LANSCE
Los Alamos Neutron Science Center

Activity Report
2015

Los Alamos
NATIONAL LABORATORY
EST 1943

About the front cover

The front cover depicts the LANSCE mesa.

LANSCE Activity Report 2015

LANSCE provides the scientific underpinnings in nuclear physics and material science needed to ensure the safety and surety of the nuclear stockpile into the future.

This report is available online: lansce.lanl.gov

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Foreword

Dear Colleagues,

The year 2015 was a year of challenges and opportunities for LANSCE. While we had significant successes, including the return to 120 Hz operations of the accelerator (for the first time in a decade) we also faced the significant challenge of the loss of the Basic Energy Sciences (BES) User Program at the Manuel Lujan Center. With the benefit of hindsight I can say that not only did we survive, we have raised the visibility of the neutron scattering work at the Lujan Center within the Laboratory community. Thanks to the dedicated efforts of the Lujan Center scientists we now have a stable material science program at the Lujan Center that directly supports LANL's mission.

The transition from BES funding to NNSA funding has changed the user program model at the Lujan Center. Despite this transition, we had 508 unique users, ran 146 experiments, and allocated 1311 flight-path days of beam to pRad, Lujan Center, and WNR. These numbers are a testament to the continued strength of LANSCE and our ability to provide unique capabilities to LANL, NNSA, and the nation.

As of this writing (November 2016) we have completed the replacement of the high-power amplifiers in the 201-MHz section of the accelerator and with that the LANSCE Risk Mitigation project. Going forward this enables us to return to a normal operating schedule, with six months of beam delivery in 2017 and seven months of beam delivery going forward.

On a personal note, Kurt Schoenberg, the LANSCE User Facility Director since 2006 retired in October of 2015. I wish Kurt the best in his retirement and thank him for his leadership over the past decade. Kurt's efforts were critical in establishing a stable platform for LANSCE during the difficult transition from BES funding and he has been a staunch supporter of the user community during his tenure. In this regard my vision is similar. For Los Alamos National Laboratory to be successful in its national security mission requires a strong capability in scientific research. LANSCE, the user community we support, and the scientific research we perform will always be an integral part of the success of Los Alamos.

- *Gus Sinnis*

Gus Sinnis
LANSCE User Facility Director

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LANL at a Glance

Los Alamos National Laboratory

Since 1943, some of the world's smartest and most dedicated technical people have accomplished the difficult, the unexpected, and at times the seemingly impossible at Los Alamos. Since its inception LANL's mission remains unchanged: to solve national security challenges through scientific excellence, and develop and apply science and technology to ensure the security of the nation. This includes the safety and surety of the nuclear deterrent, reducing global threats, and solving emerging national security challenges. The capabilities provided by LANSCE are used by a broad range of LANL programs to solve national security challenges and provide a window to the external scientific research community.

Part of the main campus of Los Alamos National Laboratory.

LANSCE at a Glance

Los Alamos Neutron Science Center

One of the major experimental facilities at LANL, the Los Alamos Neutron Science Center (LANSCE) provides a unique set of capabilities for Los Alamos National Laboratory, the National Nuclear Security Administration (NNSA), and the nation. The backbone of LANSCE is the 800-MeV proton linear accelerator. These protons feed five experimental areas: the Isotope Production Facility, Proton Radiography, the Ultracold Neutron Source, the Weapons Neutron Research Facility (WNR), which has six high-energy neutron beam lines, and the Lujan Center for Materials Research, which provides cold and thermal neutrons for materials and nuclear science research.

Most of the research performed at LANSCE is in support of NNSA missions. At WNR nuclear cross sections needed to develop a predictive capability for science-based stockpile stewardship (SBSS) are measured. Proton radiography is used to measure the time evolution of dynamic phenomena on time scales that span microseconds to hours. Understanding the performance of high explosives, material failure, and hydrodynamic instabilities are key research topics at this facility. At the Lujan Center neutron scattering is used to measure stresses and textures on components and materials used to support the SBSS program. At all of the facilities we have the ability to perform classified experiments, using actinides and high explosives, that cannot be performed at other accelerator-based facilities.

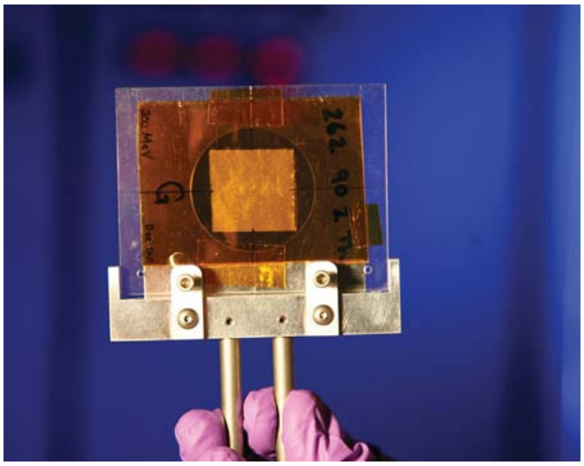
In addition to supporting NNSA missions, LANSCE provides the Laboratory with a window to the basic research community. The WNR, Lujan, and Proton Radiography facilities are NNSA-designated national user facilities. This enables us to devote a fraction of the available beam to support university-based scientific research. The Isotope Production Facility is supported by the Department of Energy Nuclear Physics program and produces isotopes for medical needs and research purposes. Finally the ultracold neutron facility has the world’s most intense source of ultracold neutrons and performs fundamental research in nuclear physics.

The Los Alamos Neutron Science Center is located on one of the historic mesas of Los Alamos.

LANSCE at a Glance

Isotope Production Facility

The Isotope Production Facility (IPF) at LANSCE produces radioactive isotopes for medicine and research. IPF supplies a variety of radioisotopes to medical researchers around the world. Moreover, IPF continues to be a leader in developing and producing new and unique isotopes for international research and development.

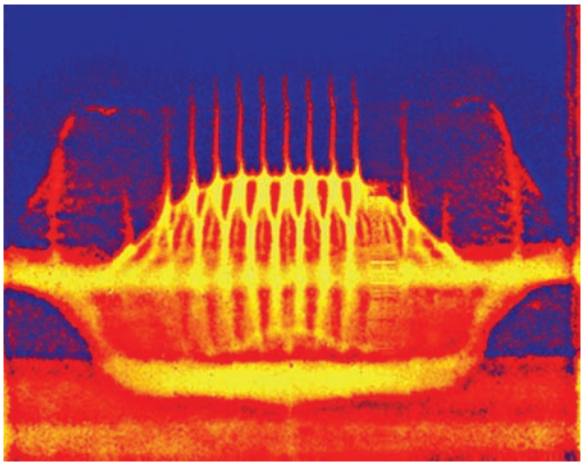


Lujan Center

The Lujan Center uses a pulsed spallation neutron source equipped with time-of-flight spectrometers for neutron-scattering studies of condensed matter. A powerful technique, neutron scattering probes the microstructure and dynamics of condensed matter. Applications for neutron scattering include materials science, engineering, condensed matter physics, chemistry, biology, and geology.

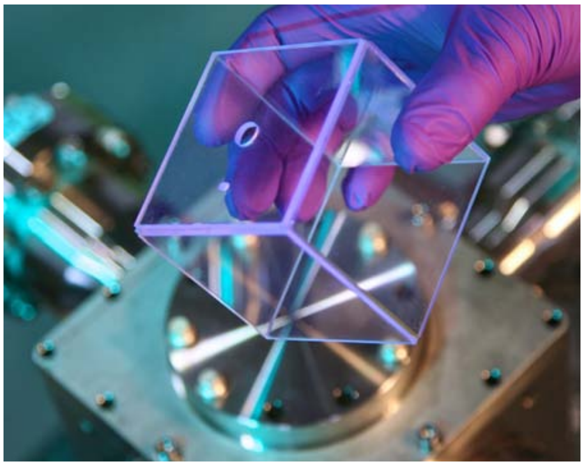
Proton Radiography Facility

The Proton Radiography Facility (pRad) and project use 800-MeV protons provided by the LANSCE accelerator facility at LANL to diagnose more than 300 dynamic experiments in support of national and international weapons science and stockpile stewardship programs.



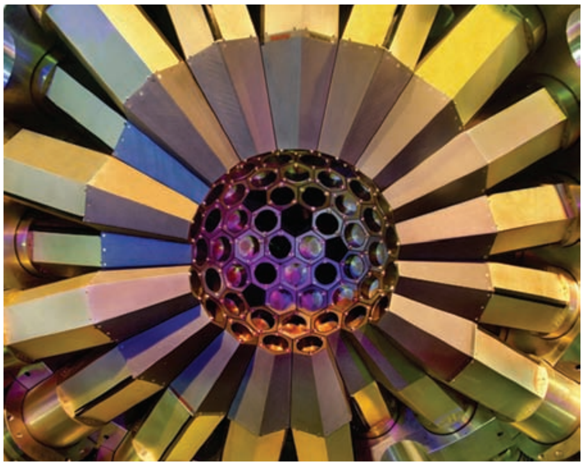
LANSCE at a Glance

Ultracold Neutron Source



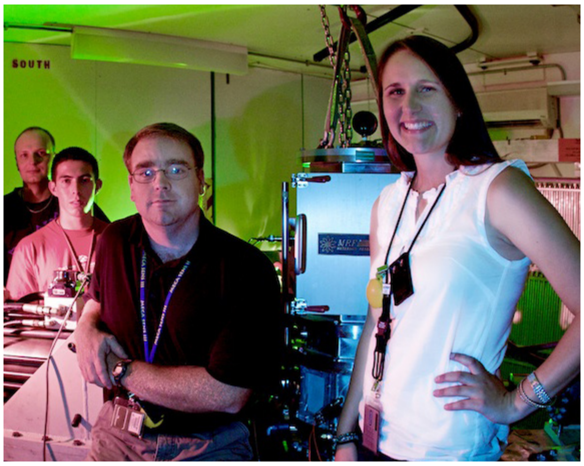
LANSCE and eight other-member institutions have come together under an international collaboration to construct the Ultracold Neutron Source (UCN). UCN provides the most intense source of ultracold neutrons in the world. Researchers have measured ultracold neutron production in UCN for the first time. The ultracold neutron extraction port at LANSCE delivers neutrons from the new ultracold neutron source for experiments that could answer questions about the fundamental constants of nature and aid in the quest for new particles.

Weapons Neutron Research Facility



The Weapons Neutron Research Facility (WNR) provides neutron and proton beams for basic, applied, and defense-related research. Neutron beams with energies ranging from approximately 0.1 MeV to more than 600 MeV are produced in Target 4 (an unmoderated tungsten spallation source) using the 800-MeV proton beam from LANSCE's linear accelerator. In the Target 2 area (Blue Room), samples can be exposed to the direct 800-MeV proton beam.

User Program



LANSCE's User Program ensures that research it oversees represents the cutting-edge of nuclear and materials science and technology. The User Program plays a key role in training the next generation of top scientists, and attracting the best graduate students, postdoctoral researchers, and early-career scientists.

Capabilities and Collaborations
2015

Capabilities and Collaborations

Capabilities and Collaborations at a Glance

Capabilities

New capabilities at LANSCE provide the tools and technology to open new paths for our valued customers while concurrently attracting new collaborators.

Collaborations

Researchers at LANSCE, in conjunction with collaborators from around the world, produce cutting-edge science that leads the way toward extraordinary new discoveries.

Capabilities and collaborations for 2015

- LANSCE resumes 120-Hz operations
- 2015's run cycle represents one of the most prolific for NNSA research
- LANSCE capabilities help researchers discover how trees transport water
- Muon imaging system is going live at Fukushima Daiichi
- LANSCE researchers are developing a new means of detecting traumatic brain injury

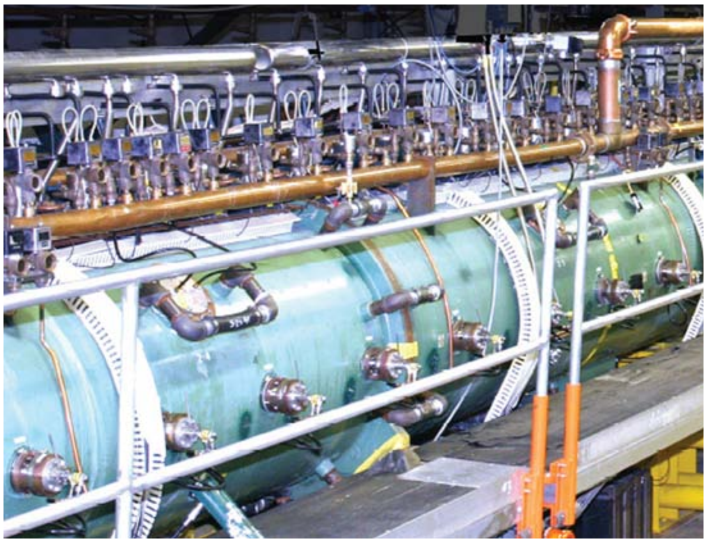
At left: LANSCE technicians performing a safety check on the Cockroft-Walton generator.

Capabilities and Collaborations

LANSCE resumes 120-Hz operations

In early December, LANSCE resumed 120-Hz operations, thus 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 Division (AOT) 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.



The LANSCE linear accelerator (linac).

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 (TPC) and the Chi-Nu array. Both are NNSA Weapons Program Science Campaigns-funded instruments. The fission TPC 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.

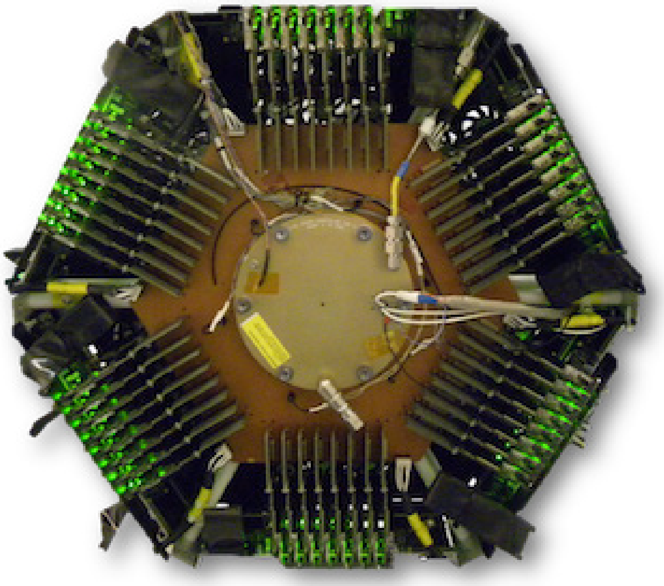
The new diacrode amplifier-based RF systems for the drift tube linac, part of the LINAC Risk Mitigation activities that enabled a return to 120-Hz operations at LANSCE.

Capabilities and Collaborations

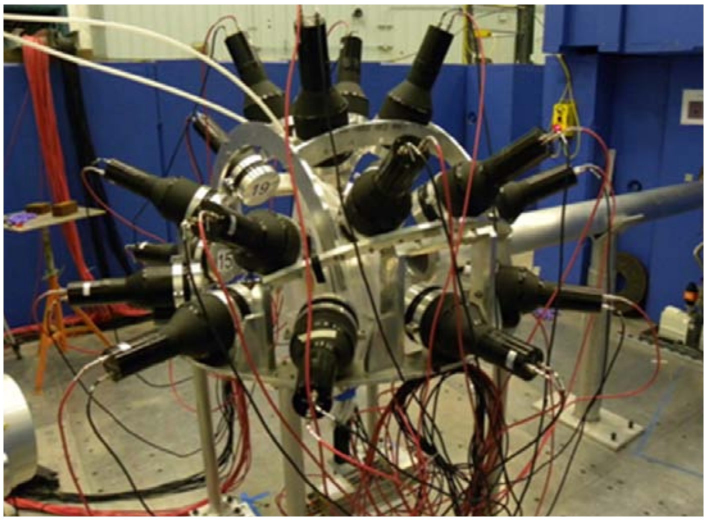
The 120-Hz operation also enables the development of new research facilities using the LANSCE LINAC. The improvements are an example of the Laboratory's LINAC accelerator expertise that could be used to design, build, and operate the Matter-Radiation Interactions in Extremes (MaRIE) x-ray free-electron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

Participants include the following: J. 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 RTBF program funded the LINAC Risk Mitigation work. LANSCE activities support the Laboratory's Nuclear Deterrence and Energy Security mission areas and the Nuclear and Particle Physics, Science of Signatures, and Materials for the Future science pillars.



Fission Time Projection Chamber.



Chi-Nu Detector Array.

Capabilities and Collaborations

2015 LANSCE run cycle was one of the most prolific for NNSA research

The broad neutron energy spectrum available at LANSCE enabled scientists to perform eight different studies during the last run cycle, which ran from October 2014 to February 2015. The results revealed materials and nuclear properties of plutonium (Pu) – from surface studies on 50-mg plutonium thin films to prompt neutron spectra for fission of the isotope plutonium-239 (^{239}Pu).

Neutron production targets at WNR and the Lujan Center provide complementary neutron energies spanning 1 meV–600 MeV, enabling advances in fundamental and applied materials research and stockpile stewardship science. The science-based Stockpile Stewardship Program combines advanced scientific and experimental capabilities with high-performance supercomputing to help scientists and engineers understand and resolve issues associated with the nation's nuclear deterrent.

A broad range of program development activities aligned the Lujan Center materials' user program with the NNSA mission, making the most run cycle one of the most prolific for plutonium research, with great benefits to NNSA programs. For example, researchers used the surface neutron reflectometer Asterix to perform the first neutron reflectometry characterization of less than 50-mg plutonium oxide (PuO_2) thin films. Such preliminary work is critical to characterizing interfaces and understanding the effect of the existence or development of nonhomogeneous phases at different surface depths of real parts. These phases might affect processes and degradation such as hydride formation or oxidation. Scientists employed the small-angle neutron scattering instrument, the low-Q diffractometer (LQD), and Asterix to perform feasibility studies of highly neutron absorbing materials (dysprosium and erbium). LQD allows scientists to characterize mesoscale defects created by aging or damage in these materials. The first experiments on plutonium samples at LQD and Asterix proved that it is feasible to characterize the effects of aging and annealing in the mesoscale in the upcoming run cycle.

Diffraction and inelastic neutron scattering measured the local structure and phonon density of states of plutonium/gallium (PuGa) alloys using highly neutron absorbing ^{239}Pu as a function of temperature on the neutron powder diffractometer (NPDF) and FDS. Scientists characterized the microscopic origin of the stabilization mechanisms and the local effects of radiation damage or stress. They also examined the mechanism behind the phase transitions that remain elusive from average structure studies and which are impossible to obtain using x-rays. The team used the filter difference spectrometer to investigate the phonon density of states (pDOS) on PuGa compounds, extending the data range over which the pDOS has been observed in such compounds. This information informs first-principle calculations leading to the vibrational models and theoretically obtained equations of state needed to simulate dynamic experiments. Overall, the work demonstrated the feasibility of using available ^{239}Pu, which is highly neutron absorbing, rather than the lower absorbing and rare isotope plutonium-242 (^{242}Pu), to perform neutron scattering experiments. These combined sophisticated modeling efforts and data-reduction methods enable the Lujan Center to respond to future NNSA needs effectively and efficiently.

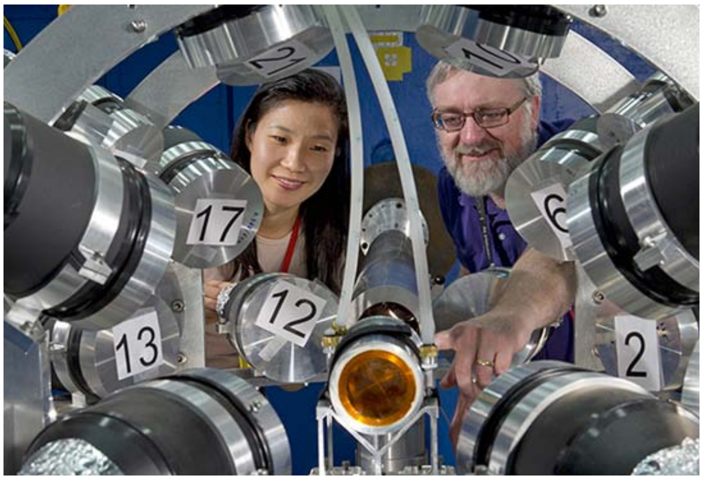
The high-energy neutrons at WNR enabled the team to achieve nuclear science milestones. The Chi-Nu detector array, developed by LANL and Lawrence Livermore National Laboratory (LLNL) to measure the prompt fission neutron spectra of ^{239}Pu, greatly benefitted from the development of a new integrated data acquisition system. The LANSCE risk mitigation project enabled an increase of a factor of 2.5 in the beam rate. The scientists achieved important NNSA milestones on the prompt fission neutron spectra of the uranium isotope, uranium-235 (^{235}U) and preliminary ^{239}Pu results.

The fission TPC is a NNSA instrument developed in collaboration with LLNL to achieve 1% accuracy in determining ^{239}Pu cross sections. The chamber delivered measurements leading toward the achievement of a Level 2 milestone. Successful preliminary results provided ^{239}Pu/^{235}U cross-section ratios.

Postdoc D. Olds sets up a LQD experiment.

Researchers fielded the Spectrometer for Ion Determination in fission Research and the total kinetic energy release in fission in both the Lujan Center and WNR. They obtained data enabled by the facilities' complementary neutron sources and broad energy range. During the recent run cycle, experiments determined the total kinetic energy dependence on incident neutron energy for fission of ^{239}Pu and the fission product yields of ^{239}Pu using the 2E-2v method.

Researchers from Physics, Materials Science and Technology, and Materials Physics and Applications divisions conducted the experiments, and AOT enabled the operation of LANSCE. NNSA funded the 2015 run cycle, which supports LANL's Nuclear Deterrence mission area and Nuclear and Particle Futures and Materials for the Futures science pillars through work sustaining Stockpile Stewardship needs for actinide material and nuclear property data.



