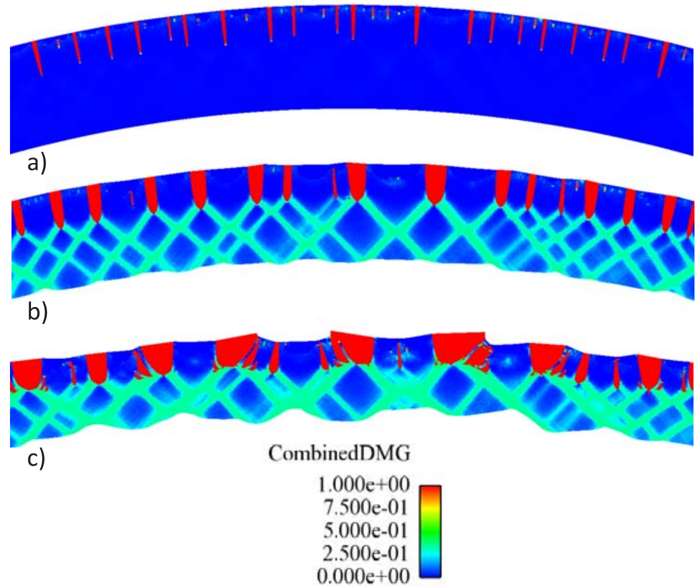
Modeling quasi-brittle damage behavior in metals

Los Alamos National Laboratory (LANL) scientists have developed a new material strength and damage model that accounts for brittle-ductile transitions in the mechanical response of quasi-brittle metals. Fracture behavior is accounted for by evolving tensile and compressive damage separately using energy-based criteria and tensor representation theory. Uniquely, this continuum-scale material model can account for mesoscale deformation and damage mechanisms. For example, strength and plasticity are built on a mechanism-based, viscoplastic framework that can account for mechanisms such as deformation twinning.

This novel model has also been recently implemented into Lagrangian Applications Project (LAP) codes. This framework allows for the study of brittle failure and brittle-ductile transitions in the material response, something that has not been previously possible in macro-scale continuum codes at LANL. Because tensile and compressive damage evolve separately, visualization of mesoscale deformation mechanisms such as crack formation and shear banding is possible. Due to the viscoplastic framework, strength and plasticity responses in this model produce smooth transitions between the elastic and plastic regimes of stress-strain curves. Early comparisons of simulation results to flyer-plate experimental data are favorable.

This work is an example of Science on the Roadmap to MaRIE, LANL's proposed experimental facility for Matter-Radiation Interactions in Extremes. This model is an example of a computational tool that can be informed and validated by the experimental results produced by MaRIE. Such a connection between modeling and experimental efforts would enhance LANL's understanding of material behavior under extreme conditions, and also provide a distinctive capability to predict overall material response.

This work is funded by the Advanced Simulation and Computing (ASC) Program through the Integrated Codes (IC) and Physics and Engineering Models (PEM) program elements. This work supports LANL's Nuclear Deterrence and Stockpile Stewardship mission area and the Materials for the Future science pillar by providing a predictive tool that



Damage evolution of a section of a thin walled beryllium cylinder with a constant internal pressure applied at times: a) 10.0 μs, b) 18.5 μs, c) 25.5 μs. The red regions show tensile damage, specifically crack formation. Green regions show shear band formation.

accounts for the effects of brittle-ductile transitions in material response. Researchers on this project include Abigail Hunter (Computational Physics, XCP-1), Alek Zubelewicz (retired from Physics and Chemistry of Materials, T-1), and Esteban Rougier (Geophysics, EES-17).

Technical Contact: Abigail Hunter

LANSCE resumes 120-Hz operations

The Los Alamos Neutron Science Center (LANSCE) resumed 120-Hz operations in early December, providing the neutron flux to meet a Level 2 NNSA milestone and enabling faster completion of a variety of nuclear physics experiments running at the accelerator-based user facility. LANSCE provides the scientific community with intense sources of neutrons for experiments supporting civilian and national security research.