H. Y. Lee and J. O'Donnell check the Chi-Nu instrument at the WNR.

Capabilities and Collaborations

Combined capabilities reveal how trees transport water

Los Alamos researchers have made the first simultaneous measurements of Ultra-Low-Field Nuclear Magnetic Resonance (ULF-NMR) and neutron imaging to visualize the movement of water in trees. Water use by trees is a key part of the hydrological process linking soil to climate and local weather. Despite decades of research and method development, nondestructive, *in vivo* measurements of water uptake and flow in trees are unavailable for field-based measurement. The lack of measurements limits progress toward understanding this important climate factor. Measurement challenges arise from the opacity of wood and the intricate nature of the water transport system, where opposing pressure gradients in adjacent tissues are responsible for water uptake from the soil and delivery of carbohydrates produced in the leaves.

To overcome these methodological challenges, LANL researchers from Earth System Observations, (EES-14), Applied Modern Physics (P-21), and Inorganic, Isotope and Actinide Chemistry (C-IIAC) have developed an ULF-NMR system suitable for use in ambient, outdoor environments to monitor nondestructively longer-term changes in the water contents of living trees non-destructively. Other NMR systems work in regulated temperatures, requiring a cooled magnet and maintaining the system at constant temperature. The ULF-NMR system does not need cooling. The journal *Review of Scientific Instruments* reported this system.

Laboratory scientists moved toward field application by calibrating the NMR signal for water uptake by different tissues. Therefore, the team and colleagues from Nondestructive Testing and Evaluation (AET-6), Materials Science in Radiation and Dynamics Extremes (MST-8), and LANSCE Weapons Physics (P-27) conducted simultaneous neutron radiography and ULF-NMR measurements of D_2O (i.e., deuterium, also known as "heavy water") uptake by living branches at LANSCE.

The researchers used the 60-meter Lujan Center Flight Path 5 neutron beam line. Both NMR and neutron imaging allow differentiation between D_2O and H_2O (the more common isotope of water). Alternate watering of branches with these two water sources enabled the researchers to measure the flow rates with both systems simultaneously and compare them. The team also added a surfactant to the source water, thereby changing its surface tension and inducing bubble formation (cavitation) in the branch's water-conductive tissue. This condition induced failure of the conductive tissue to simulate drought conditions in nature.

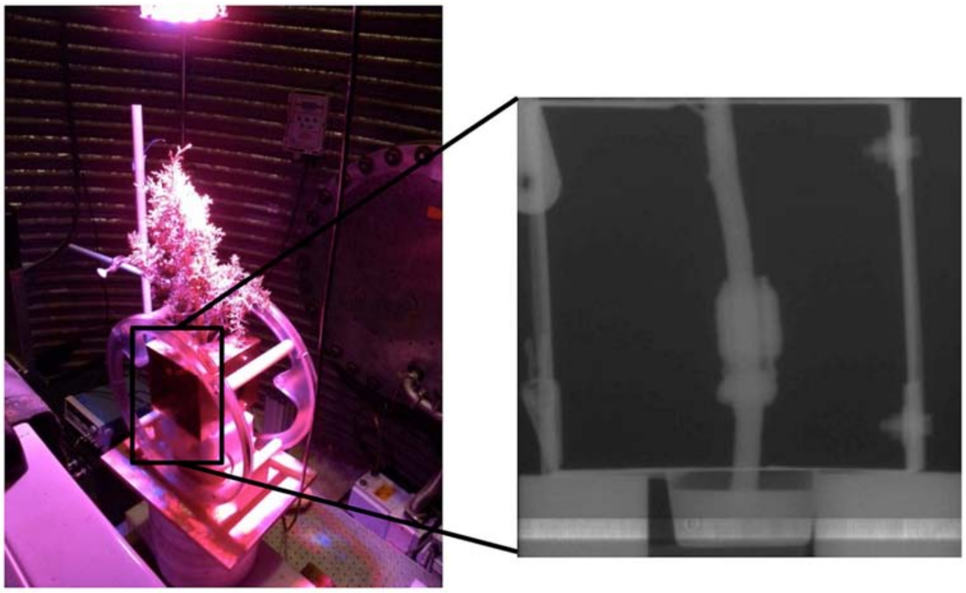
This measurement of NMR during active neutron imaging was the first of its kind. Simultaneous decline in the NMR and neutron signal (see the graph on the following page) proved the feasibility of the method. Exploration of the rates of change in signal amplitudes indicates that approximately 70% of the NMR signal is due to water moving rapidly towards the leaves in the water-conductive tissue. The remaining approximately 30% of the NMR signal results from slowly moving or bound water within cells and/or tissues related to carbohydrate transport and storage. The success of these measurements proves the concept of non-destructive water flow detection with ULF-NMR and the utility of simultaneous NMR and neutron imaging measurements. This new capability opens up myriad possibilities for enhanced visualization of water and carbohydrate transport processes in trees.

The Los Alamos research team for the combined ULF-NMR and neutron imaging studies include the following: S. Sevanto (EES-14), M. Espy and M. Malone (P-21), L. Turin Dickman (EES-14), J. Hunter (AET-6), R. Nelson (P-27), J. Yoder (C-IIAC), and S. Vogel (MST-8).

Reference: “Low-field Nuclear Magnetic Resonance for the In Vivo Study of Water Content in Trees,” *Review of Scientific Instruments* **85**, 095110 (2014).

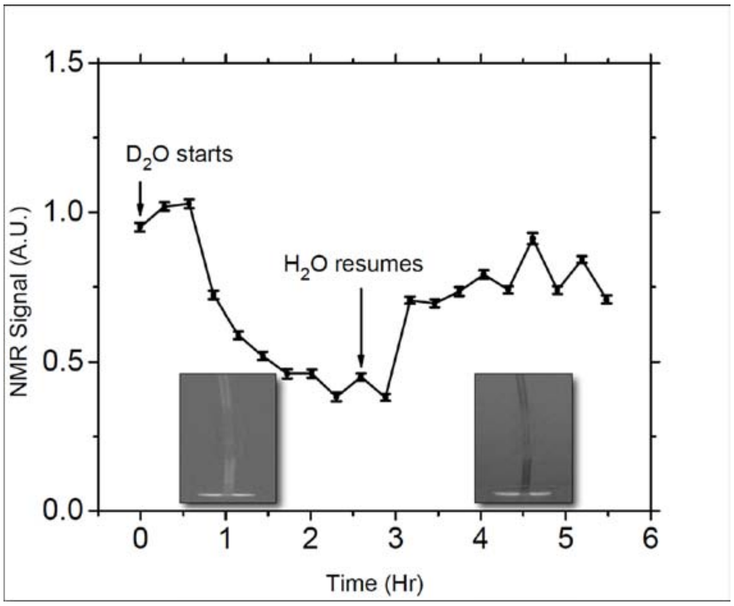
Authors include the following: *J. Yoder (C-IIAC), M. W. Malone and M. A. Espy (P-21), and S. Sevanto (EES-14).*

The Laboratory Directed Research and Development program funded the work, which supports the Laboratory's Global Security mission area and the Science of Signatures science pillar through the capability to monitor the impact of drought on vegetation. A Principal Associate Directorate for Science, Technology, and Engineering (PADSTE) small-equipment grant purchased the neutron imaging equipment. NNSA Weapons Campaign 8 (Enhanced Surveillance) sponsored the development and operation of the neutron imaging detector.



This photograph shows the NMR and neutron-beam setup. The neutron detector (left) picks up neutrons, which enter at the right. The NMR system surrounds the juniper branch.

Inset to the right shows the neutron radiograph setup. The branch sits in the middle. The bars on both sides are the NMR shield. The NMR coil is the thickening on the branch.



NMR signature and two neutron images of the branch taken during NMR measurements. Neutron radiographs were made at the time indicated on the scale. D_2O uptake is revealed in the radiographs as the white color in the branch, H_2O as the black color. The NMR signal declines when D_2O is replacing H_2O, and increases as the plant is re-watered with H_2O. The different images show the progress of D_2O uptake, which appears as lighter regions (left). Rewatering with H_2O appears as darker regions in the differenced image (right).

Capabilities and Collaborations

Lab’s muon imaging system going live at Fukushima Daiichi

A muon imaging system pioneered at the Laboratory will be deployed to Japan’s Fukushima Daiichi power plant by the end of 2015. An earthquake and tsunami in 2011 severely damaged the plant, leading to concerns that molten nuclear fuel spread from the reactor core to the pressure and containment vessels. The goal of the deployment is to reveal the amount, condition, and location of the highly radioactive nuclear fuel remaining inside the reactors, without exposing workers to the high radiation fields inside the reactor facilities.

Muon radiography uses secondary particles called muons that are generated when naturally occurring cosmic rays collide with upper regions of Earth’s atmosphere. The muons create images of the objects that the particles penetrate. LANL researchers exploit multiple scattering of the muons in an object of interest to obtain 3-D images. C. Morris (Subatomic Physics, P-25) first developed this technique more than 10 years ago.

The Laboratory Threat Reduction Team in P-25, together with Toshiba Corporation and Decision Sciences International Corporation (DSIC), will image reactor unit No. 2 using cosmic muons. The Los Alamos technique will provide Tokyo Electric Power Company with a map so that workers can safely remove of nuclear fuel from the damaged plant.

The imaging system is being assembled at a Toshiba facility in Japan. It consists of two approximately 7m x 7m tracking detectors made of gas-filled drift tubes provided by DSIC, which are read out by Toshiba electronics. One detector will be deployed in front of the reactor building, with the other on the second floor of the turbine building on the opposite side of the reactor unit. The Laboratory team developed tracking software and recently tested it on data taken with a smaller prototype.

Laboratory participants include the following: J. D. Bacon, J. M. Durham, J. M. Fabritius II, E. Guardincerri, C. Morris, K. O. Plaud-Ramos, D. C. Poulson, Z. Wang, and S. Fellows (all P-25).

Muon tomography and development of its application at Fukushima were made possible in part through LANL's LDRD program. Work for Others funding from Toshiba Corporation and the Tokyo Electric Power Company sponsored other aspects of the research.

The work supports the Laboratory’s Global Security mission area and the Science of Signatures science pillar. The Lab’s muon tomography technology is also deployed in locations around the world to help detect smuggled nuclear materials.

Capabilities and Collaborations

This detector is currently mounted in a horizontal mode at the Toshiba facility in Yokohama, where the detectors are assembled.
(Courtesy of M. Saltus, DSIC)

Los Alamos National Laboratory postdoctoral researcher E. Guardincerri (right), and undergraduate research assistant S. Fellows (left) prepare a lead hemisphere inside a muon tomography machine.

Capabilities and Collaborations

Interface engineering enables a path forward for magnetoelectric multiferroics

Los Alamos scientists and collaborators have discovered a way to realize magnetoelectric coupling and net magnetic moment in antiferromagnetic $BiFeO_3$ (BFO). This finding has potential utility for designing high-density data storage platforms of the future. The journal *Scientific Reports* reported the research.

BFO has outstanding ferroelectric properties. However, there is virtually no net moment to interact with an applied magnetic field. This lack of a magnetic handle impedes its development for potential applications. Therefore, researchers developed a composite of two materials [$La_{0.7}Sr_{0.3}MnO_3$ (LSMO) and BFO], neither of which independently exhibits a dielectric response to a magnetic field. Polarized neutron reflectometry measurements of the composite reveal significant net uncompensated magnetization in BFO. The authors concluded that the large uncompensated magnetization of BFO in the superlattice is a consequence of unique features associated with the superlattice; e.g., its growth, strain, architecture, proximity to a ferromagnet, etc. Below 179 K, LSMO is ferromagnetic and BFO exhibits net uncompensated magnetization; the magnetization of BFO is opposite to that of the LSMO. The magnetic order parameters have the same dependence with temperature, suggesting that LMSO induces the uncompensated magnetization of BFO. The magnetization enables a magnetic field to change the dielectric properties of the superlattice. The team cited this phenomenon as an example of synthetic magnetoelectric coupling.

The finding represents a new path to produce synthetic magnetoelectric coupling in a nanocomposite at 10 K. With this approach, it is not longer necessary to discover a single-phase multiferroic for useful applications. Instead, the more-manageable challenge becomes applying interface engineering to intimately couple dissimilar materials.

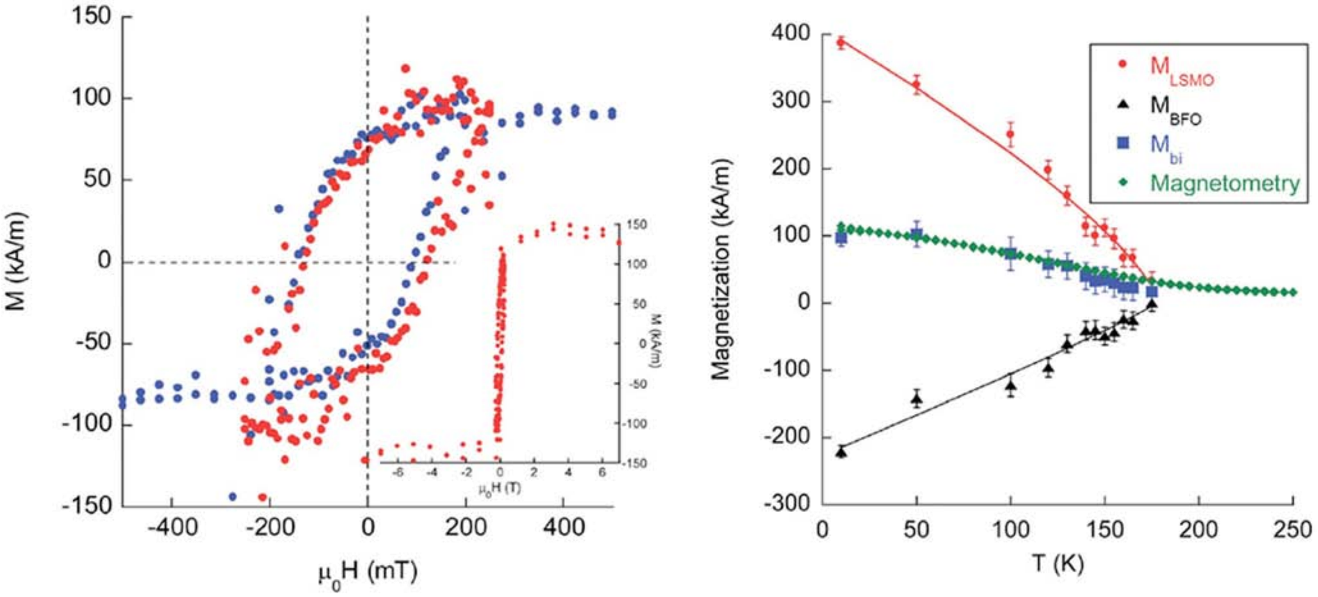
The team concluded that the controlled creation of magnetic moment in BFO is an important step toward the design and implementation of integrated oxide devices for next-generation magnetoelectric data storage platforms.

Reference: "Synthetic Magnetoelectric Coupling in a Nanocomposite Multiferroic," *Scientific Reports* **5**, 9089 (2015).

Authors include the following: P. Jain (Materials Synthesis and Integrated Devices, MPA-11); Q. Wang, Z. Bi, and Q. Jia (Center for Integrated Nanotechnologies, MPA-CINT); T. Ahmed and J. Zhu Physics of Condensed Matter and Complex Systems, T-4); M. Fitzsimmons (formerly of Lujan Center); M. Moldan (Universidad Complutense de Madrid, Spain); A. Glavic (Oak Ridge National Laboratory, ORNL); C. Urban (University of California,San Diego, UCSD), and M. Varela (Universidad Complutense de Madrid and ORNL).

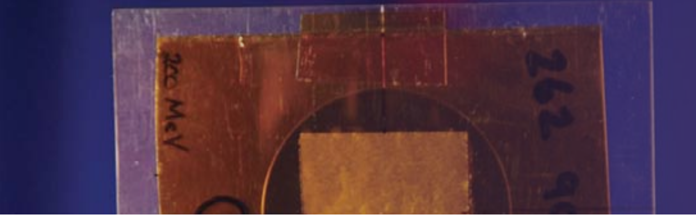
The Laboratory's LDRD program funded the work, which was performed, in part as CINT, an Office of Science User Facility operated for the DOE Office of Science. This work has benefited from the use of the Spallation Neutron Source at ORNL and the Lujan Center, which were at the time funded by the Scientific User Facilities Division of the DOE's Office of Basic Energy Sciences; and the National High Magnetic Field Laboratory at Los Alamos, which the National Science Foundation sponsors.

The work supports the Laboratory's Energy Security mission area and the Materials for the Future science pillar through the use of materials with tailored functionality to enable technological innovations in information storage, sensing, and computing.



The graph on the left plots magnetization vs. magnetic field for superlattice measured from ±0.5 T and ±7 T (red and inset) at 10 K. The temperature dependence of the magnetizations is represented as circles for LMSO and triangles for BFO layers in the superlattice. Squares represent the thickness—the weighted average of the magnetization, with diamonds representing the moment of the sample measured with magnetometry normalized by the volume of the superlattice film.

Isotope Production Facility 2015



IPF at a Glance

Los Alamos National Laboratory has produced radioactive isotopes for medicine and research. IPF at LANSCE supplies a variety of radioisotopes to medical researchers and other scientists all over the world and has been a leader in developing and producing new and unique isotopes for research and development Since 2009, the Office of Nuclear Physics has administered the nation's isotope program for the Office of Science.

LANL's Isotope Production and Applications Program is unique:

- IPF at LANSCE uses a 100-MeV proton beam at 250 µA to produce isotopes from an 800-MeV-capable accelerator.
- The Radiochemistry Complex, located at TA-48, houses a dedicated processing facility with 13 hot cells that can shield up to 1000 Ci of Co-60. The hot cells are cGMP/FDA compliant for production of active pharmaceutical ingredients.
- The Plutonium Facility, located at TA-55, is developing the ability to process large-scale AM-241.
- In-house expertise in nuclear physics, radiochemistry, radionuclide applications, actinide science, and targetry development.

Isotopes produced at LANL are used as environmental tracers:

- As-73 is used to investigate environmental contamination and transport of toxic arsenic.
- Na-22 and other environmentally relevant isotopes are needed to understand flowpaths for geochemical and hydrologic modeling.
- Al-26 is used to elucidate the impacts of acid rain.
- Si-32 is needed for oceanographic tracing, which contributes to a better understanding of climate change and its aggregate impacts on the environment.

Isotope production at LANL ensures the following:

- A safe, secure and reliable domestic supply of radionuclides Sr-82 and Ge-68 that reduces our dependence on foreign-supplied isotope materials and services.
- A source of surrogate materials and analytical standards for use in testing and validation of procedures.
- A supply of radiotracers for environmental impact studies after radiation dispersal events and for model validation and related applications.
- Radionuclides and technical expertise needed for nuclear forensic applications.

Extensive application of software systems to model:

- The behavior of targets under extreme thermal, mechanical, and radiation conditions.
- Yields of primary products and impurities in a variety of irradiation environments.

At left: D. Reass works the manipulators of the IPF hot cell.

Recent LANSCE run cycle was one of the most prolific

The Laboratory's Isotope Production team produces radioisotopes for use in research and medicine. The team has developed a promising new way of using an important radioactive isotope of bismuth in cancer therapy. Nuclear Medicine and Biology has published their findings.

High-energy alpha (α)-particles emitted by the decay of radioactive isotopes can be harnessed to destroy malignant cells. This therapeutic strategy, known as α-therapy, is the subject of much study. The Federal Drug Administration (FDA) recently approved the α-emitter radium-223 dichloride ($^{223}RaCl_2$) for the treatment of bone metastases arising from a particular type of cancer. The short-range (several cell diameters) and high linear energy transfer (approximately 100 keV/μm) of emitted α-particles suggests their use in the treatment of micrometastatic disease, where the decay energy could be limited to the targeted cells. However, the limited availability of α-emitting radionuclides with appropriate physical properties for therapy hinders their development for clinical application. Binding these radioisotopes to chelating agents (molecules that can form several bonds to a metal ion) and appropriate biological targeting vectors to direct the complexes to the malignant cells present technical challenges. Better chelation and targeting methods for the radioisotopes could achieve significant medical benefits for therapy.

Bismuth-213 (^{213}Bi) has potential for targeted α-therapy. The short half-life is suitable for use with small-molecule and peptide-based targeting agents. Its half-life and small decay chain minimize toxic side effects that may arise from long-lived daughter nuclides. ^{213}Bi can be obtained from a commercially available generator system comprised of its longer-lived parent actinium-225 (^{225}Ac). Some clinical trials have demonstrated the utility of ^{213}Bi for cancer treatment. However, challenges associated with the aqueous chemistry of the metal ion and binding Bi^{3+} using ligands (ions or molecules that bond to a central metal ion) have hampered its use in targeted α-therapy.

The Los Alamos team examined a new series of nitrogen-rich macrocyclic ligands (depicted as L in the top figure on the next page) and explored its coordination chemistry with Bi^{3+}. Researchers compared the binding of Bi^{3+} provided by the new ligands with that of some commonly used ligands (as shown in the top row of the top caption on the following page).

Unlike other commercially available ligands such as DOTA, these new ligands are selective for Bi^{3+} even in the presence of the parent radioisotope Ac^{3+}. Density functional theory calculations corroborate the experimentally observed selectivity of these ligands for Bi^{3+} compared with Ac^{3+}. This selectivity is important to minimize detrimental effects of $^{225}Ac/^{213}Bi$ generator breakthrough that could lead to inadvertent patient dosing with small quantities of long-lived ^{225}Ac.