The resumption is the result of LINAC Risk Mitigation activities. Improvements include a new, fully designed radio frequency (RF) power amplifier, new water systems for the drift tube linac, and upgrades to the linear accelerator control systems. Scientists, engineers, and technicians from Accelerator Operations and Technology (AOT) Division designed, tested, and installed the sophisticated systems. The result enabled a return to high-power operations that had ceased in 2006 due to aging high-power radio frequency equipment.

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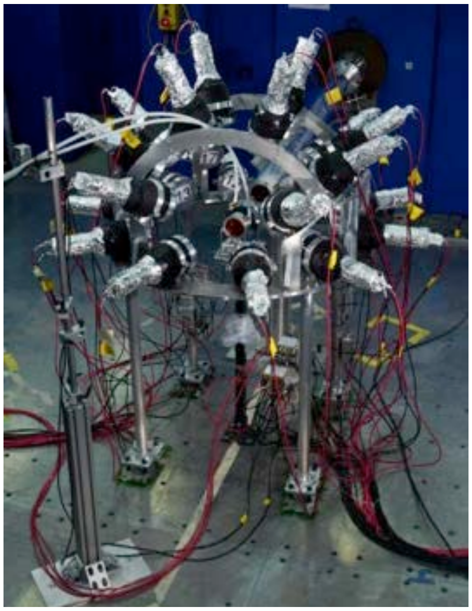
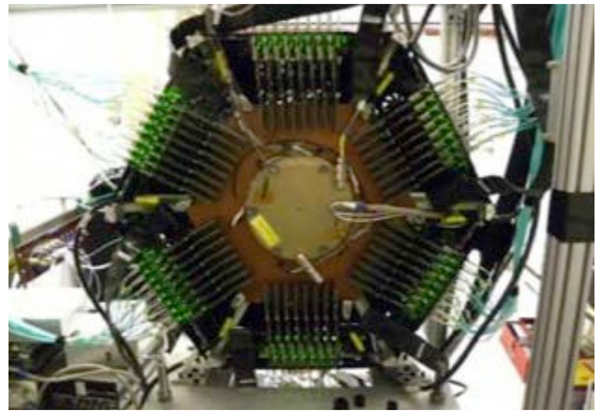
LANSCE... cont.



Fission Time Projection Chamber



Chi-Nu Detector Array

The new Diacrode amplifier-based RF systems for the DTL, part of the LINAC Risk Mitigation activities that enabled a return to 120-Hz operations at LANSCE.

The high-power neutron flux from the higher proton pulse repetition rate enables improvements in data collection by a factor of 2.5 for the fission Time Projection Chamber and the Chi-Nu array. Both are NNSA Weapons program Science Campaigns-funded instruments and active collaborations between Los Alamos and Lawrence Livermore national laboratories. The fission Time Projection Chamber is designed to allow more precise fission cross-section measurements than were possible with previously used techniques. This benefits both NNSA Defense programs and DOE Nuclear Energy programs through increased understanding of energy generation and accuracy in modeling of reactors and weapons. Chi-Nu measures the energy spectrum and number of neutrons emitted in fission, improving confidence in the outgoing fission neutron spectrum as a function of incident neutron energy.

The 120-Hz operation also enables the development of new research facilities utilizing the LANSCE LINAC. The improvements are an example of the Laboratory's LINAC accelerator expertise that could be used to design, build, and operate the MaRIE XFEL, the world's highest energy hard (42-keV) x-ray free-electron laser, which is at the core of the Lab's proposed Matter-Radiation Interactions in Extremes experimental facility for control of time-dependent material performance.

John Lyles and staff (RF Engineering, AOT-RFE) led the high power RF systems effort; Mechanical Design Engineering (AOT-MDE), Instrumentation and Controls (AOT-IC), and Mechanical and Thermal Engineering (AET-1) staff performed water systems and instrumentation and control work. The NNSA Readiness in Technical Base and Facilities (RTBF) program funded the LINAC Risk Mitigation work. LANSCE activities support the Lab's Nuclear Deterrence and Energy Security mission areas and the Nuclear and Particle Physics, Science of Signatures, and Materials for the Future science pillars.