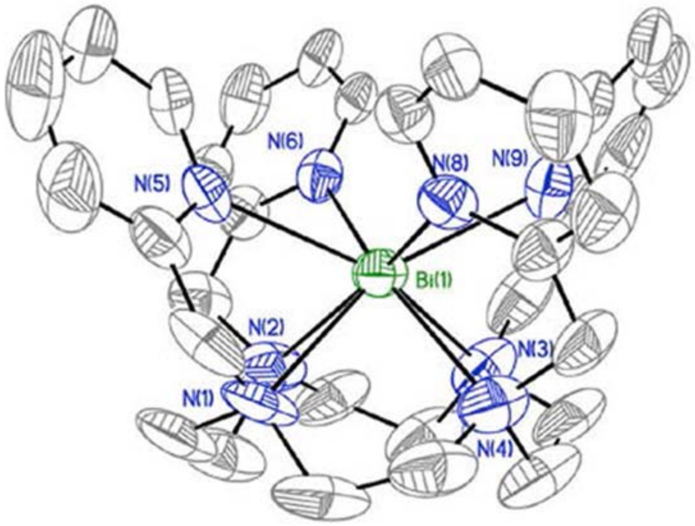
Researchers found that subtle electronic modifications across the series of ligands cause significant effects on the solution behavior of their Bi^{3+} complexes. Among the four new ligands tested, L^{py} (bottom figure on the following page) exhibits optimal Bi^{3+}-binding kinetics and complex stability. The investigators concluded that this class of nitrogen-rich ligands might be used for the rapid, selective, and stable chelation of radiobismuth for targeted α-therapy. The information gained from the research provides insight for the rational design of ligands for therapeutic radioisotopes.

Reference: "Bismuth Radioisotopes," *Nuclear Medicine and Biology* **42**, 428 (2015).

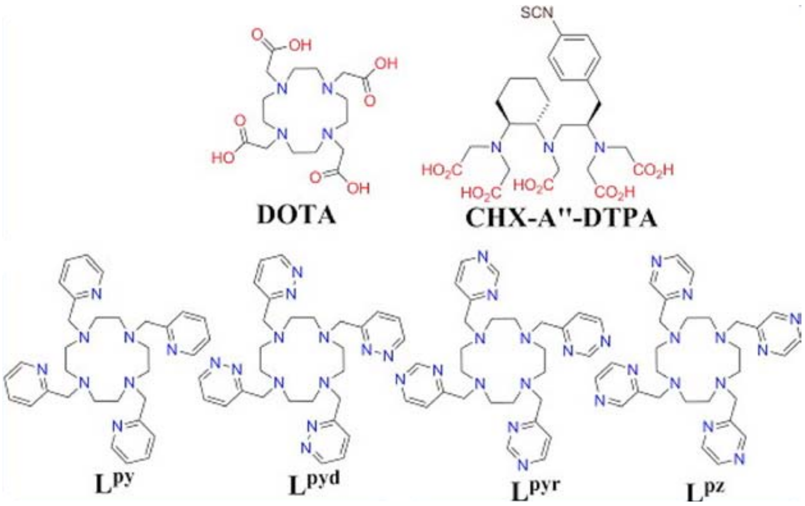
Authors include the following: J. J. Wilson, M. Ferrier, V. Radchenko, J. R. Maassen, J. W. Engle, F. M. Nortier, and M. E. Fassbender (C-IIAC); E. R. Batista and R. L. Martin (Physics and Chemistry of Materials, T-1); K. D. John and E. R. Birnbaum (Science Program Office-Office of Science, SPO-SC).

The DOE Office of Science Isotope Development and Production for Research and Applications subprogram and the Heavy Element Chemistry Program of the DOE's BES funded different aspects of the work.

The Laboratory's LDRD program sponsored a postdoctoral fellowship, and some researchers received Seaborg Institute Fellowships. The work supports the Lab's Materials for the Future area through the development of isotopes for radiation therapy treatment.



Structures and abbreviated names of ligands investigated.



Crystal structure of Bi^{3+} bound to L^{py}; the chemical formula is denoted as $[Bi(L^{py})(OTf)](OTf)_2]$.

Developing longer-lived isotopes for medical diagnostics

The Laboratory irradiates targets at IPF to produce isotopes for medical applications. Some isotopes are used in radionuclide generator systems to supply short-lived isotopes for medical imaging or therapy. A generator is a self-contained system housing a longer-lived parent isotope and a shorter-lived daughter. The daughter can be periodically extracted onsite as needed, leaving the parent behind to generate another daughter. Generators are a convenient way to make short half-life isotopes available due to their cost effectiveness and independence from accelerator or nuclear reactor facilities.

Some generator systems can produce short half-life isotopes for Positron Emission Tomography (PET) medical imaging. For example, the germanium-68 (^{68}Ge)/gallium (^{68}Ga) system provides ^{68}Ga (half-life of 67.6 minutes). The ^{68}Ga can be attached to targeting biomolecules via bifunctional chelating agents to image cancer and infection. LANL and Brookhaven National Laboratory (BNL) routinely produce the parent radionuclide ^{68}Ge (half-life of 270.8 days) for the generator.

Researchers have proposed the titanium-44 (^{44}Ti)/scandium-44 (^{44}Sc) pair (see the top figure on the following page), to make available the PET isotope ^{44}Sc (halflife of 3.97 hours). This system shows similarities to ^{68}Ge/^{68}Ga, but it also exhibits significant differences. The ^{44}Sc half-life is almost four times that of ^{68}Ga. The longer half-life could enable tracking slower biological processes and permit more complex radiopharmaceutical preparations post-elution. The ^{44}Ti halflife of roughly 60 years could provide a long-term radionuclide source for the daughter ^{44}Sc. However, such a long half-life creates economic and engineering challenges due to the large quantity of long-lived ^{44}Ti that must be secured on the generator column. High ^{44}Ti activities also require high particle beam currents and long irradiation times.

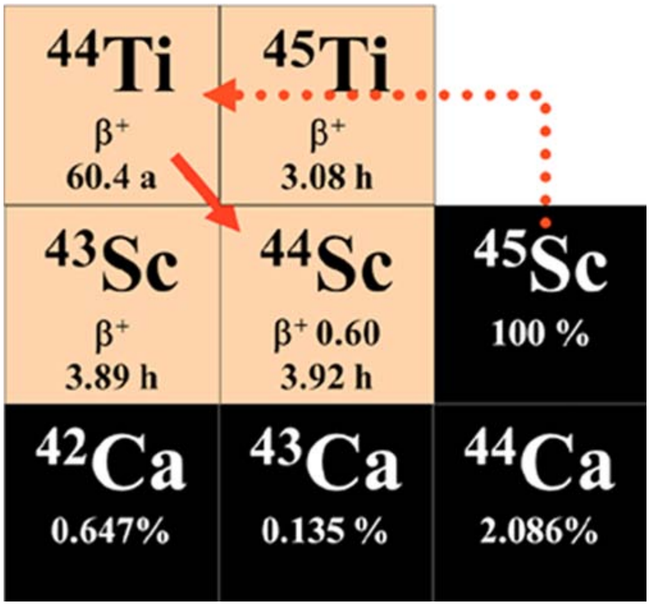
LANL and BNL are examining the production of parent ^{44}Ti at quantities to make possible pre-clinical and clinical evaluations of ^{44}Sc as a PET agent possible. The team performed two proton beam irradiations of natura abundance Sc metal targets at LANL's IPF during the 2014–15 run cycle. Lower proton energies maximized the efficiency of the ^{44}Ti reactions.

The irradiations produced more than 10 mCi of ^{44}Ti, a significant amount compared with current worldwide stocks. In parallel, BNL is working on the design and fabrication of additional proton beam targets for the future bulk manufacturing of ^{44}Ti activity.

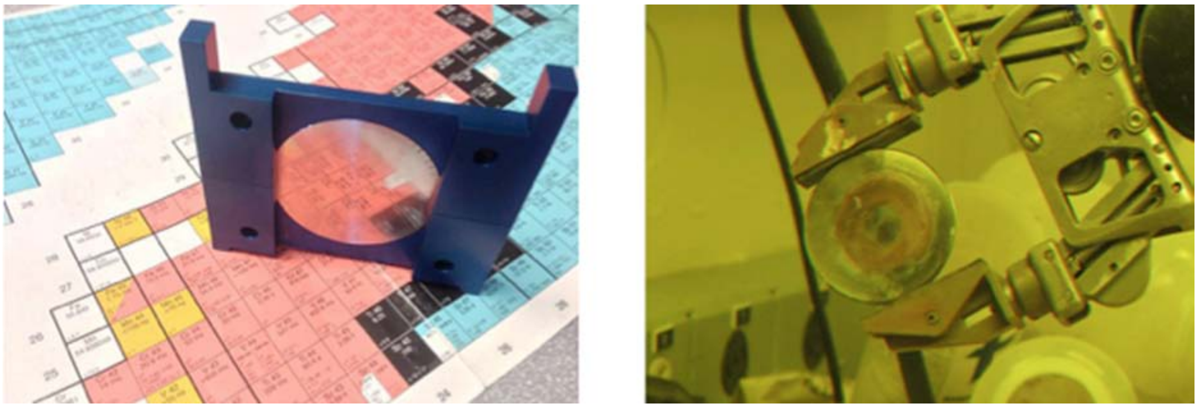
Accumulated ^{44}Ti must be chemically recovered from the irradiated scandium target. The team used the first target to develop chemical separation methods to isolate microgram quantities of ^{44}Ti from many grams of scandium. LANL and BNL research indicates that ion-exchange column chromatography would be the most efficient separation technology. Scientists are optimizing the chemical separation. After isolation and purification from byproduct radionuclides, long-lived ^{44}Ti will be fixed to a solid support for the repeated elution of daughter nuclide ^{44}Sc. The researchers are considering different extraction systems to ensure long-term sorption of ^{44}Ti and near-quantitative recovery of the ingrown ^{44}Sc imaging isotope. The team plans prototype sorption systems to evaluate performance and ^{44}Ti breakthrough evaluation, the two main parameters determining the quality of a radionuclide generator design. Once the team has found and demonstrated a successful system, test generators could be made available for ^{44}Sc labeling and biological studies.

Los Alamos researchers include the following: V. Radchenko, J. W. Engle, J. R. Maassen, C. M. Naranjo, F. M. Nortier, and M. E. Fassbender (C-IIAC); and E. R. Birnbaum and K. D. John (SPO-SC).

The DOE Office of Science, Nuclear Physics via the Isotope Development and Production for Research and Applications Program, funded the work, which supports the Laboratory's Global Security mission area and the Materials for the Future and Nuclear and Particle Futures science pillars through the development of isotopes for medical applications.



Production and decay pathway for the generator system ^{44}Ti/^{44}Sc.



Scandium target before (left) and in a hot cell after irradiation (right).

Lujan Neutron Scattering Center 2015

LANSCE
Los Alamos Neutron Science Center

Lujan Center

Lujan Center at a Glance

The Lujan Center uses a pulsed spallation neutron source equipped with time-of-flight spectrometers to perform neutron scattering studies of engineered materials. Neutron scattering is a powerful technique for probing the microscopic structure and dynamics of materials. Applications include materials science, engineering, condensed-matter physics, chemistry, biology, and geology.

The instruments at the Lujan Center operate in time-of-flight mode, receiving neutrons from a tungsten spallation target. Four moderators provide epithermal, thermal, and cold neutrons to specialized beamlines.

At the core of the Lujan Center is a spallation neutron target, moderator, and reflector system (TMRS) and the LANSCE linac. The accelerator operates at an energy of 800 MeV, with typical beam currents of 100 µA on the TMRS.

The Lujan Center's highly optimized tungsten spallation target provides a high peak flux with a broad wavelength bandwidth per frame. Two liquid hydrogen moderators provide high-intensity cold-neutron beams ideally suited for nuclear physics, reflectometry, inelastic scattering, and small-angle scattering. Water moderators provide thermal and epithermal neutrons for neutron imaging, nuclear physics, and diffraction beamlines. In addition, because of its low repetition rate, 20-Hz, long-wavelength neutrons can be used without significant frame overlap, allowing the collection of data over a broad range of time constants and length scales ideally suited for total scattering and diffraction studies.

The Lujan Center offers access to a large variety of specialized sample environments, including low temperatures down to 40 mK, magnetic fields up to 7 T, high temperature furnaces up to 2,400^{o}C and uniaxial stress (F_max=250 kN) and fluid, as well as anvil cell pressure capabilities (30 GPa-2,000K).

At left: A. Smith prepares the sample chamber on HIPPO.

Magnetic measurements detect hydrogen contaminants in plutonium

Researchers from Condensed Matter and Magnet Science (MPA-CMMS) and Nuclear Materials Science (MST-16) used magnetization, x-ray, and neutron diffraction measurements enabled by the Laboratory's materials-science capabilities to demonstrate a technique for detecting low concentrations of plutonium hydride in samples. The technique, published in the *Journal of Applied Physics,* is relevant to plutonium applications, workers who handle plutonium, and long-term plutonium storage. Contaminants, such as oxygen, hydrogen, and carbon, can degrade the mechanical properties of plutonium, resulting in consequences that can negatively affect health and safety.

Los Alamos researchers examined the effects of plutonium metal exposed to low levels of hydrogen during the radioactive decay process. The team showed that ferromagnetic remanence – the residual magnetization left in a ferromagnetic material (a permanent magnet) after exposure to a magnetic field – could detect small quantities of hydrogen against the background of pure plutonium. Pure plutonium is non-magnetic. However, Los Alamos researchers in the early 1960s discovered that plutonium acquires a magnetic moment when it reacts with hydrogen to create plutonium hydride. Therefore, magnetic measurements can be used to detect the presence of hydride formation in plutonium metal.

Researchers used the NPDF and neutron diffraction at LANSCE to characterize the metallic crystal structures samples of polycrystalline delta (δ)-plutonium stabilized with gallium (Ga). The samples had the expected face-centered cubic (fcc) structure and lattice parameters. The scientists exposed the samples to hydrogen under partial vacuum at 450 °C to ensure reproducible hydrogen solubility for the magnetization measurements. They loaded one sample to a hydrogen (H)/Pu atom ratio of 0.01 ± 0.0003, and encapsulated the second plutonium sample without H loading. After sealing the samples in Ti containers to prevent radioactive contamination of the surroundings or exposure of the samples to air, the team measured the magnetization of the capsules as a function of magnetic field and temperature at the NHMFL-Pulsed Field Facility at Los Alamos. They used a commercial vibrating sample magnetometer in a physical properties measurement system. The results confirmed that the 2.0 at. % Ga-stabilized H-free δ-Pu samples are nonmagnetic between 4-300 K.

The results demonstrated that commercial magnetization measurement techniques are sensitive to the conversion of tiny amounts (0.0015 mole fraction) of hydrogen in Ga-stabilized δ-Pu to ferromagnetic PuH_x. This easily reproducible technique is a useful quantitative diagnostic to determine the content of small amounts of PuH_x in samples.

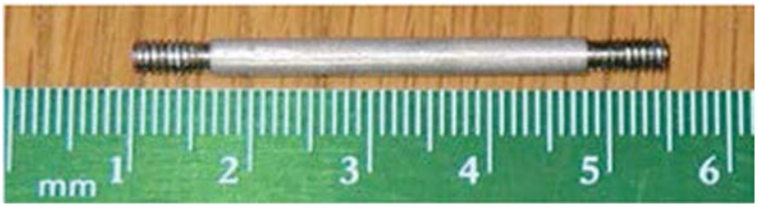
Reference: “Detecting Low Concentrations of Plutonium Hydride with Magnetization Measurements,” *Journal of Applied Physics* **117,** 053905 (2015).

Authors include the following: J. W. Kim (MPA-CMMS, now at Rutgers University), E. Mun (MPA-CMMS, now at Simon Fraser University, Canada), J. Baiardo, V. Zapf, and C. Mielke (MPA-CMMS); A. Smith, S. Richmond, J. Mitchell, and D. Schwartz (MST-16).

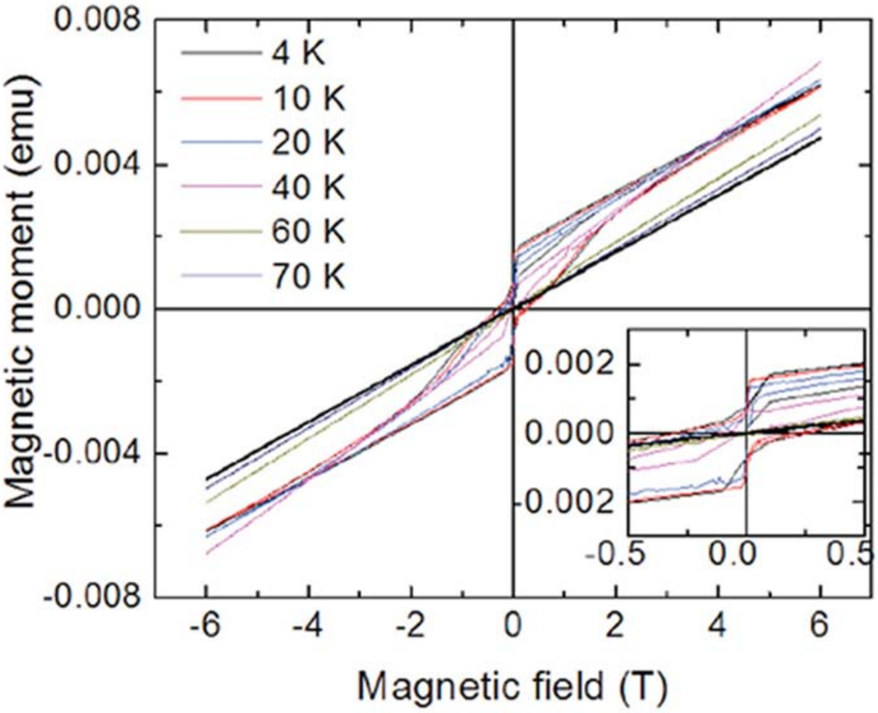
The Laboratory's LDRD program funded the LANL work. Magnetization measurements were performed at NHMFL, funded by the NSF, the State of Florida, and the DOE.

The neutron diffraction work was conducted on the NPDF at the Lujan Center, funded by DOE's BES.

The work supports the Laboratory's Nuclear Deterrence mission area and the Materials for the Future and Science of Signatures science pillars through investigation of materials in the nation’s nuclear weapons stockpile.



A plutonium sample is sealed in a titanium Ti container for magnetization measurements.



This graph plots magnetic moment as a function of magnetic field of δ-Pu with 1 at. % H exposure in a Ti sample holder (b), minus the magnetization of the sample without H exposure in Ti sample holder (a). Measurements were conducted at after zero-field cooling (in H < 10^{-3}T) from room temperature and sweeping the magnetic field around a 6 T hysteresis loop starting from H = 0. The inset shows a zoomed view of the magnetic hysteresis, with a linear background subtracted.

Lujan Center

Oxygen-deficient $BaTiO_{3-x}$ as an efficient bifunctional oxygen electrocatalyst

Development of cost-effective and highly active catalysts for electrochemical energy storage and conversion applications is a critical element in currently studied sustainable energy technologies. Metal-air batteries represent the most promising energy storage systems for portable electronics, electrical vehicles, and stationary applications for storing clean energy obtained from wind, solar, and power plants.

Unlike traditional intercalation electrodes in lithium-ion batteries, the porous air cathode in the metal-air cell can take reactant oxygen (O_2) from the atmosphere, instead of storing it in the electrodes. The unique configuration results in a vastly improved theoretical specific energy density of 1086, $Wh \cdot kg^{-1}$ for zinc-air and 5028 $Wh \cdot kg^{-1}$ for lithium-air batteries, two of the most promising metal-air systems. However, these advanced electrochemical energy technologies greatly rely on the oxygen reduction reaction (ORR) and oxygen evolution reaction (OER), a pair of the most important and technologically pertinent electrochemical reactions. Unfortunately, the ORR and OER typically have very high overpotentials with slow kinetics, requiring catalysts containing large amount of precious metals such as platinum and iridium. The prohibitive expense and limited supply of these precious metals make for unsustainable catalysts for modern society.

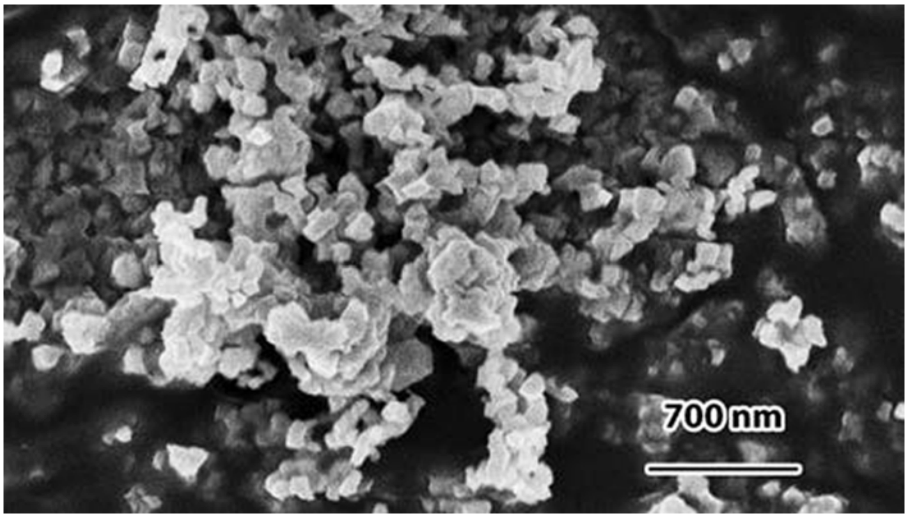
Perovskite oxides are nonprecious metal catalysts that have emerged as the most promising bifunctional ORR and OER catalysts for electrochemical energy conversion and storage. Laboratory researchers and collaborators have synthesized a new type of oxygen-deficient perovskite ($BaTiO_{3-x}$) using a sol-gel method, followed by a reductive heat treatment. The journal *Nano Energy* published the research.

The bottom figure on the following page shows that the oxygen-deficient $BaTiO_{3-x}$ perovskite catalysts exhibit high-catalytic activity simultaneously for ORR and OER in alkaline electrolyte. Especially significant, the measured OER activity on the perovskite catalyst exceeds the IrO_2 catalyst at relatively low potential and with a much-improved onset potential. The team conducted neutron diffraction experiments on the high-intensity powder diffractometer at the Lujan Center to elucidate the structure of the oxygen-deficient $BaTiO_{3-x}$ catalysts. The results indicate that the hexagonal $BaTiO_{3-x}$ phase is oxygen deficient with a stoichiometry of $BaTiO_{2.76.}$ The authors suggest that oxygen vacancies in the perovskite crystal structure lead to vastly enhanced electrocatalytic activity toward the ORR and OER. This work demonstrates a new type of highly efficient perovskite bifunctional catalyst for electrochemical energy storage and conversion through oxygen reduction and evolution reactions.

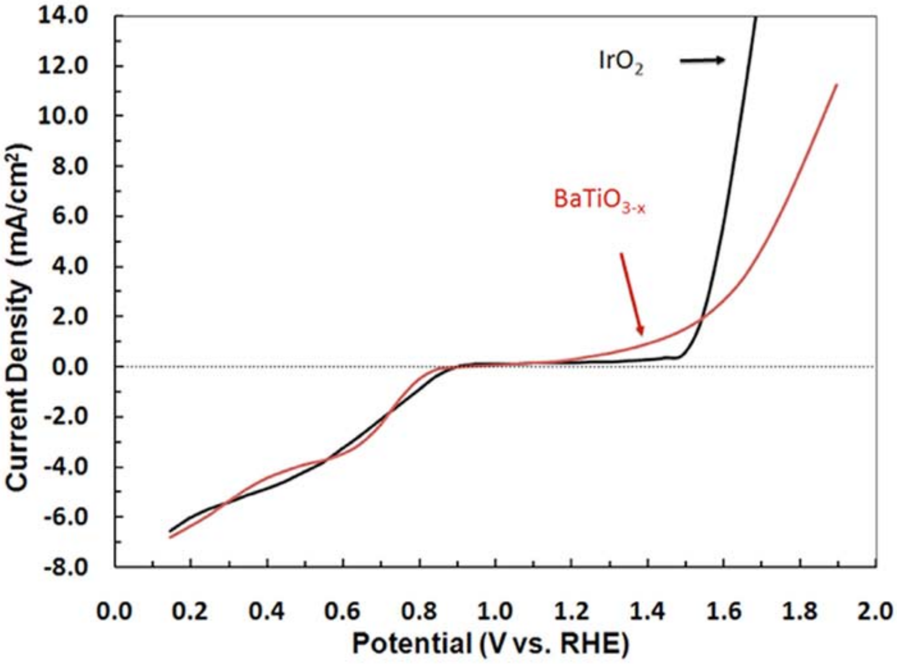
Reference: "Oxygen-deficient $BaTiO_{3-x}$ Perovskite as an Efficient Bifunctional Oxygen Electrocatalyst," (Rapid Communication) *Nano Energy* **13,** [4] 423 (2015).

Authors include the following: C. Chen, R. Dickerson, P. Papin (Metallurgy, MST-6); G. King (Materials Science in Radiation and Dynamics Extremes, MST- 8); S. Gupta, W. R. Kellogg, and G. Wu (State University of New York – Buffalo).

The Laboratory's LDRD Program funded the research, which supports the Laboratory's Energy Security mission area and Materials for the Future science pillar through the development of materials for energy storage. This work benefited from the use of the Lujan Center's high-intensity powder diffractometer instrument at LANSCE, which was developed through a joint NNSA-DOE BES instrument construction project.



Scanning electron micrograph image for a typical oxygen-deficient $BaTiO_{3-x}$ catalyst particle. State-of-the-art iridium oxide (IrO_2) catalysts, used for reference, have excellent OER activity comparable or even better than earlier reports.



Steady-state polarization plots of the ORR and OER for IrO_2 and $BaTiO_{3-x}$ catalysts in 0.1 M NaOH electrolyte at 25°C and 900 rpm.

Lujan Center

Using neutrons to predict the lifetime of bridges

Civil Engineering, the magazine of the American Society of Civil Engineers, highlighted the advantages of using neutron diffraction to evaluate large-scale engineering structures, such as the behavior of suspension bridge cables under extreme conditions. Columbia University researchers and Los Alamos collaborators analyzed bundled cables from the heavily trafficked George Washington Bridge that crosses the Hudson River to connect New York City and New Jersey.

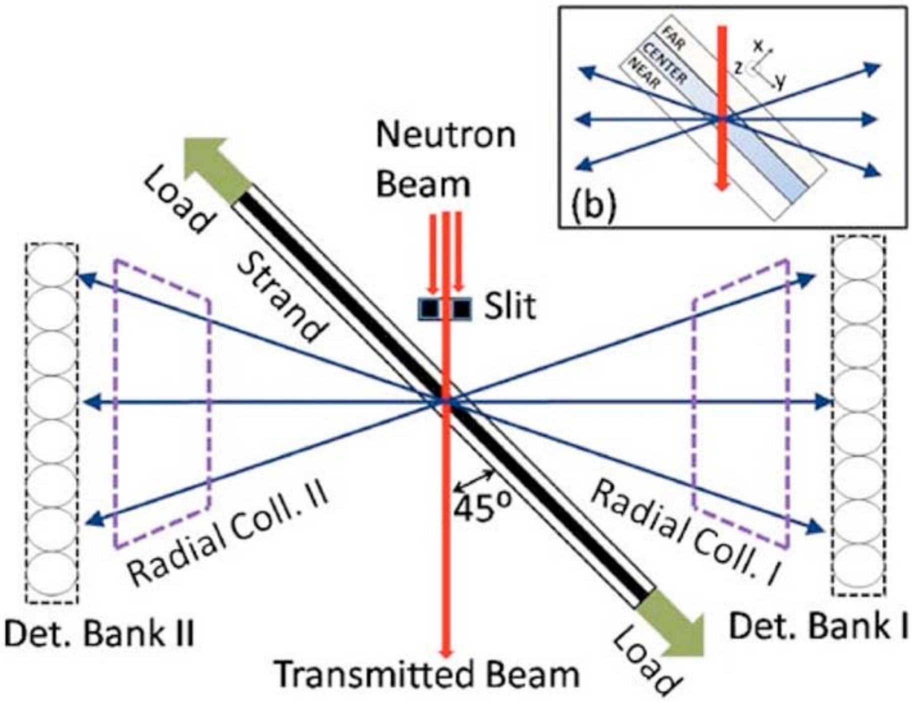
The research constitutes the first use of neutron diffraction on engineering-level samples from an existing civil structure. It was performed in part using the spectrometer for materials research at temperature and stress (SMARTS) at the Lujan Center. Neutron diffraction has an advantage of providing a nondestructive and nonintrusive means to gather crucial data from strands buried deep inside the cable. Other measurement approaches, such as inserting strain gauges, cause additional friction between wire strands, which ultimately can alter the boundary conditions.

The measurements revealed that prior assumptions about load sharing between individual strands in the cable bundle were conservative and have led to underestimations of bridge lifetime. Researchers theorize that friction and cable curvature and compaction might play a role in how the broken wires regain their load-carrying capacity. The neutron-diffraction study produced validation data that aid the development of predictive models for aging infrastructure. These results are important to the federal and state transportation departments that address pervasive structural deficiencies in the nation's bridges.

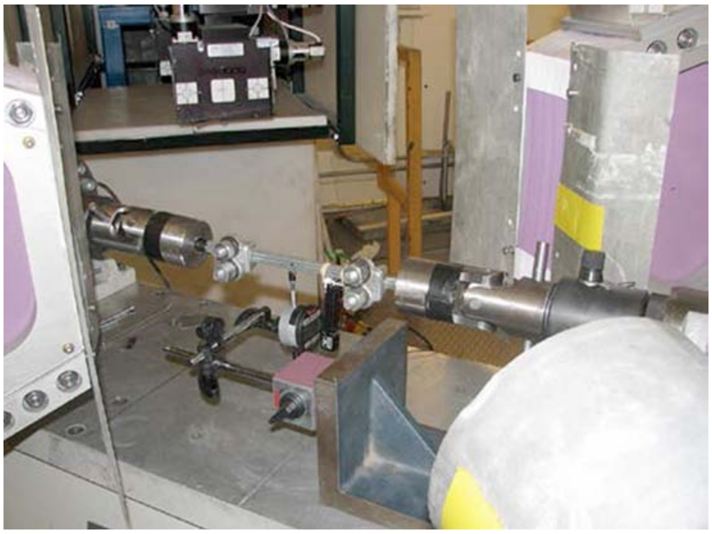
Los Alamos researchers include the following: B. Clausen and D. Brown (MST-8) and T. Sisneros (P-25). *Civil Engineering,* founded in 1930, is circulated to more than 140,000 civil engineers around the world.

Reference: "Subatomic Particles Aid Investigation of Large Bridge Components," by Laurie Shuster, *Civil Engineering,* April 21, 2015.

The NSF funded the research at Columbia University. The work benefited from the use of the Lujan Center, which is sponsored by DOE BES. The research supports the Laboratory's Global Security mission area and the Materials for the Future science pillar by demonstrating experimental measurements that are vital for the validation of structural and materials models.



In the schematic of the SMARTS diffractometer, the intersection of the incident beam and the acceptance fans of the radial collimators define the probe volume (inset). The entire load frame is mounted on a precision translator and can be moved to bring the center of each wire into coincidence with the probe volume. Detector bank II measured the longitudinal strains in this schematic.



Sample mounted in the load tester of the SMARTS diffractometer.

Additively manufactured U_6Nb heat-treated in situ in SMARTS

A LLNL and LANL team heat-treated uranium-niobium (6 wt.%) alloy (U_6Nb) in situ in SMARTS at the Lujan Center. The team's work aimed to understand the materials processing methods that LLNL performs. The results provided valuable data for improving LLNL's additive manufacturing techniques.

Additive manufacturing 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. The resulting parts produced via additive manufacturing should be thoroughly characterized because the process is very different from traditional manufacture.

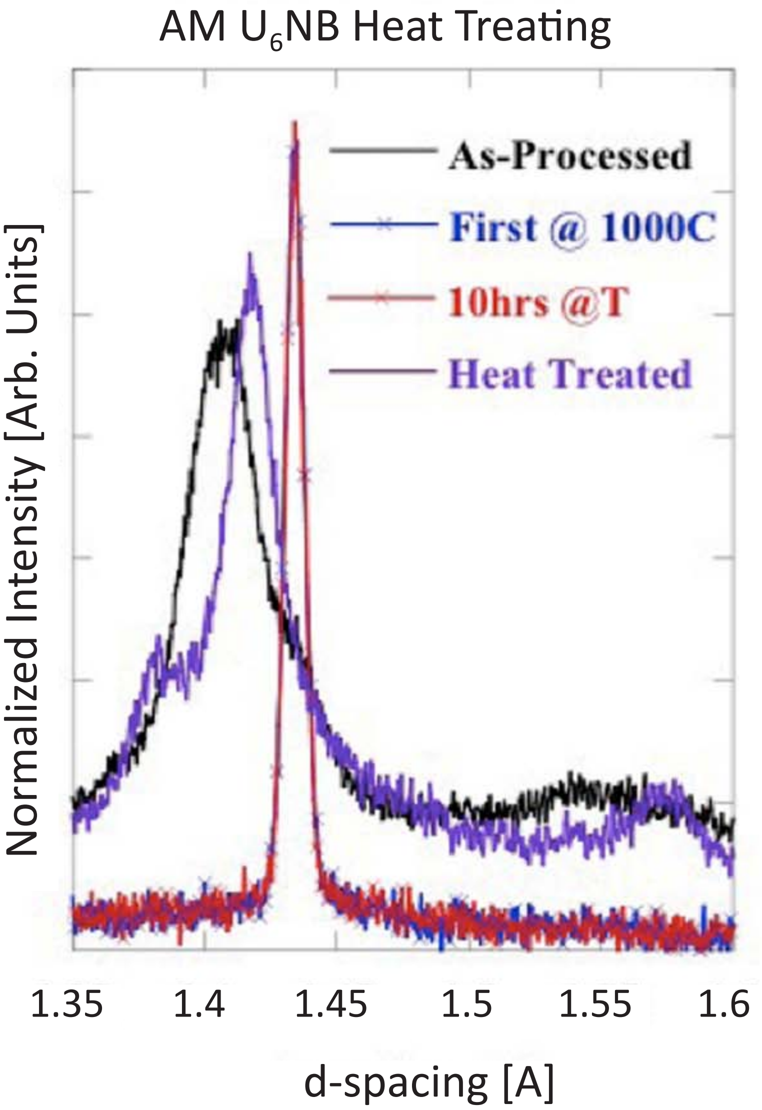
Traditionally processed U_6Nb usually has a monoclinic (α'') crystal structure. Previous experiments at SMARTS showed that as-processed, the U_6Nb material additively manufactured at LLNL has a two-phase structure consists of roughly equal amounts of the monoclinic and tetragonal (γ0) crystal structure. Following the LLNL heat-treatment (10 hours at 1000°C), the material is single phase γ0.

The team heated an as-processed sample 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 (approximately 5 minutes) on SMARTS. The figure on the following page 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 are indistinguishable from that 10 hours later. The final diffraction pattern after the heat-treatment is consistent with the sample heat treated ex situ at LLNL. The researchers concluded that the aspects of the microstructure that can be monitored with diffraction – Nb concentration, internal stress, dislocation density, and texture – did not change during the hold at 1000°C. Therefore, the researchers conclude that the change must have occurred during the heating phase.

LLNL can use these results to better design the heat-treatment process to achieve the final microstructural goal. Moreover, the work represents the philosophy driving MaRIE, the Laboratory's proposed experimental facility for control of time-dependent material performance. The philosophy is to understand the manufacturing process to enable 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.

The NNSA Primary Assessment Technologies Campaign funded the work, which supports the Laboratory's Nuclear Deterrence mission area and Materials for the Future and Science of Signatures science pillars.

Researchers include the following: A. Wu (LLNL), D. Brown, and B. Clausen (MST-8).



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

Combined crystallographic and NMR studies of carbonic anhydrase

Proton transfer is a fundamental mechanism at the core of many enzyme-catalyzed reactions. It is exquisitely sensitive to pH, electrostatics, active-site geometry, and chemistry. Carbonic anhydrases (CAs) are ubiquitous enzymes that catalyze the interconversion of carbon dioxide (CO_2) and hydrogen carbonate (HCO_3). Human CAs are involved in a great variety of physiological processes: respiration, ureagenesis, gluconeogenesis, cerebrospinal fluid production, and general acid/base homeostasis. The CA enzyme has evolved a fast and efficient way to conduct protons through a combination of hydrophilic amino acid side chains that coordinate a highly ordered hydrogen-bonded water network. LANL scientists and collaborators have studied the structure of CA using a combination of neutron crystallography and NMR to gain a better understanding of proton transfer and how subtle changes in ionization and hydrogen-bonding interactions can modulate enzyme catalysis. *Proceedings of the National Academy of Sciences* published the research.

In the Human Carbonic Anhydrase II (HCA II) enzyme, a proton derived from water bound to a zinc (Zn) atom in the active site is transferred to the bulk water surrounding the enzyme. The proton transfer network involves several highly ordered water residues, as well as amino acid residues tyrosine 7 (the 7th amino acid in the molecule) and histidine 64 (the 64th amino acid) from the enzyme. Histidine 64 becomes protonated, swings out into the bulk water, and releases the proton.

To understand the process, the authors probed the protonation state of all tyrosine amino acids in HCA II and measured their pKa (acidity constant) in solution, with particular focus on tyrosine 7. They combined these studies with analysis of new neutron crystallographic structures, which enable direct visualization of hydrogen atoms in proteins. The information provides insight into the effect of pH on important active-site residues. The team measured NMR spectra from pH 5.4–11.0. Identification of all eight tyrosines in HCA II allowed interrogation of their individual behaviors in solution and a comparison of the results with the crystal structures. The data revealed that tyrosine 7 has a pKa three units lower than the other tyrosines and matches that of histidine 64 to participate in the proton transfer.

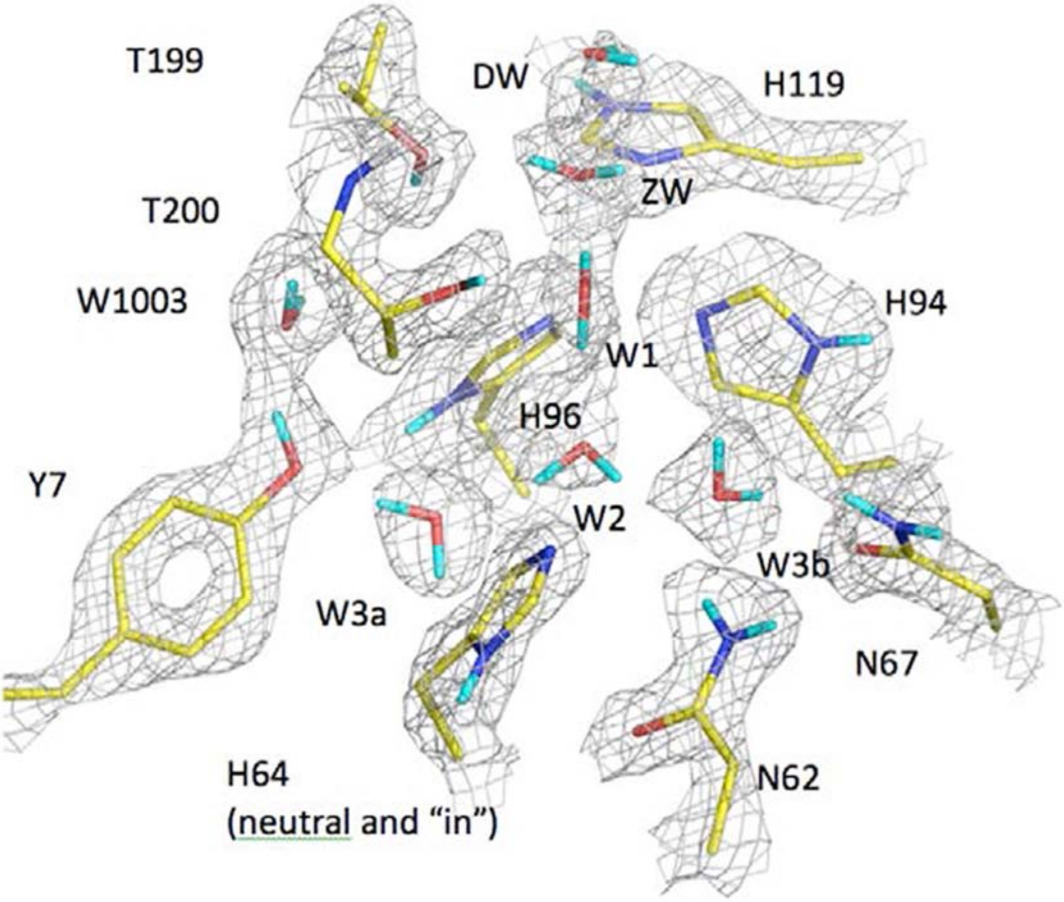
This is the first example demonstrating the powerful combination of NMR spectroscopy and neutron crystallography to gain insight into the electrostatics of a protein active site and how such electrostatics affect the charged states and hydrogen bonding of amino acid residues. The results show that the protonation states of histidine and tyrosine residues are sensitive to both pH and the presence active-site Zn atom. These factors change how histidine and tyrosine residues hydrogen bond to water and other amino acids. The research shows that it is possible to study these changes directly and at high resolution.

Reference: "Joint Neutron Crystallographic and NMR Solution Studies of Tyr Residue Ionization and Hydrogen Bonding: Implications for Enzyme-mediated Proton Transfer," *Proceedings of the National Academy of Sciences* **112,** 5673 (2015).

Authors include the following: R. Michalczyk, C. Unkefer, and J-P. Bacik (B-11); A. Kovalevsky and Z. Fisher (formerly B-11); collaborators from Forschungszentrum Jülich GmbH, Technische Universität München, ORNL, and University of Florida.

Researchers prepared amino acids for NMR studies at the LANL Stable Isotope Resource. P. Silks (B-11) provided stable-isotope-labeled tyrosine used in some labeling experiments. The research used two instruments – x-ray Diffractometer and 700-MHz NMR—that PADSTE purchased as an institutional investment.

The DOE Office of Science sponsored the Protein Crystallography Station at the LANSCE, and a LANL LDRD Early Career grant funded research. The work supports the Laboratory's Global Security mission area and the Science of Signatures science pillar via the elucidation of the structure and mechanisms of important human enzymes.



Active site of HCA II enzyme shows crucial tyrosine 7 (Y7) and histidine 64 (H64) residues and a well ordered water network that includes molecules labeled DW, ZW, W1, W2, W3a, W3b, and W1003.

Lujan Center

Neutron scattering showcased as Editor's Pick in special *Biointerphases* issue

In research recognized as an Editor's Pick in a special "in focus" issue of *Biointerphases* on bio surface analysis, Laboratory researchers and their colleagues describe recent advances using neutron scattering to study the structure of soft condensed materials. The research included model bio-related systems and in situ investigations of biological interfaces and living cells under mechanical stress.

Understanding these systems at nanometer scales is important for solving many complex biological problems, developing innovative medical treatments, and advancing the development of highly functionalized biomimetic technologies. Example applications include the following: 1) neutron scattering to study simple systems such as the shear stability of lipid membranes, which has implications in the design of biocompatible functional coatings; and 2) studies of cancer cell adhesion and response to fluid shear stress, which has implications for understanding the behavior of aggressive brain tumors.

Neutron surface scattering measurements typically examine simple, homogeneous model systems. Studying complex living objects—for example, endothelial or cancer cells in dynamic shear conditions mimicking the flow of blood—presents an extraordinary challenge. The strengths of neutron scattering are its non-pertubative nature, the ability to probe large surface areas of buried interfaces with nanometer resolution, and the possibility of manipulating the scattering contrast via isotopic substitutions. These properties enable the examination of structural details not accessible with most other techniques. The information may provide a new way to investigate and understand living tissue in situ. Understanding these complex systems could lead to advances in the treatment of cancer, atherosclerosis, and other disorders associated with the cardiovascular system.