Technical contacts: Kurt Schoenberg and John Erickson

Neutron surface scattering studies demonstrate promise to address important aspects of actinide surface chemistry

Actinides and actinide oxides exhibit some of the most intriguing and challenging chemistry known. Frequently their compositions are not stoichiometrically precise, and their oxide structures can change dramatically under various environmental conditions. Studies of actinide surfaces and surface initiated chemical evolution of bulk materials, at the core of the LANL mission, are even more challenging. The scientific challenge is to identify, measure, and understand the aspects of their surface chemistry—which can depend on preparation methodology and aging conditions—without disturbing their microstructures. For example, the details of chemical evolution on ^{239}Pu surfaces, particularly the Pu valence state, are important for understanding stockpile aging, given the reversible auto-reduction of PuO_2 to Pu_2O_3 under various environments. The other key science question involves reactivity of different actinides with gases and liquids at the atomic and nanoscales.

Recent data generated using the ASTERIX and SPEAR neutron spectrometers at the Los Alamos Neutron Science Center (LANSCE) represents the first measurement of PuO_x, UO_x and Th films using neutron reflectometry (NR). The results hold promise that neutron surface scattering

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Neutron surface... cont.

techniques (with reflectometry, grazing incidence diffraction, and grazing incidence small angle scattering) will give unique insight into these important systems from sub-*nm* to *µm* length scales. Such studies of actinides surface chemistry and reactivity are relevant to a broad spectrum of problems: from environmental remediation to stockpile stewardship.

Neutrons provide a distinct advantage over x-rays in structural characterization of lighter elements and accessibility of buried interfaces, making them an excellent probe for studying and mapping different hydride and oxide forms at surfaces and interfaces of heavy metals. Neutrons, due to their excellent penetrability and comparable scattering cross sections for actinides and isotopes of interest (O_2, H_2, D_2, etc.), are ideally suited to study Å length scales changes in the chemistry of these materials.

Preliminary studies of neutron reflectometry of $^{239}PuO_x$, UO_x and Th thin films were performed at LANSCE using ASTERIX and SPEAR. Several nanometer-thick films of PuO_x were grown on a zirconia substrate with approximately 1 cm^2 surface area (total mass of PuO_x less than 50 micrograms) by polymer assisted deposition. The films of UO_x and Th were prepared by DC-magnetron sputtering. These films were investigated by neutron reflectometry and off-specular neutron scattering to determine their thickness and composition. In case of the PuO_x film (Figure 1), the preliminary neutron scattering data analysis quantifies the characteristics of a high quality film. The scattering length density (SLD) distribution normal to the surface is homogenous and matches almost exactly the literature value for crystalline $^{239}PuO_2$. No lower density region between PuO_2 and zirconia substrate or other chemically different layer at the air interface were observed. The air/PuO_2 and zirconia/PuO_2 roughness were ~20 and ~5 Å *r.m.s*, respectively. Very small off-specular scattering testifies to a high degree of in-plane order within the film.

In the case of Th films in situ time dependent neutron reflectivity was used to measure changes in the SLD and thickness of the material during a controlled oxidation process (Figure 2). As the oxidation progressed, several sub-stoichiometric thorium oxides, ThOx ($x<1$), preferentially formed between the thorium metal and its dioxide layer were observed. The SLD value of these new oxides increased until a constant value for ThO was reached. These NR experiments demonstrated that the kinetically favored ThO can be preferentially generated over the thermodynamically favored ThO_2. The near perfect stoichiometric lattice and relative low O solubility in the ThO_2 top layer limits the availability as well as diffusivity of O species interacting with ThO, and hence prevents or slows the successive further oxidation. The conclusion of this work is that solid-state thorium monoxide, measured for the first time, is produced at material interfaces. The practical implication of this material, for example