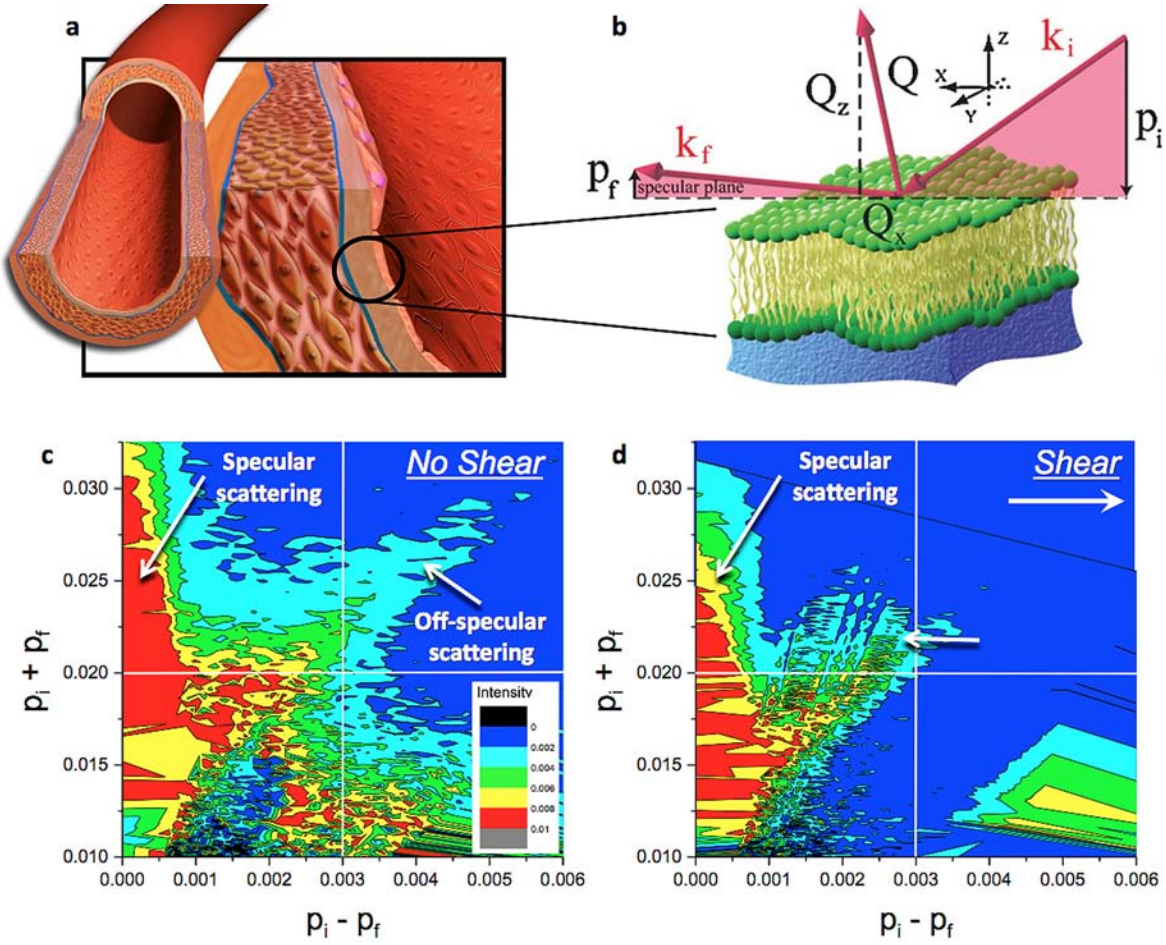
Neutron surface scattering can examine structural changes in soft materials (including those of biological importance) and provide essential structural information to complement the capabilities of MaRIE, the Laboratory's proposed facility for materials studies at the mesoscale. Researchers could use these concepts and experimental approaches to conduct new studies that would provide better understanding of biomedical questions, suggest innovative treatment, or advance the development of novel highly functionalized technologies inspired by nature.

Reference: "Analysis of Biosurfaces by Neutron Reflectometry: From Simple to Complex Interfaces," *Biointerphases* **10,** 019014 (2015).

Authors include the following: A. Junghans, S. Singh, and J. Majewski (MPA-CINT); E. B. Watkins (MPA-11); M. J. Waltman (B-11); H. L. Smith California Institute of Technology; L. Pocivavsek (University of Pittsburg Medical Center); and R. D. Barker (Institute Laue-Langevin, France).

This research benefited from the use of the Surface Profile Analysis Reflectometer (SPEAR) in the Lujan Center at LANSCE. DOE BES funded the Lujan Center.

The work supports the Laboratory's Science of Signatures and Materials for the Future science pillars through the study of complex and living systems.



Scientists used neutron scattering at the Lujan Center to study complex bio-interfaces, including the behavior of monolayers of living cells under the stress induced by the flow of liquid mimicking blood. The human vascular system is constantly exposed to blood flow and is inherently reliant on the solid mechanical and fluid mechanical stresses for normal healthy function.

(a) The innermost layer of blood vessels consists of a single monolayer of endothelial cells, the most susceptible to mechanical stress due to the flow of blood. Neutron reflectivity enables researchers to visualize the part of the live cells attached to a solid support and to mimic the conditions of the vascular flow during scattering measurements.

(b) Specular scattering reveals the mechanism of how the extracellular matrix changes in thickness and density at different temperatures and shear rates. This provides crucial information to understand how endothelial adhesion works and how it might be influenced for biomedical applications. The off-specular data depict changes in the in-plane arrangement of the cells.

The graphs for (c) and (d) show experimental two-dimensional intensity maps of neutrons scattered from endothelial cells at static and shear conditions, respectively. The significant extension of the off-specular signal (right top corner) as (c) compared to (d) indicates more in-plane fluctuations (or disorder) at static conditions. When the cells are under stress due to the flow of liquid, they become more uniformly ordered and aligned.

Lujan Center

Uranium-niobium experiments validate models for aging degradation and material processing

A decade-long experimental campaign to understand and predict thermal aging of U-Nb alloys at Los Alamos has provided unique data-validating innovative thermodynamic and kinetics modeling. These alloys behave similarly to stainless steel, with good corrosion resistance and ductility in the initial condition. However, the U-Nb alloys suffer from severely degraded properties after thermal exposures. The phase transformations responsible for aging are quite complicated even though the alloy contains only two major elements. The significant body of experimental data gained at Los Alamos and elsewhere makes this material a good test case for critical comparisons of the theory of solid-state phase transformations with experiment. The insights gained will improve models of processing and aging of U-Nb and a wider variety of alloys. *Proceedings of the International Conference on Solid-Solid Phase Transformations in Inorganic Materials 2015* published the work.

Researchers encapsulated several hundred U-Nb alloy specimens in quartz and aged them under controlled conditions ranging from 100 to 625°C in the Sigma facility at LANL. Sampling the entire phase transformations pathway from initial time to equilibrium required long-term aging, up to 5 years. The team characterized the microstructure via light and electron microscopy, and measured the phase amounts and compositions by x-ray diffraction.

The top figure on the following page shows the updated equilibrium phase diagram. The team evaluated the new model using the CALculation of PHAse Diagrams (CALPHAD) framework, which ensures an optimal fit accounting for both phase equilibria data (black data points) and thermochemical data (not shown). For the first time in this system, researchers incorporated first-principles calculations of density functional theory into the overall assessment. The long-term LANL aging data (inset) validated a key prediction of the model, the γ_2 phase boundary on the niobium-rich side.

The team performed phase field simulations of microstructural evolution of the α (orthorhombic) and γ (body-centered cubic, bcc) phases and their compositions to better understand the complicated kinetic paths that lead to final equilibrium at temperatures between ambient and 647°C. As early as 1972, experiments had revealed that the system paused at a metastable phase, $\gamma_{1\text{-}2}$, of intermediate composition, approximately 50 atomic % Nb. The new study has amplified this puzzling result, shown in the orange region in the phase diagram figure. Because these compositions fall within the unstable region of the phase diagram (γ-bcc miscibility gap), researchers need a new approach to explain the observation of a persistent metastable $\gamma_{1\text{-}2}$ phase and the total phase transformation sequence. The team conducted phase field kinetics modeling, employing as inputs the same thermodynamic model used to predict the phase diagram (as shown in the top figure on the following page), in addition to a variety of diffusion parameters also modeled in this study.

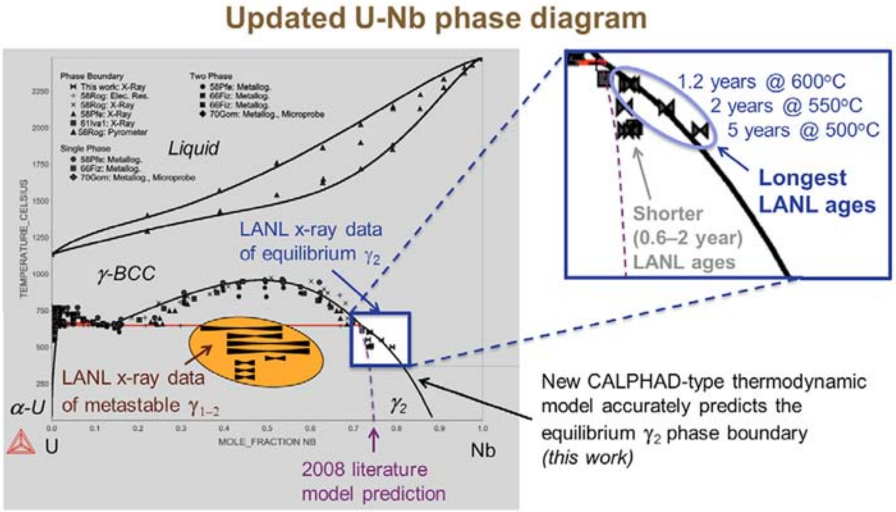
The bottom figure on the following page depicts phase-field kinetics simulations of a U-Nb diffusion couple at 450°C without (left) and with (right) the use of strain-adjusted free energies in the simulation code. As time increases (moving front to back), the alpha phase grows at the expense of the gamma phase, and the gamma increases its niobium content to conserve mass. How much the gamma composition changed was the major question. The results using the baseline thermodynamic model by itself (left side) failed to predict the $\gamma_{1\text{-}2}$ phase, and instead evolved the system straight to the equilibrium γ_2 phase. To explain the persistence of the $\gamma_{1\text{-}2}$ phase, the authors hypothesized that strain energy between the misfitting α and γ crystal structures would shift Gibbs free energy of the γ-bcc phase in ways that would stabilize of the $\gamma_{1\text{-}2}$ phase. These modifications to the CALPHAD model (right) enabled improved phase-field predictions consistent with the experimental evidence. The team concluded that this is a plausible approach, which could be applied to other actinide alloys and other engineering alloys.

Reference: "A Hierarchical Computational Thermodynamic and Kinetic Approach to Discontinuous Precipitation in the U-Nb System," *Proceedings of the International Conference on Solid-Solid Phase Transformations in Inorganic Materials 2015.*

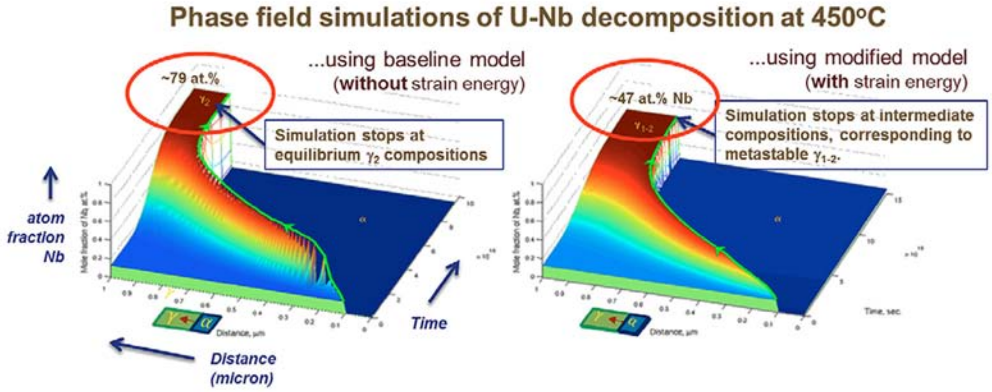
Los Alamos authors include the following: R. Hackenberg (6), H. Volz (Weapons Test Engineering, W-14), A. Llobet (Neutron Science and Technology, P-23), A. Smith (MST-16), and G. King (MST-8), with collaborators from Texas A&M University (T. Duong, R. Arroyave, and S. Gibbons), LLNL (A. Landa and P. Turchi), CALTECH (S. Bajaj), and the Royal Institute of Technology in Sweden (A. Ruban and Levente Vitos). T. Tucker, Pallas Papin, B. Forsyth, A. Kelly, T. Beard, J. Cooley, and K. Clarke (MST-6) contributed to the specimen preparation, aging, and characterization at LANL.

The modeling portion of this work formed the PhD dissertation of T. Duong at Texas A&M University; Hackenberg and Turchi served as external examiners. The experimental portion of the work was performed at LANL and funded through the NNSA Enhanced Surveillance Campaign (T. Zocco, LANL Program Manager).

The research supports the Laboratory's Nuclear Deterrence and Energy Security mission areas, and the Materials for the Future science pillar, by understanding and predicting the effects of material processing, aging, and corrosion on the properties, performance, and functionality of the materials. A synergy of unique actinide R&D experiments coupled with multi-scale modeling enabled the work.



Updated U-Nb phase diagram.



Phase-field kinetics simulations of a U-Nb diffusion couple at 450°C without (left) and with (right) the use of strain adjusted free energies in the simulation code. The vertical axis and color indicates the composition, and by extension the phase (blue has ~0 at.% Nb and is α-U; turquoise, yellow, and red are richer in Nb and represent the γ-bcc phase.)

Proton Radiography 2015

LANSCE
Los Alamos Neutron Science Center

pRad at a Glance

For more than a decade LANL has used high-energy protons as a probe in flash radiography for a decade. pRad uses 800-MeV protons provided by the LANSCE accelerator facility to investigate dynamic experiments in support of national and international weapons science and stockpile stewardship programs. Through this effort, significant experience has been gained in using charged particles as direct radiographic probes to diagnose transient systems.

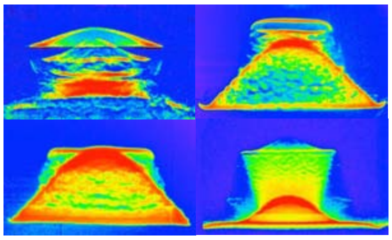
The proton radiography effort at LANSCE has operated as a user facility since 2003 and has recently been designated as one of the three DOE user facilities at LANSCE. Each year, a proposal call is distributed and the submitted proposals are reviewed by a program advisory committee.

Currently, the user community extends from the DOE-NNSA national laboratories, LANL, Lawrence Livermore National Laboratory, Sandia National Laboratories, and Oak Ridge National Laboratory to international users [Atomic Weapons Establishment (AWE), Commissariat à l'énergie atomique et aux énergies alternatives (CEA) and All-Russian Scientific Research Institute for Experimental Physics (VNIIEF)] and has recently grown to include DoD laboratories [(Army Research Laboratory (ARL) and Eglin Air Force Base (AFB)], as well as university interest (Harvard, Imperial College, and Technical University of Darmstadt).

pRad is training the next generation of national security scientists. Every year, high school, undergraduate, and graduate students, as well as postdocs, visiting scientists, and professors, join the pRad team to conduct exciting experiments. pRad attracts new talent to research in shock physics, weapons physics, dynamic materials, and stockpile stewardship.

Fundamental materials research

Invented at LANL, proton radiography provides a unique understanding of the fundamental behavior of materials. This set of radiographs (below) taken after various metals (clockwise from top left, aluminum, copper, tantalum, tin) were shocked from below reveals radically different behavior; for example, the aluminum sample splits into layers while the tin sample melts.



Dynamic experiments

For a single experiment, the pRad facility is able to make multiple images over time – currently, up to 37 images. Taken together, these images form a time-lapse movie that illuminates ultra-fast phenomena.

Understanding shocked materials

Protons penetrate through materials driven by high explosives—giving insights into their behavior under dynamic conditions. Proton radiography makes possible quantitative measurements of material densities under extreme conditions, providing a diagnostic capable of measuring the performance of untested weapons components or aged components in the stockpile. This precision makes possible a range of fundamental science measurements as well.

Characterizing components

Multiple proton pulses provide super high-speed movies of the interiors of explosions for stockpile stewardship without underground testing. The penetrating power of protons makes possible detailed radiographic images of experiments conducted in sealed metal containment vessels, to study damage features in explosively shocked samples.

At left: J. Goett aligns optical components used to characterize the prototype 10-frame ultra-high-speed camera.

pRad

Enhanced imaging for dynamic physics research at the Proton Radiography Facility

Researchers have successfully installed and operated a new and improved high-speed imaging system at pRad.

The imaging system is designed for dynamic experimental studies. These advances significantly enhance the pRad capabilities for users in the materials and shock physics communities.

The Laboratory pioneered proton radiography, which is well suited to the study of dynamic processes in materials. The technology features excellent contrast and the capability to radiograph dynamic events on short time-scales (e.g., a few microseconds) multiple times during its evolution. With the LANSCE accelerator's capabilities, the number of radiographs is limited only by the camera technology.

The large-format, 10-frame hybridized focal plane array design of the new imaging system offers much improved spatial and charge resolution, higher quantum efficiency, lower noise, and faster repetition rate over the current state of the art, with integration times below 50 ns.

The new camera design, slated to replace an earlier 3-frame design, allows experimenters more than 40 radiographs per event, as opposed to the 21 provided in the current system, and with fewer cameras.

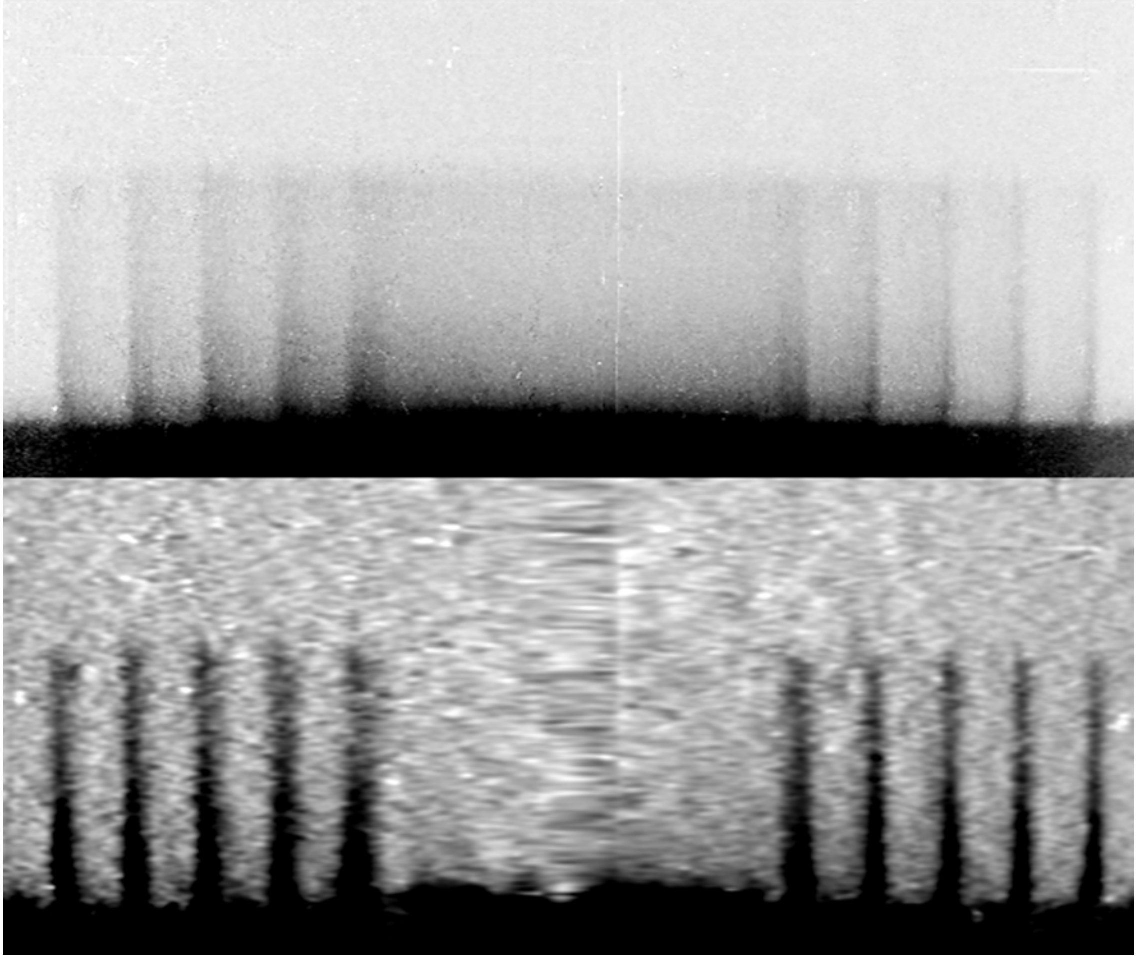
The goal for the current experimental run cycle was to prove that the camera could operate in the harsh ionizing environment of the proton beam. Physics Division researchers made an aggressive push to prepare the camera to take data in a dynamic experiment.

In its first deployment, the camera recorded the evolution of Richtmeyer-Meshkov instabilities at late times (image). The team will focus on quantitative characterization of the camera's capabilities (i.e., measurements of transfer curves) and integration of the sensor into a production-camera design.

Materials experiments at the Laboratory's proposed MaRIE experimental facility would demand unprecedented time-resolved imaging capabilities. MaRIE is designed for the study of time-dependent mesoscale materials science. Many of the technologies featured in this new imaging prototype (e.g., improvements in in-pixel memory and quantum efficiency) are promising additions to the suite of technologies researchers could utilize in conceptual designs of MaRIE.

The Laboratory's P-23 and P-25 groups, Teledyne Imaging Sensors, Fishcamp Engineering, and SNL collaborated to develop this new imaging system.

NNSA Science Campaign 3 funded the work, which supports the Laboratory's Nuclear Deterrence mission area and the Materials for the Future and Science of Signatures science pillars through dynamic materials and shock physics investigations.



The team (Principal Investigator B. Buttler, P-23) performed two identical experiments at about 7 atm (atmospheric pressure) of helium. Two shots—one from 0–5.5-µs with an interframe time of 275 ns (21 images and a static) and one from 5.8–13.8 µs (21 images)—will be combined.

The 10-frame camera, which was fielded on the second, from 5.9–9.5 µs with an interframe time of 400 ns, is a link between the two, to verify repeatability. The image taken using the 10-frame camera shows (top) areal density and (bottom) Abel inverted.

pRad

Elena Guardincerri: Tracking muons to reduce nuclear threats and help preserve architectural treasures

When Elena Guardincerri was a physics PhD student at the University of Genova, she considered muons a nuisance. She built muon detectors to snare these secondary cosmic rays, which were interfering with her experiments to study elusive neutrinos. Now, as a member of the P-25 Muon Tomography team, she is developing a muon detector to assist in saving a 37,000-ton masonry cathedral dome, known as Il Duomo, in Florence, Italy, from severe cracks and earthquake damage. Her novel method uses muons as a probe to image reinforcement elements inside thick-walled structures.

"Elena is an extremely creative physicist," said her team leader Chris Morris, who invented multiple scattering muon imaging, which exposes smuggled nuclear material even when it is concealed by shielding material.

Muons can identify dense objects and make distinctions between substances, such as water and melted nuclear fuel, and unlike x-rays, they can penetrate deep inside materials, generating images of thick objects. Cosmic muon radiography does all of this without damaging structures and without the need of an artificial radiation source.

Guardincerri helped write software for the muon trackers built in Japan by Toshiba that will obtain precise images of the Fukushima Daiichi nuclear power plant, a critical step before disaster cleanup can begin safely. In other high-profile work, Guardincerri is "contributing enormously to the P-DO threat reduction effort," Morris said. For instance, she is testing how well muons can scout for nuclear weapons effects underground.

Guardincerri credits former team member Cas Milner for proposing muon tomography for the dome—one of several ideas the Laboratory presented to an Italian delegation of conservation experts in 2013.

Designed by the secretive master builder Filippo Brunelleschi, the 15th-century dome of Santa Maria del Fiore Cathedral is an architectural marvel, and it is has been affected by ever-expanding cracks for centuries. Some scholars believe, based on historical documents, that iron reinforcements might be inside the dome's thick masonry, but investigations with metal detectors failed to yield conclusive evidence either for or against this view. To determine the dome's strength and need for further reinforcements, the cathedral's preservationists are looking to LANL to help determine the exact location of the iron–if it exists–and compile a more detailed crack profile, which will be used in their models.

In 2015, Guardincerri visited Florence to explain to the cathedral's conservation committee why she believes LANL's muon tracker technology could provide precious information regarding the inside of the dome. She presented vivid images of iron bars embedded in a replica wall built at LANL. The committee approved the design of a pair of portable trackers, each weighing no more than 220 pounds, one of which will be suspended inside the cathedral near Giorgio Vasari's Last Judgment fresco.

"This will be a great stage to show the world that this [muon imaging] works," said Guardincerri, who grew up in a nearby town.

With LDRD Early Career Award funding, she is redesigning the muon trackers, which currently weigh 800 pounds each. Following a recent visit to the National Geographic Society, she and National Geographic are exploring ways to collaborate on the project based on a mutual interest in innovative imaging technology as well as in the history of Florence.

She and colleague Matt Durham (P-25) explained how the one-detector method that has been used for pyramids is better for a wider field of view and the award-winning LANL technology is better for seeing details in smaller structures. By sandwiching a structure between two detectors and measuring the muon rays entering and exiting a structure, the LANL muon tracker distinguishes dense objects with a resolution that other muon imaging methods cannot achieve. For the dome application in particular, "our technique is more accurate and the spatial resolution is much better," Guardincerri said.

To reveal structural secrets of the Florence cathedral and help protect it against further damage, E. Guardincerri is designing lightweight muon trackers made of two-inch-diameter carbon fiber drift tubes for measuring the dome's thick-walled passageways.

PHELIX at pRad enhances movie-making of materials in extreme environments

A new pulsed power driver for pRad is producing images of higher spatial resolution than previously attainable, serving as a valuable tool for scientific experiments key to understanding and maintaining the U.S. nuclear stockpile.

An air-insulated capacitor bank, the Precision High Energy Density Liner Implosion eXperiment (PHELIX) provides greater than 400 kJ of stored energy, thus (1) generating peak currents above 5 MA to implode centimeter-size liners at 10 to 40 µs and (2) attaining speeds of 1–4 km/s. The experiments are self-confined. Researchers can tune the magneto-hydrodynamic push on the liner to match experimental needs via adjustments of the charge voltage for each shot. When combined with proton radiography technology, PHELIX produces more than five times the axial imaging data at higher spatial resolution in one experiment than what was previously available with Atlas, the Laboratory's former pulsed-power facility for liner-on-target experiments.

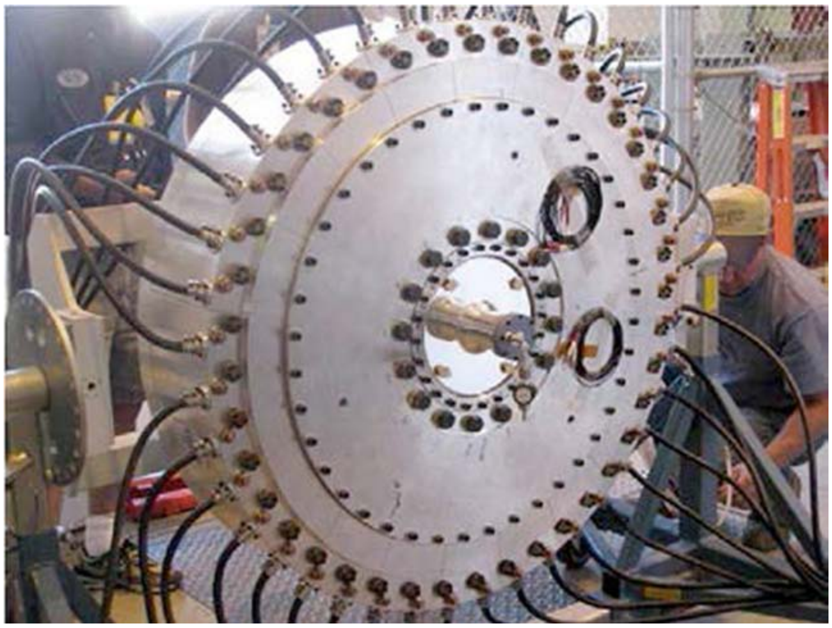
D. Oro (P-23) gave an invited talk featuring this capability at the Shock Compression in Condensed Matter conference in Tampa, FL. Damaged surface hydrodynamic experiments performed with PHELIX explored shocked-ejected particle transport into gas in converging geometries. Researchers employed a cylindrical liner-on-target configuration for these experiments. Scientists used micron-sized tungsten particles in place of shock-formed ejecta to control the initial conditions. A 100-µm-thick layer of tungsten powder coated the inner surface of the cylindrical target. The liner impacts the target, generating a shock that launches the tungsten particles off the target surface. The researchers captured the time history of the trajectory of the converging shocked-ejected particulate in 21 proton radiographs recorded during the experiment.

The team has executed three experiments of this type: into 1) vacuum, 2) argon at 8.3 bars, and 3) xenon at 8.3 bars. The image quantity and quality from pRad provide a level of detail in time and space not available previously for these types of experiments. The experiments employ pRad's X3 magnifier. PHELIX can also be operated with the X7 magnifier to trade off field-of-view for higher resolution. Study of the details of hydrodynamically evolving features under extreme conditions is important for validating hydrodynamic algorithms in weapons computer codes. PHELIX gives researchers another tool to achieve these conditions in a controlled fashion that is compatible with advanced diagnostics such as pRad. PHELIX has the advantage of its small size (approximately that of a travel trailer), which can be placed in the pRad beamline for experiments and removed to make way for others. The Laboratory's previous pulsed power machines, Atlas and Pegasus, required large rooms and fixed positioning.

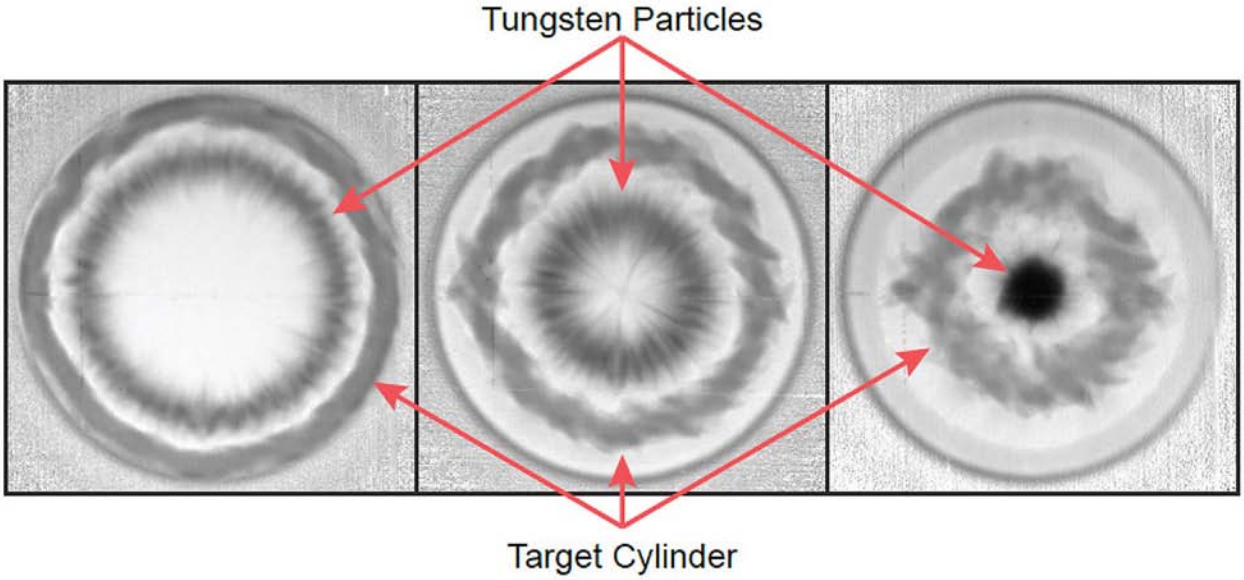
The work is an example of Science on the Roadmap to MaRIE, the Laboratory's proposed Matter-Radiation Interactions in Extremes facility that would provide the capability to image over microseconds timescales thick samples of materials undergoing a dynamic event.

Funded by Science Campaign 1: Primary Assessment Technologies (LANL Program Manager S. Sterbenz), the creation of PHELIX involved a collaboration of the Laboratory's Physics, Computational Physics, Accelerator Operations and Technology, and Materials Science and Technology divisions; and National Security Technologies LLC.

The pRad capability is primarily funded by the NNSA Science Campaigns. PHELIX supports the Laboratory's National Security mission area and the Materials for the Future and Science of Signatures science pillars through investigation of shock-ejected particulates.



The above photo shows the PHELIX transformer, at the center of which is the liner load cassette. This image was taken during initial testing, before the boxcar was installed. The black coaxial cables connect the transformer to capacitor banks (not shown).



Three of the 21 proton-radiographs taken down the liner load central axis during the experiment. The images were taken—from left to right—at approximately 30 µs, 34 µs, and 39 µs after the start of current flow. In the first image, the cloud of tungsten particles and target cylinder enter the field of view. In the second image, the fastest traveling particles have reached the center. In the third image, most of the tungsten particles have accumulated at the center.

Ultracold Neutron Source 2015

LANSCE
Los Alamos Neutron Science Center

UCN at a Glance

LANSCE is home to some of the most intense sources of cold neutrons—these are among the coldest of subatomic particles. The LANSCE UCN source is a unique facility that produces high-energy spallation neutrons and uses solid deuterium to cool the neutrons by a fold of one billion. The resulting UCN have two distinct properties that allow them to be studied precisely: 1) they move at speeds of only a few meters per second and 2) they are completely confined by magnetic fields and material bottles for many hundreds of seconds at a time. These properties lead to very precise low energy particle physics experiments that search for small differences between measurement and prediction, and these precision measurements are a powerful tool for investigating new physical processes that can complement and rival experiments at high-energy colliders such as CERN.

There are several new and ongoing experiments at the UCN source that measure decay correlations and other properties of the neutron. This program of measurements probes the particle physics underlying neutron decay, and it has important implications for high-energy physics and cosmology. In addition, because of the interaction between UCN and material surfaces, the facility is used to study materials relevant to high-precision experiments, and it also will provide a detailed understanding of neutron-induced fission on actinides.

UCNA

UCNA measures the beta-asymmetry, or the correlation between the neutron spin and the decay beta-particle. UCNA exploits the properties of UCNs to produce a decay geometry competitive with more conventional cold neutron beam experiments.

UCNτ

UCNτ uses a magnetic trap to confine neutrons so that they do not interact with material surfaces while under storage.

UCNB

The UCNB experiment improves upon the spectrometer used for UCNA to investigate more correlations in neutron decay. In UCNB, the protons also emitted during the decay of the neutron are also detected in coincidence with the decay electrons.

UCNb

UCNb measures the potential distortion of the neutron beta-decay energy spectrum caused by physics beyond the Standard Model.

UCNS

A new program at LANSCE, the UCN source uses UCNs to finely control fission in actinides such as plutonium and uranium to investigate sputtering and damage of material surfaces, topics essential to the NNSA's mission.

LANL nEDM

A new effort is underway at LANL, taking advantage of the unique LANSCE UCN source, to develop a room-temperature nEDM experiment with a sensitivity of δdn~3 x 10^{-27} e-cm, a 10-fold improvement over the current limit set by an experiment at ILL.

SNS nEDM

A new neutron EDM (nEDM) experiment is being developed to be installed at the Fundamental Neutron Physics Beamline at the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory, with a goal sensitivity of δdn~5 x10^{-28} e-cm. UCNs from LANSCE have been used to test prototype UCN storage cells.

At left: Z. Tang installs the UCN flapper assembly into the new UCN source, in preparation for testing the UCN transport properties of the new source.

Ultracold Neutron Source at LANSCE enables new experiments

Los Alamos researchers employ capabilities at LANSCE to design and construct new experimental instruments for studies to produce a better understanding of the fundamental forces at work in the universe. These experiments rely on the power and flexibility of the UCN Source, which offers a high density of ultracold neutrons with the world's highest degree of polarization and low background from the spallation source

Ultracold neutron lifetime experiment

The ultracold neutron lifetime (UCNτ) experiment seeks to measure the neutron lifetime with accuracy 1 second or less. Ultracold neutrons are free neutrons with kinetic energies on the order of 100 neV or velocities around a few m/s. Enrico Fermi recognized that such particles can be reflected from surfaces like light and trapped in containers or "material bottles." Trapped ultracold neutrons have been used to measure how long a neutron lives, a fundamental constant that is a part of the standard model of particle physics predictions and a parameter influencing processes such as helium production in the early universe and the rate of energy production in the sun.

Systematic errors caused by ultracold neutron-material surface interactions have limited measurement accuracy. Several experiments have given conflicting answers, deviating from each other by more than five sigmas. Los Alamos, Indiana University, and other collaborators have built the world's first asymmetric magnetic bottle to store ultracold neutrons. The bottle completely removes the ultracold neutron-surface interactions and addresses other known systematic errors to provide a new venue to determine the neutron lifetime. Several detector technologies have been developed at Los Alamos for this unique experiment, including a new multilayer surface detector for ultracold neutrons (image on the following page). This detector replaces existing ultracold neutron detectors and has been deployed for ultracold neutron flux monitoring, development of ultracold neutron guides, and ultracold neutron lifetime research.

With these improvements in place, researchers plan to measure the neutron lifetime with unprecedented accuracy. These capabilities will also enable new experimental studies of physics beyond the Standard Model.

Neutron electric dipole moment experiment

An extremely sensitive probe of new physics, an electric dipole moment (EDM) measures the separation of positive and negative charges within a system. The neutron EDM (nEDM), a similar measurement within the neutron, is said to have "killed more theories than any other single measurement." A joint experimental and theoretical LDRD-Directed Research project probes new sources of time reversal violation with the nEDM.

The project is developing a new nEDM experiment with a sensitivity of 3 x 10^{-27} e-cm, a 10-fold improvement over the current limit. Performing this experiment requires a stored neutron density of approximately 100 UCN/cc. Achieving this density necessitated an improved neutron guide to transport neutrons from the source to the experimental measurement area. Los Alamos researchers developed, fabricated, and tested a new design to provide the improved performance required for the nEDM experiment.

Making a joint between guide components with a minimum gap has been a challenge in constructing a neutron transport system. Even a gap of a few tenths of a millimeter for every meter of a guide section leads to a significant loss of transported neutrons. The team based the new Los Alamos guide on the standard conflat flange design and modified it to minimize the gap between adjacent guide sections. Scientists stored the ultracold neutrons in guide sections and measured the lifetime of the stored ultracold neutrons (approximately 100 seconds), revealing a significant improvement over similar previous measurements using the current guide joint design.

Lead experimenters are S. Clayton, T. Ito, M. Makela, C. Morris, A. Saunders, Z. Wang (P-25); M. Hoffbauer (Chemical Diagnostics and Engineering, C-CDE); and S. Seestrom (P-DO).

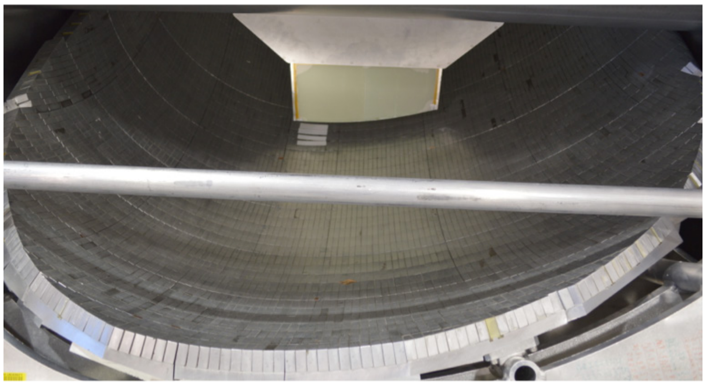
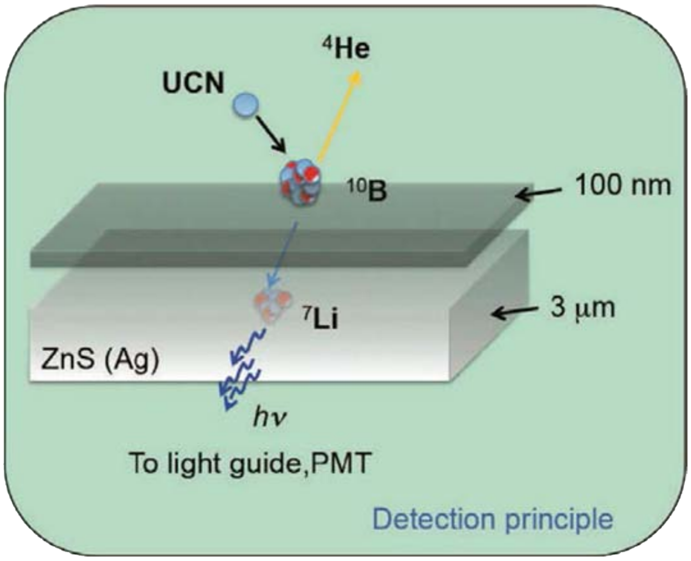


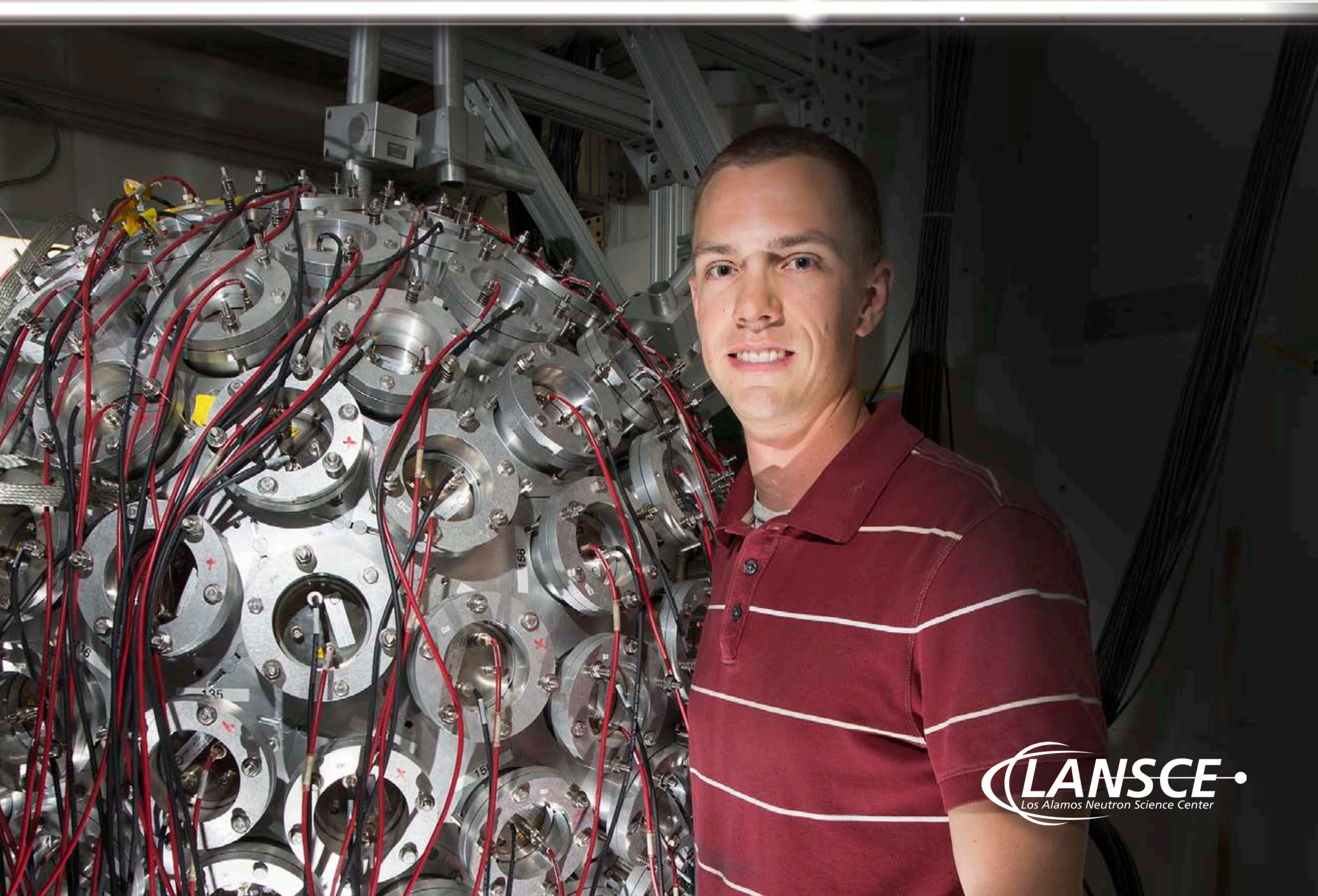
Photo of the UCNτ permanent magnet array installed in a vacuum vessel with a boron-10/ZnS:Ag detector (top, center of the photo) in its lowered position. During storage of UCNs, the detector is in a raised position above the trap, and the UCNs are confined to the volume below the top edge of the bowl-shaped array. After a short (few seconds) or long (~1000 seconds) storage period, the detector is lowered into the trapping volume to count surviving neutrons.