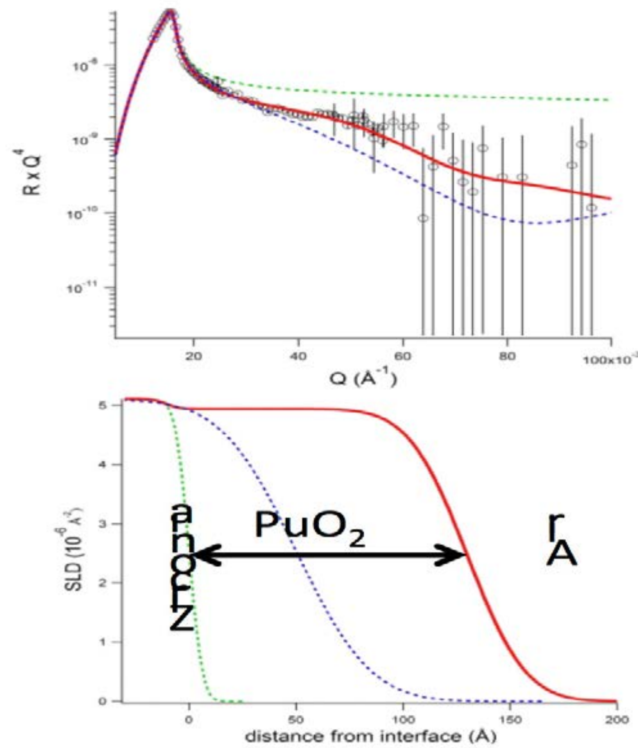

Figure 1: Top- PuO_x NR data (symbols with error bars) and fits (lines) corresponding to scattering length density models presented at the bottom. Green and blue–pure zirconia interfaces with different roughness values. Inclusion of the PuO_2 layer (red) was essential to fit the data.

used as nuclear fuel, could provide an ideal combination of features between metal fuel and oxide fuels. These include the thermo-physical properties relative to metal fuel and chemical stabilities similar to oxide fuel. ThO fuel shows many advantages with enhanced performance over the traditional oxide fuels: namely, high-fissile density (good breeding performance), high-thermal conductivity, and high-melting point with adequate chemical stability.

Using NR, researchers were able to demonstrate the capability to determine the chemical speciation signatures on a complex uranium oxide family. Namely, both the surface and underlying layers of the uranium oxides were characterized with Å-level-resolution. This capacity cannot be achieved using x-ray scattering since it is not capable of distinguishing between U_3O_8 and α-U_3O_8 especially at the nanometer scale. Moreover, the Å-resolution measurement of the chemical speciation and its spatial distribution for nuclear materials of technological importance could foster a revolution in understanding their oxidative behavior by providing new capabilities to exploit rich forensic information and extend fundamental knowledge to assess or interpret the signatures, while leaving the opportunity to employ additional, possibly destructive methods of analysis. The development

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Neutron surface ... cont.

of this method may also be applicable to a broad range of other scientific disciplines.
The work is an example of science on the roadmap to MaRIE, the Laboratory's proposed experimental facility for control of time-dependent material performance. Using MaRIE's advanced capabilities, the combination of x-ray and neutron surface scattering methods will provide unprecedented, time-resolved access to structural properties of actinides and their surfaces from atomic- to meso- scales. A complete picture of the chemical depth profiles and surface topography of hydrides and oxides formed at metal interfaces can be provided. The highly penetrative nature of neutrons together with high energy x-rays will facilitate these studies over a wide range of chemical environments, pressures, and temperatures.

Researchers include Daniel Schwartz, David Moore, and Joe Martz (Nuclear Materials Science, MST-16); Brian Scott, Eve Bauer and Erik Watkins (Materials Synthesis and Integrated Devices, MPA-11); Ann Junghans (Polymers and Coatings, MST-7), Peng Wang (formerly Lujan Center, LC-LANSCE), Kirk Rector and Heming He (Physical Chemistry and Applied Spectroscopy, C-PCS), David Allred (BYU, Provo), and Jarek Majewski (Center for Integrated Nanotechnologies, MPA-CINT).

This research was supported by the Primary Assessment Technologies Campaign, the Los Alamos Laboratory Directed Research and Development program and a G. T. Seaborg Institute postdoctoral fellowship (to H. He). This work benefited from the use of the time-of-flight neutron reflectometer SPEAR and ASTERIX at Lujan Neutron Scattering Center at LANSCE until 2014 funded by the DOE Office of Basic Energy Sciences and Los Alamos National Laboratory under DOE Contract DE-AC52-06NA25396.

Technical contact: Jarek Majewski

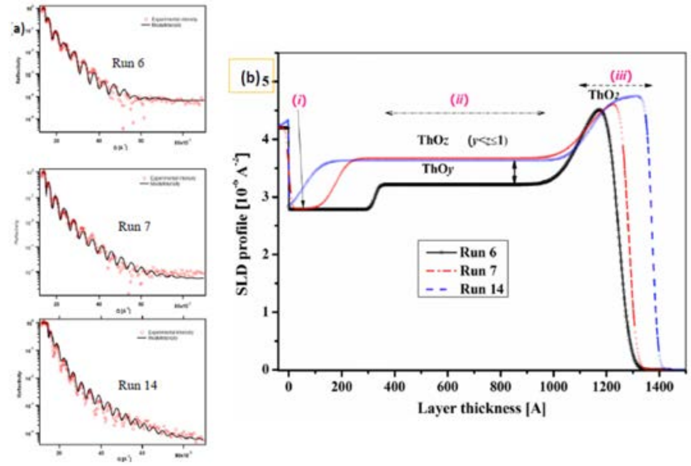

Figure 2: (a) NR spectra in the form of *R* vs. Q_z obtained on thorium coated mono-crystalline α-quartz at mid-stage (Run #6) and near-final-stage (after Run 7) of controlled oxidation after a given exposure to ~100 ppm O_2 in Ar; Run 6: 150°C after ~300 min; Run 7: 150°C after ~250 min; Run 14: 150°C after ~700 min. The data is represented by open circles. The solid lines through the data points are the best-fits based on the real space SLD models presented in (b). The zero thickness is set at the quartz substrate/Th film interface.

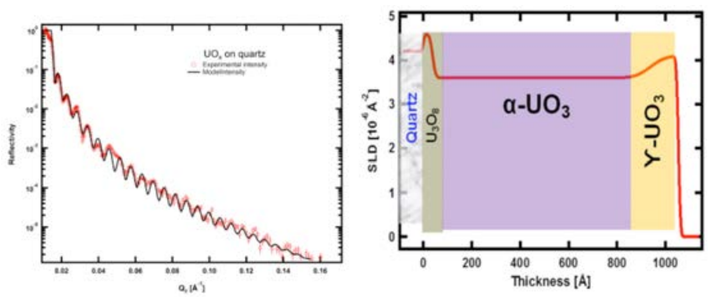

Figure 3: (a) NR spectrum in the form of R vs. Q_z from UO_x coated mono-crystalline α-quartz. The data is represented by open circle with error bars indicating one standard deviation. The solid lines through the data points are the best-fit corresponding to the SLD profiles shown in (b).

Additively manufactured U6Nb heat treated in situ in SMARTS

Results aid materials processing techniques

In an attempt to understand materials processing being done at Lawrence Livermore National Laboratory (LLNL), additively manufactured U6Nb was recently heat treated in situ in the Spectrometer for Materials Research at Temperature and Stress (SMARTS), at the Los Alamos Neutron Science Center. The results provided valuable data for improving LLNL's additive manufacturing techniques, and is companion work done on similar material at the Advanced Photon Source as illustrated in the photo at the top of page 4.

Additive manufacturing (AM) represents a relatively new fabrication paradigm in which parts are built from the ground up to final geometry, as opposed to traditional manufacture, where large blanks are produced and machined to final dimensions. AM needs to be scientifically examined because the process is very different from traditional manufacture.