The Laboratory's LDRD program funded both experiments, which support the Laboratory's Global and Energy Security mission areas and Nuclear and Particle Futures science pillar.



The multilayer boron-10 (^{10}B) surface detector for ultracold neutrons consists of a thin-film ^{10}B top layer supported by a luminescent layer of zinc sulfide: silver (ZnS:Ag). One of the charged particles α or lithium-7 (^{7}Li) generated from the neutron capture stops in the ZnS:Ag layer and emits light that passes through a light-guide or a transparent window before detection by photomultipliers. A ^{10}B thickness of 100 nm and a ZnS:Ag thickness of a few microns are sufficient for this purpose.

Weapons Neutron Research Facility 2015



WNR at a Glance

The Weapons Neutron Research Facility (WNR) consists of a high-energy "white" neutron source (Target-4) with 6 flight paths, three low-energy nuclear science flight paths at the Lujan Center (Target-1), and a proton reaction area (Target-2). The neutron beams produced at WNR Target 4 complement those produced at the Lujan Center because they are of much higher energy and have shorter pulse widths. The neutron sources are driven by the 800-MeV proton beam of the LANSCE linear accelerator or linac.

Neutron beams with energies ranging from approximately 0.1 MeV to greater than 600 MeV are produced in Target-4. The neutron production target at Target-4 is a bare unmoderated tungsten cylinder that is bombarded by the 800-MeV pulsed proton beam from the LANSCE linear accelerator and produces neutrons via spallation reactions. Because the proton beam is pulsed, the energy of the neutrons can be determined by time-of-flight techniques. The time structure of the proton beam can be easily changed to optimize a particular experiment. Presently, Target-4 operates with a proton beam current of approximately 1.5 µA, 1.8 sec between pulses, and approximately 14,000 pulses/sec. Target-4 is the most intense high-energy neutron source in the world and has 6 flight paths instrumented for a variety of measurements. With the completion of planned accelerator radio-frequency generator upgrades, the beam current to Target-4 will be increased by a factor of 2.5 to provide beam currents up to 5 µA.

In the Target-2 area (Blue Room), samples can be exposed to the 800-MeV proton beam directly from the linac or a beam that has been compressed in time from the Proton Storage Ring (PSR). Although the total beam current is limited by the shielding in Target-2, the PSR beam provides significantly more peak intensity than the direct beam from the accelerator. Target-2 is used for proton irradiations and hosts the high-flux Lead Slowing-Down Spectrometer. For lower energy proton experiments, proton beams with energies as low as 200 MeV have been transported to Target-2.

At present there are three flight paths at the Lujan Center devoted to Nuclear Science research. The other flight paths support the DOE / Basic Energy Sciences Materials Science User Program. These flight paths view a moderated target and have neutron energies that range from sub-thermal to approximately 500 keV.

With these facilities, LANSCE is able to deliver neutrons with energies ranging from small fractions of an electron volt to several hundreds of MeV, as well as a proton beam with a wide range of time and intensity characteristics.

At left: S. Mosby demonstrates the DANCE detector.

WNR

Determining how much energy is released during the fission of plutonium

The energy released when a heavy element such as plutonium undergoes nuclear fission could be used to drive both reactors and nuclear weapons. Most of this energy is released in the form of kinetic energy of the fission fragments formed during the process, and almost all the local heating in reactor fuel is deposited as fission fragments decelerate inside the core. Although in the past TKE in fission has been measured carefully for low incident energy neutrons in the past, there is almost no information for high- energy neutrons such as those produced in nuclear fusion. The lack of data at high neutron energies is mainly due to the safety concerns associated with handling plutonium, as well as the limited number of high intensity fast neutron sources. LANSCE is one of a handful of facilities in the world that routinely performs experiments on plutonium and provides high-intensity, fast neutron beams. For the first time, scientists at LANSCE have now measured how the total kinetic energy of ^{239}Pu changes as a function of incident neutron energy spanning up to 30 MeV. The journal Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment has published a description of the instrument and methodology for the experiment.

A team of P-27 researchers conducted the experiments. Oregon State University prepared the plutonium sample, which consisted of a thin deposit of the material on a carbon film attached to an aluminum ring. The researchers mounted the sample in a double-sided ionization chamber and irradiated it with neutrons at the Lujan Center and WNR facilities at LANSCE. They measured the total kinetic energy release per fission. The experiment ran for several weeks and successfully collected data for all the incident neutron energies of interest. The high efficiency of the instrument, combined with intense LANSCE beams and a new data acquisition system, enabled fission output measurements across 11 orders of magnitude in incident neutron energy.

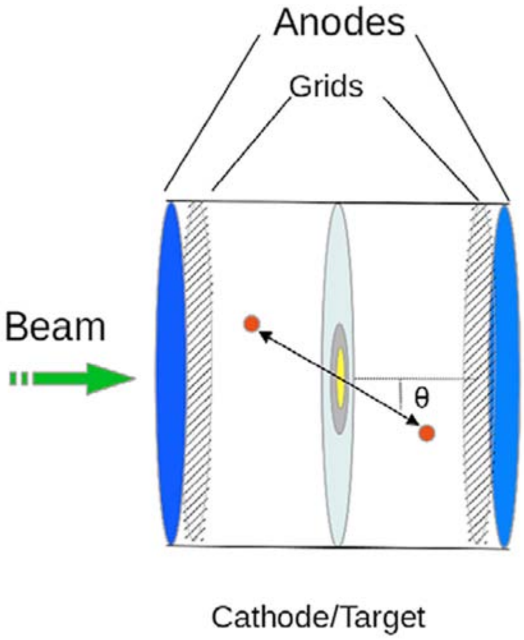
The new experiment confirmed what theory had predicted: that kinetic energy released in the fission of plutonium is significantly reduced as the incident neutron energy is increased. As a consequence, less kinetic energy than previously thought is released when fission is induced by fusion neutrons.

Reference: "A Fission Fragment Detector for Correlated Fission Output Studies," Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, **757**, 75 (2014).

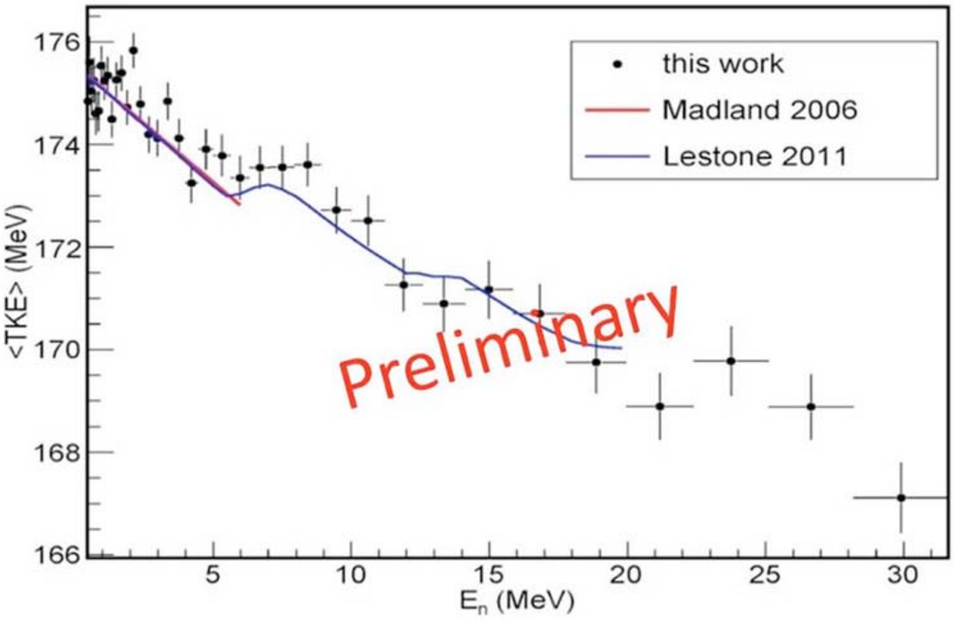
Authors include the following: S. Mosby, F. Tovesson, A. Couture, R. Meharchand, K. Meierbachtol, J. M. O'Donnell, B. Perdue, and D. Richman (P-27); D. L. Duke and D. Shields (P-27 and Colorado School of the Mines); and V. Kleinrath (P-27 and Idaho State University).

NNSA Campaign 1: Primary Assessment Technologies (Program Manager S. Sterbenz) funded this research. This work benefited from the use of the LANSCE accelerator facility, which is sponsored by DOE, NNSA, Office of Science, and Office of Nuclear Energy, Science and Technology sponsor. F-J. Hambsch (Institute of Reference Materials and Measurements, Geel, Belgium) constructed the ionization chamber used for this experiment, and Walter Loveland (Oregon State University) prepared the plutonium and uranium samples that made the experiment possible.

Extending measurements to incident neutron energies well beyond thermal enables testing of modern theoretical models. The new nuclear data support the Laboratory's Nuclear Deterrence mission area. Nuclear science research at LANSCE is a key capability that supports the Laboratory's Nuclear and Particle Futures science pillar. This research will be part of Dana Duke's PhD thesis at Colorado School of Mines where she studies total kinetic energy release and other characteristics of the nuclear fission process using LANSCE capabilities.



Schematic view of the ionization chamber used to measure total kinetic energy release in fission. The red circles represent the fission fragments emitted from a thin layer of plutonium (shown in yellow).



Preliminary results for the TKE in fission of ^{239}Pu. The experimental result is compared with theoretical calculations.

First tests of thermal-neutron-induced semiconductor failures

LANSCE has an unparalleled ability to assess semiconductor failures from high-energy neutrons. LANSCE utilizes high-energy neutron sources produced at Target-4 in WNR. Industrial users have been testing electronics at WNR since the 1990s. Now, Los Alamos researchers have used a flight path developed at Target-1 at the Lujan Center to measure the failure rate in semiconductor devices at thermal neutron energies.

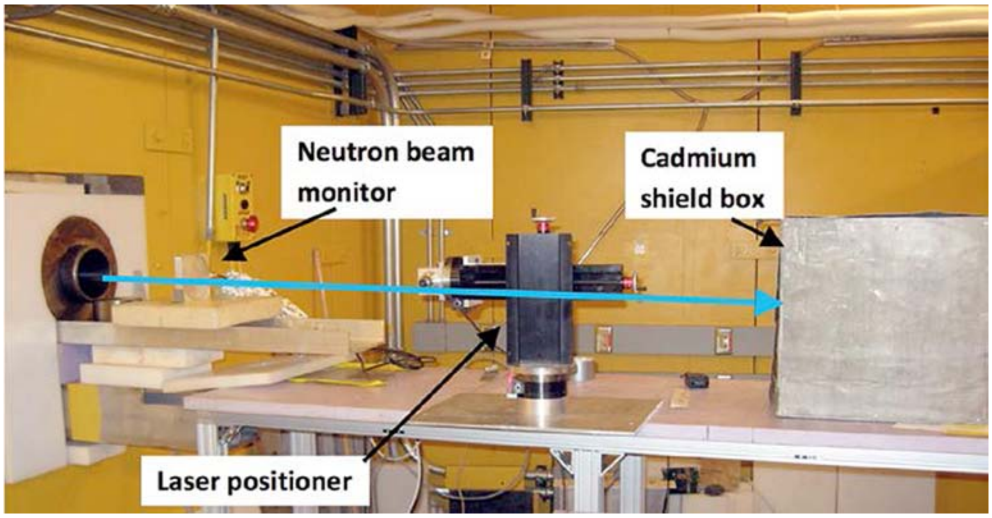
For the first time, Laboratory researchers and scientists from Honeywell Aerospace have measured the effect of thermal neutrons (neutrons in thermal equilibrium with their environment). The long-time LANSCE industry user performed a thermal neutron test on an integrated circuit previously characterized at a reactor. The LANSCE and reactor test results agreed in the number of observed failures per thermal neutron. The successful demonstration of this capability could enable LANSCE to expand its role in testing of semiconductor radiation effects.

High-energy neutrons, produced in the atmosphere by cosmic rays striking oxygen and nitrogen atoms in the air and undergoing a nuclear reaction, can thermalize (lose energy to achieve thermal equilibrium with their environment) in the surrounding materials and interact with the semiconductor devices. Boron-10 (^{10}B) (20% of natural boron) is found in semiconductor devices. This isotope is of particular concern for many applications because of its vulnerability to thermal neutrons. Boron-10 has a large thermal neutron cross section and produces a charged particle that can cause failure when it is deposited in a sensitive semiconductor volume. Efforts to remove boron from semiconductor devices have been unsuccessful.

H. Quinn (Space Data Systems, ISR-3) and M. Devlin, M. Mocko, and S. Wender (P-27) took measurements for a variety of semiconductor devices. They recorded the number of device failures with and without a cadmium (Cd) shield. Cadmium has a large absorption cross section at thermal and below neutron energies. Therefore, the difference in the failure rate with and without Cd in the beam reflects the effect of thermal neutrons. As expected, preliminary results revealed a range of failure rates for different semiconductor devices. Based on these data, the failure rate in a specific environment, such as space, could be determined. If the failure rate is thought to be too high, a different device may have to be used for some applications.

LANSCE developed this new technology in response to the semiconductor community, which continues to view neutrons as a serious threat to the reliability of integrate circuits. As semiconductor feature sizes become smaller and operating voltages become lower, the odds of failure increase. The new LANSCE results benefit space and avionics electronics applications.

Industry partly funded the work. This is an example of putting the Laboratory's unique capabilities to use for science in service to society. The work supports the Laboratory's Global Security mission area and the Nuclear and Particle Futures science pillar. The research benefited from the use of the Lujan Center, which is funded by NNSA.



Inside the experimental cave on Flight Path 12 at the Lujan Center, where Los Alamos has established a capability to test thermal-neutron-induced semiconductors. The LANSCE beam enters from the left and passes through a neutron monitor before entering a cadmium shield box housing the semiconductor test board.

S. Wender has been aligning beams for companies from around the world since the early 1990s, when LANSCE became known as one of the few places where researchers can characterize semiconductor components and study various failure modes caused by neutron radiation.

WNR

Neutron spectra measurements obtain uranium-235 data in previously unexplored region

Researchers used a challenging combination of two time-of-flight measurements on the Chi-Nu experiment at LANSCE to demonstrate important aspects of the physics behind nuclear reactions at the low end of the fission neutron spectrum (below 0.5 MeV). The preliminary, unpublished experimental results on ^{235}U appear to uphold what nuclear reaction models had predicted–that this end of the spectrum is similar to fission induced by thermal neutrons.

The discovery of nuclear chain reactions in the fission of uranium and plutonium nearly 80 years ago made nuclear reactors and nuclear weapons possible. When a nucleus undergoes fission, several neutrons are released. These neutrons can induce fission in neighboring nuclei to create a chain. The probability of subsequent reactions depends on the energy of the fission neutrons. This is what the Chi-Nu experiment is designed to measure. Neutrons emitted in fission can have a wide range of energies, and the distribution of these energies (the spectra) can vary with the energy of the incident neutron that causes the fission.

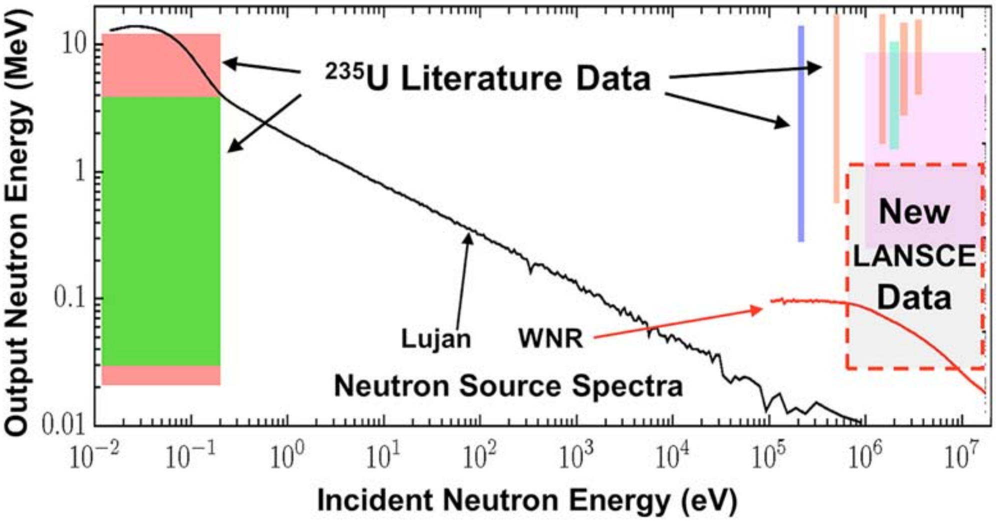
Chi-Nu's array of 22 lithium glass neutron detectors used in this work is specialized for the part of the neutron emission spectrum below 0.5 MeV. The team performed the experiment at LANSCE/WNR neutron source of pulsed fast neutrons. The recent upgrade of the LANSCE accelerator enabled an increase in the intensity of the neutron source by a factor of 2.5. An advanced data-acquisition system based on waveform digitizers took advantage of this improved accelerator performance. LANL and LLNL scientists used a "double" time-of-flight approach at WNR. The researchers identified the energy of the neutrons causing the fission (first time-of-flight) and measured the energy of the emitted neutrons (second time-of-flight). The first time-of-flight measurement from the neutron source to the fission chamber gives the energy of the neutron inducing the fission. The second measurement, the time from the fission detector to the neutron detector 40 cm away, determines the energy of the fission neutrons. Nuclear models had predicted that the spectrum would not change rapidly with incident neutron energy. This is the first experimental verification of that theory.

In future experiments, scientists will use a different array of Chi-Nu detectors to measure the higher energy part of the ^{235}U fission neutron spectrum. Researchers aim to resolve significant discrepancies reported in the literature. They also plan to investigate both the low- and high-energy regions of the neutron spectra for fission of ^{239}Pu, an isotope that presents measurement challenges because of the natural alpha-particle radioactivity of the samples.

Los Alamos researchers include the following: R. Haight, H. Y. Lee, T. Taddeucci, J. O'Donnell, S. Mosby, M. Devlin, N. Fotiadis, R. Nelson, and S. Wender (P-27); T. Bredeweg (Nuclear and Radiochemistry, C-NR); D. Neudecker (Nuclear and Particle Physics, Astrophysics and Cosmology, T-2); M. White (Materials and Physical Data, XCP-5); and C. J. Solomon (Monte Carlo Codes, XCP-3).

NNSA Science Campaign 1: Primary Assessment Technologies (LANL Program Managers M. Chadwick, S. Sterbenz, and M. White) funded the research, which supports LANL's mission areas of Nuclear Deterrence, Global Security, and Energy Security, as well as the Laboratory's Nuclear and Particle Futures science pillar.

D. Neudecker and H. Y. Lee discuss the ^{235}U data in the Chi-Nu experimental area. Behind them is an array of neutron detectors surrounding the fission chamber.



Location of the new WNR/LANSCE data for prompt fission neutrons from neutron-induced fission of ^{235}U. The location of previous and the present data are given by the areas in the plot of incident neutron energy (horizontal axis) versus outgoing neutron energy (vertical axis). Also shown are the ranges of incident neutron energies available at the Lujan Center and at WNR.

Measuring the anisotropy in uranium-235 fission

In the 1950s, Laboratory researchers first demonstrated that the strong anisotropies exhibited in neutron-induced fission depend on the incident neutron energy and fissioning nucleus. The results, generated by measuring the fragment anisotropy of several isotopes for incident neutron energies up to 10 MeV, had implications for cross-section measurements and understanding the underlying physics of the fission process. Now, a novel instrument at LANSCE directly measures systemic fission effects that had previously been calculated only by theoretical means.

Neutron-induced fission cross sections are typically measured as ratios. Isotopes that exhibit different levels of anisotropy introduce a systematic error to the measurements. The angular distributions of the fragments are also closely related to the quantum mechanical state of the fissioning nucleus at the time of scission (where the nucleus breaks apart into two fragments). This phenomenon provides a rare window into the quantum world of the fissioning nucleus.