Traditionally processed U6Nb usually has a monoclinic (α'') crystal structure. Previous experiments at SMARTS showed that as-processed, the U6Nb material additively manufactured at Livermore has a two-phase structure comprised of roughly equal amounts of the monoclinic and tetragonal (γ_0) crystal structure. Following the Livermore heat-treatment (10 hours at 1000°C), the material is single phase γ_0.

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Additively ... cont.

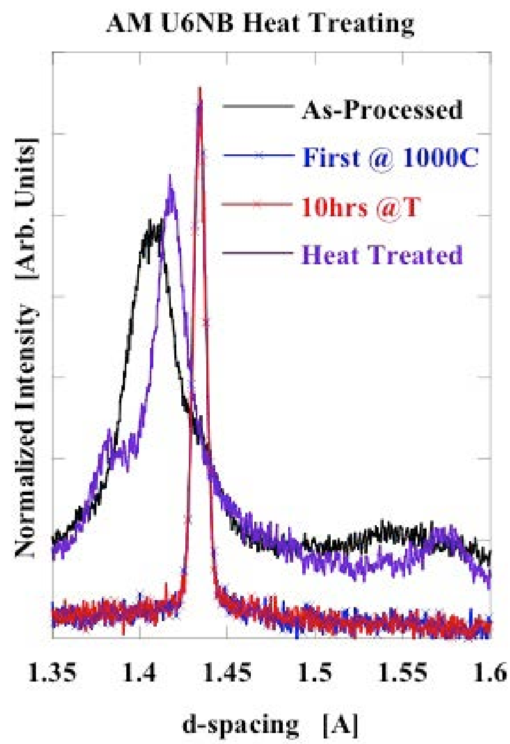
An as-processed sample was heated in-situ on SMARTS with a heating rate of 100°C/min followed by a 1000°C (in the cubic (γ) phase) hold for 10 hours. The timing of the heat treatment matches well with the data integration time (~5 minutes) on SMARTS. The figure shows several diffraction patterns, before and after heat treating, when first reaching 1000°C and after 10 hours at 1000°C.

The diffraction data when the sample first reached 1000°C is indistinguishable from that 10 hours later. Moreover, the final diffraction pattern after the heat treatment was consistent with the sample heat treated ex situ at Livermore. The conclusion is inescapable: the parts of the microstructure that can be monitored with diffraction, i.e. the Nb concentration, internal stress, dislocation density, and texture, did not change during the hold at 1000°C, and therefore, must have changed during the heating phase.

These results can be used by Livermore to better design the heat treatment process to achieve the final microstructural goal. Moreover, the work represents the philosophy driving MaRIE, i.e. understanding manufacturing process towards optimization, control, certification, and qualification. The limited data rate at SMARTS allows researchers to monitor the microstructure during the relatively long heat treatment. In contrast, the very high data rate associated with MaRIE would allow monitoring of the material deposition process itself, which happens in a fraction of a second. MaRIE (Matter-Radiation Interactions in Extremes) is the Laboratory's proposed experimental facility for control of time-dependent material performance.

The work, which was funded by the Primary Assessment Technologies Campaign, supports the Laboratory's Nuclear Deterrence mission and Materials for the Future science pillar. Researchers include Amanda Wu (LLNL) in collaboration with Don Brown and Bjorn Clausen (Materials Science in Radiation & Dynamics Extremes, MST-8).

Technical contact: Don Brown



Shown are several diffraction patterns, before and after heat treating, when first reaching 1000°C and after 10 hours at 1000°C, demonstrating that the parts of the microstructure that can be monitored with diffraction must have changed during the heating phase.

To learn more about MaRIE, please see marie.lanl.gov, or contact Cris Barnes, capture manager, at cbarnes@lanl.gov.

Roadmap to MaRIE, featuring science and technology highlights related to Los Alamos National Laboratory's proposed experimental facility, is published by the Experimental Physical Sciences Directorate. For information about the publication, please contact adeps-comm@lanl.gov.

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