The TPC project aims to measure the ^{239}Pu fission cross section. The fission Time Projection Chamber (fission TPC) tracks charged particles and their energy deposition. The unique instrument enables direct measurements of almost all the systematic effects associated with the fission cross section, including the anisotropy. Previous cross section measurements typically corrected for anisotropy using theoretical calculations rather than obtaining it experimentally. The anisotropies of ^{239}Pu and ^{235}U must be determined to achieve the goal of measuring the ^{239}Pu fission cross section. Researchers have used the fission TPC at LANSCE to make a significant advance toward measuring the ^{239}Pu fission cross section to 1% accuracy.

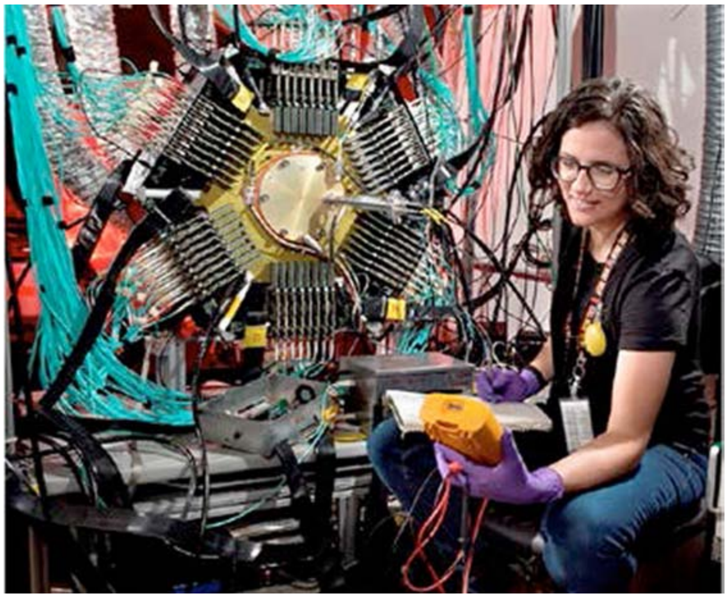
F. Tovesson, B. Manning, V. Kleinrath, and D. Duke (P-27), working with outside collaborators, measured the angular distribution of fission fragments from the neutron-induced fission of ^{235}U. This achievement marks the first continuous measurement for incident neutron energies from 200 keV to several hundred MeVs. Preliminary results for ^{235}U fission emission anisotropy, shown in the bottom figure on the following page, generally agree with the energy dependence observed in previous measurements up to 10 MeV, although the absolute value is somewhat lower. Above 10 MeV the data are scarce, making meaningful comparisons difficult. After finalizing the results for ^{235}U, the team plans to analyze ^{239}Pu, for which fewer data are available in the literature.

The fission TPC measurements could also lead theorists to a better understanding of the fission process. The angular distributions provide insight into the transition states on top of the fission barriers as the compound nucleus deforms on its path to fission. More detailed information about those states would advance understanding of the fission process and allow scientists to more reliably calculate nuclear cross sections that cannot be measured directly.

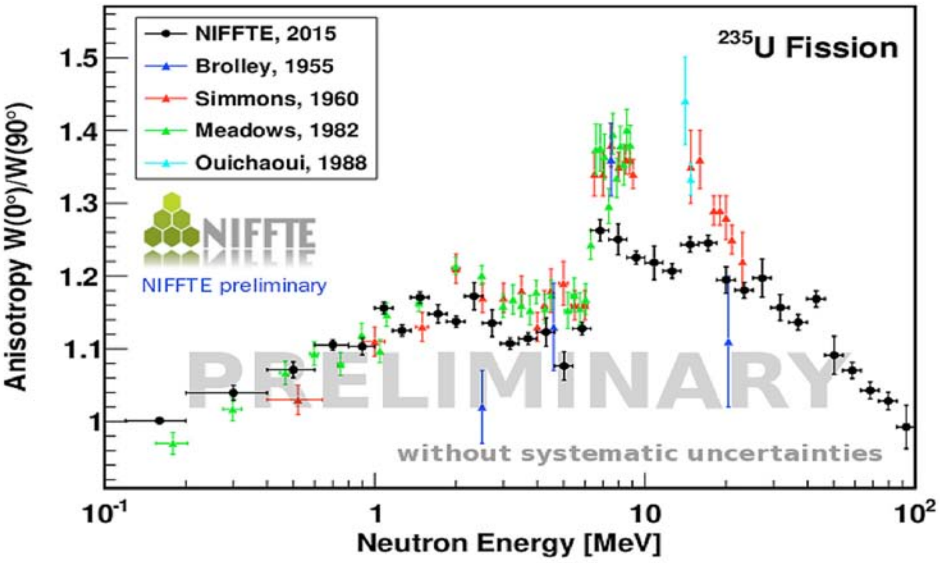
Reference: “A Time Projection Chamber for High Accuracy and Precision Cross-section Measurements,” *Nuclear Instruments and Methods in Physics Research A* **759**, 50 (2014). Lawrence Livermore National Laboratory leads the TPC project.

Authors’ institutions: LLNL, Pacific Northwest National Laboratory, California Polytechnic State University, Idaho National Laboratory, Oregon State Technology, Abilene Christian University, and LANL (D. L. Duke, T. Hill, A. B. Laptev, R. Meharchand, L. Montoya, and F. Tovesson).

NNSA Science Campaign 1: Primary Assessment Technologies in the NNSA’s Science Campaign program funded this work as part of the fission TPC project. The research supports the Laboratory’s Nuclear Deterrence mission area for stockpile stewardship and the Nuclear and Particle Futures science pillar.



V. Kleinrath with the fission TPC, which she uses to perform this work as part of her PhD thesis at Vienna University of Technology.



The preliminary results for the ^{235}U fission fragment anisotropy, defined as the emission probability of fission fragments in incident neutron beam direction over the probability of fragment emission perpendicular to the neutron beam. NIFFTE stands for Neutron-Induced Fission Fragment Tracking Experiment.

WNR

Reducing the uncertainty of backgrounds for Chi-Nu fission measurements

Measurement of background is important for effective statistical design of experiments. J. O'Donnell (P-27) has developed a method to measure backgrounds associated with coincidence as part of the Chi-Nu project at LANSCE. The method enables true in situ background measurements and a dramatic reduction in the statistical uncertainty of the background. *Nuclear Instruments and Methods A* published the research.

The work aims to determine the background under the true coincidence events without assumptions for the shape of the background or determination of arbitrary parameters. The measurement method uses flash waveform digitizers with onboard processing capabilities to acquire all the singles data for each detector, with near-zero dead time, and then record all the data on a computer. Later analysis includes a simple software search for coincidences. The analysis preserves the high statistical accuracy of the singles data; thus the statistical uncertainty on the background extracted can be very small. Data acquisition for the background measurement occurs simultaneously with the foreground measurement to provide two immediate benefits: 1) this new method is four times more effective at using beam time, in contrast with methods that dedicate a fraction of the beam time to measuring the background; and 2) it reduces systematic uncertainties (e.g., no sources of background are changed between the two phases of measurement, and the background normalization is absolute). Researchers expect that the method could be used for a large class of coincidence experiments, in which the backgrounds cannot be fully eliminated. Prompt fission spectra experiments performed at WNR as part of the Chi-Nu project are an example.

Researchers developed the Chi-Nu detector array for experiments at LANSCE to accurately measure the spectrum of neutrons emitted in neutron-induced fission of ^{239}Pu and ^{235}U.

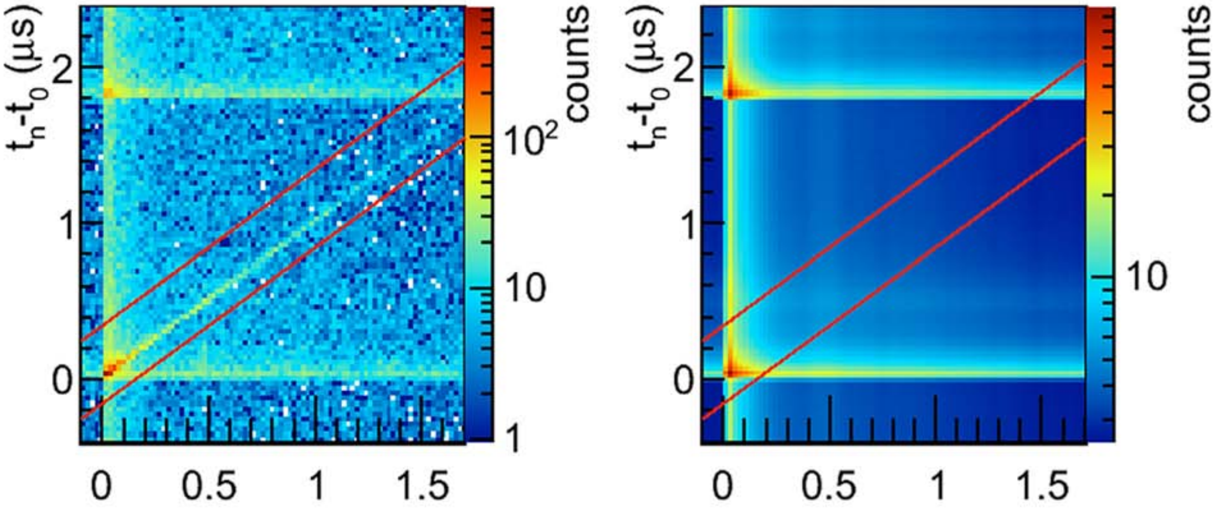
The prompt fission neutron spectrum is an important quantity, and NNSA Science Campaign 1 is funding an experimental campaign to reduce the uncertainties associated with these nuclear data. Chi-Nu uses a two-arm time-of-flight technique, detecting fission fragments to infer the incoming neutron time of flight and also to start an outgoing neutron time-of-flight measurement. In addition to detecting fission-fragment fission-neutron coincidences, there is an opportunity to observe coincidences involving alpha particles misidentified as fission fragments, neutrons from other fission events, beam neutrons scattered in the experimental area, and fission fragments generated from these scattered neutrons. The background from these chance coincidences must be measured accurately.

The top figure on the following page represents the 2-D background obtained for the preliminary ^{239}Pu fission data from the Chi-Nu project. Red diagonal lines depict boundaries that researchers use to project the results recorded on the top figure.

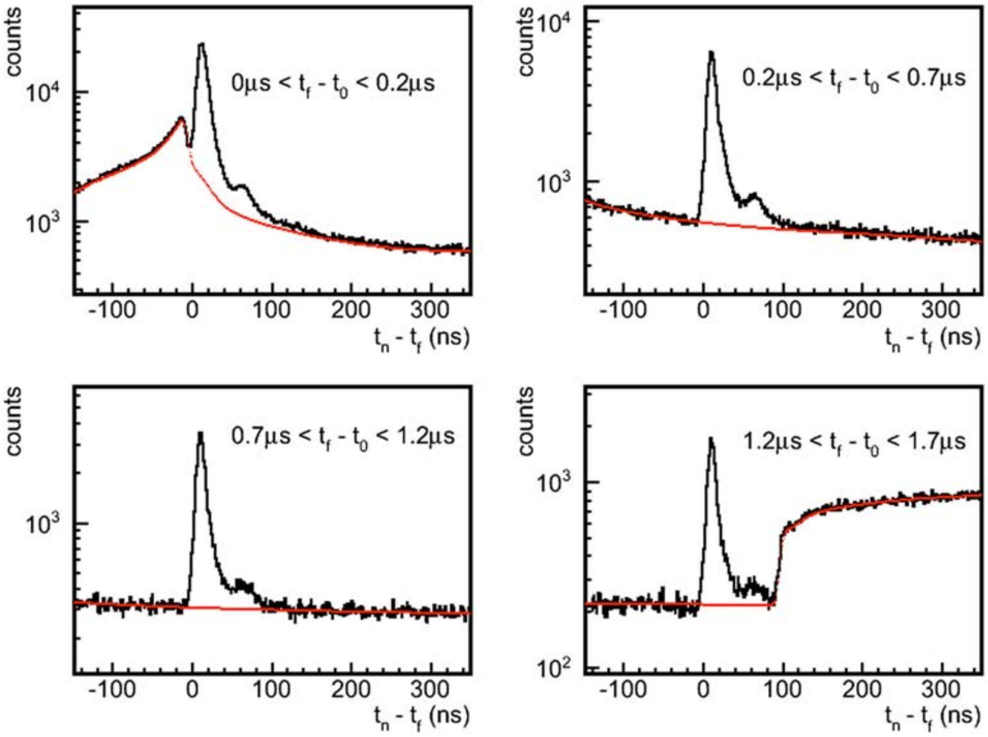
The bottom figure on the following page shows the projected 1-D backgrounds for four different regions of incoming neutron energies. Features of the background shapes can be better understood from the full 2-D backgrounds. These backgrounds are not flat, and the background shape varies with the incident neutron energy. The new background analysis method appears to account for all the significant background components and has very small uncertainties.

Reference: "A New Method to Reduce the Statistical and Systematic Uncertainty of Chance Coincidence Backgrounds Measured with Waveform Digitizers," *Nuclear Instruments and Methods* **A** (2015), article in press. J. M. O'Donnell (LANSCE Weapons Physics, P-27) authored the paper.

This work benefited from the use of the LANSCE accelerator facility and was performed under the auspices of the NNSA. The work supports the Laboratory's Nuclear Deterrence mission area and the Nuclear and Particle Futures science pillar by reducing the uncertainties of key data used to predict nuclear performance.



Measured coincidences (left) and background (right) for outgoing neutrons from neutron-induced fission of ^{239}Pu as a function of the fission time (incoming neutron time of flight), t_f-t_0, and the outgoing neutron time, t_n-t_0.



Time of flight, t_n-t_f, spectra (black) for outgoing neutrons following neutron-induced fission of ^{239}Pu in coincidence with fission fragments for different regions of incoming neutron time of flight, t_f-t_0. The measured background (red) has error bars smaller than the line width.

Mini-CAPTAIN snags first ionization track

Mini-CAPTAIN, the prototype for the Cryogenic Apparatus for Precision Tests of Argon Interactions with Neutrinos (CAPTAIN), demonstrated its first ionization track. The Mini-CAPTAIN detector is a liquid argon TPC, a device capable of imaging charged particles via a trail of ionization electrons (ionization tracks) left behind when they interact with the argon nuclei. Its success makes it one of only a handful of liquid argon detectors now operating in the world. The neutrino worldwide research community increasingly uses liquid argon as a detection medium. This result paves the way for an international neutrino experiment.

The 1,000-channel liquid argon TPC with 400-kg instrumented mass is under commission at LANL. The TPC relies on LANSCE's high-energy neutron beam, which is uniquely suited to aid understanding of how to reconstruct few-GeV neutrino interactions. Researchers will use the neutron data to measure cross-sections of spallation products that are backgrounds to measurements of neutrinos from a supernova burst and cross-sections of events that mimic the electron neutrino appearance signal in long-baseline neutrino physics. These data will enable development of strategies to count neutrons and evaluate their energies in a liquid argon TPC. This information is important for the total neutrino energy measurement in the analysis of long-baseline neutrinos. The data will enable larger and more complex neutrino experiments aimed at solving scientific grand challenges such as explaining the universe’s matter-antimatter asymmetry.

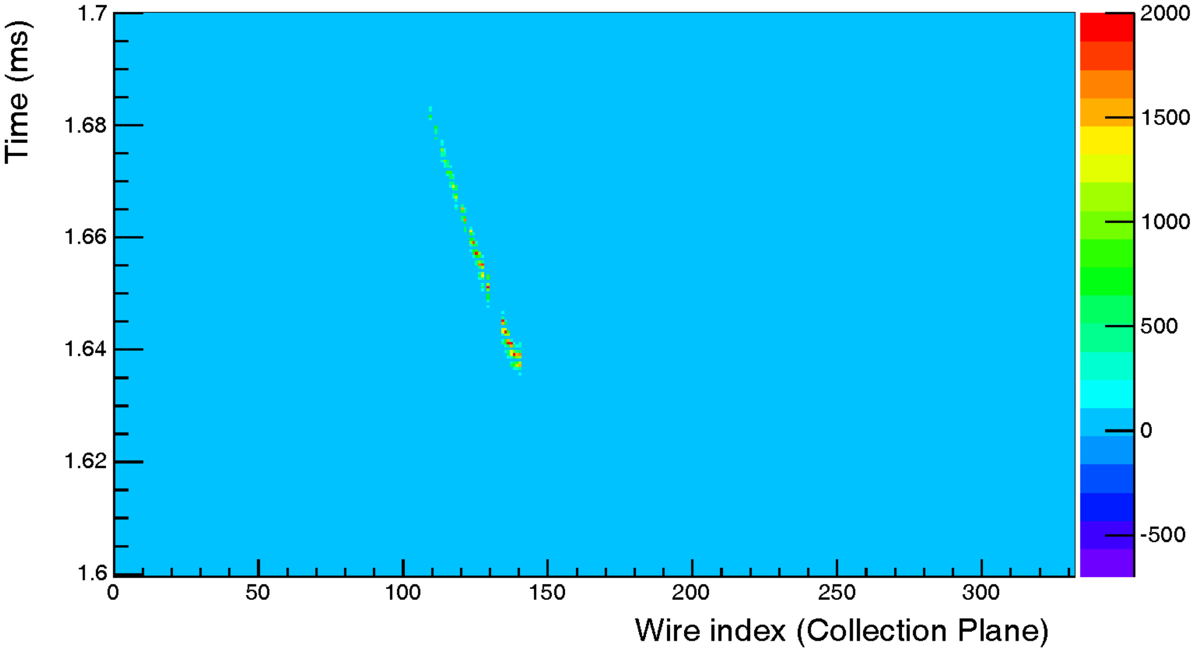
The CAPTAIN detector, a 5-ton instrumented mass liquid argon TPC with 2,000 channels, is also under construction at Los Alamos and will eventually run at the FNAL. The CAPTAIN program addresses important scientific questions associated with the long-baseline, atmospheric, and supernova neutrino science of DUNE (Deep Underground Neutrino Experiment). DUNE is an international long-baseline neutrino program designed to aid neutrino science and proton decay studies. The Laboratory develops and manages the DUNE detector systems. Los Alamos researchers working on Mini-CAPTAIN and the liquid argon TPC include C. Mauger, E. Guardincerri, G. Garvey, D. Lee, Q. Liu, W. Louis, J. Mirabal-Martinez, J. Medina, G. Mills, J. Ramsey, W. Sondheim, C. Taylor, and R. Van de Water (P-25); K. Rielage (P-23); and G. Sinnis (P-27).

The CAPTAIN program began as an LDRD program project. A. Carlson (P-25), J. Friedland, S. Gandolfi (P-23), and M. Graesser (T-2), performed work relevant to the long-baseline program. Development of the LANL detector led to the formation of a broad collaboration from organizations across the U.S. Many external collaborators, especially graduate students and postdoctoral researchers, have spent significant time at the Laboratory working on the project. The CAPTAIN program continues to involve Laboratory researchers from P and T groups.

More information: www.lanl.gov/science-innovation/scienceprograms/office-of-science-programs/high-energy-physics/captain.php.

External CAPTAIN collaborators include national laboratories (Argonne, Lawrence Berkeley, BNL, and Fermi), University of Alabama, University of California – Davis, Irvine, Los Angeles, and San Diego; University of Hawaii; University of Houston; Indiana University; Louisiana State University; University of Minnesota; University of New Mexico; University of South Dakota; South Dakota State University; and Stony Brook University.

The Laboratory's LDRD program and the DOE Office of Science High Energy Physics funded different aspects of the LANL research. The work contributes to DOE Office of Science missions and supports the Laboratory’s Nuclear and Particle Futures science pillar via neutrino science studies.



First demonstration of an ionization track from a laser calibration system in the Mini-CAPTAIN detector. A high-intensity ultraviolet laser pulse traversing the time projection chamber created the data. The color of the track represents the amplitude of the signal. Mini-CAPTAIN currently runs with one collection plane and one induction plane.

User Program and Demographics

2015

LANSCE

Los Alamos Neutron Science Center

User Program and Demographics

User Program at a Glance

LANSCE's User Program ensures that the research it oversees represents the cutting-edge of nuclear and materials science and technology.

DOE's designated national user facilities are

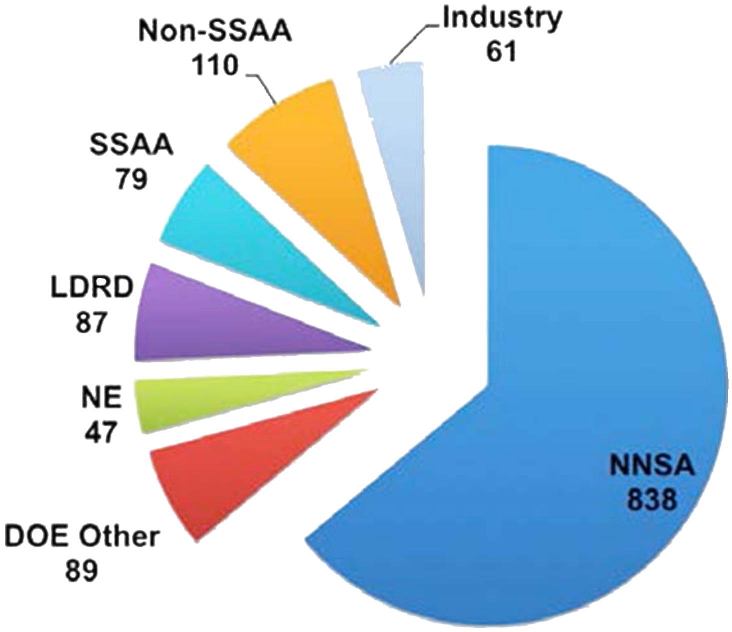
- Lujan Center
- pRad
- WNR

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

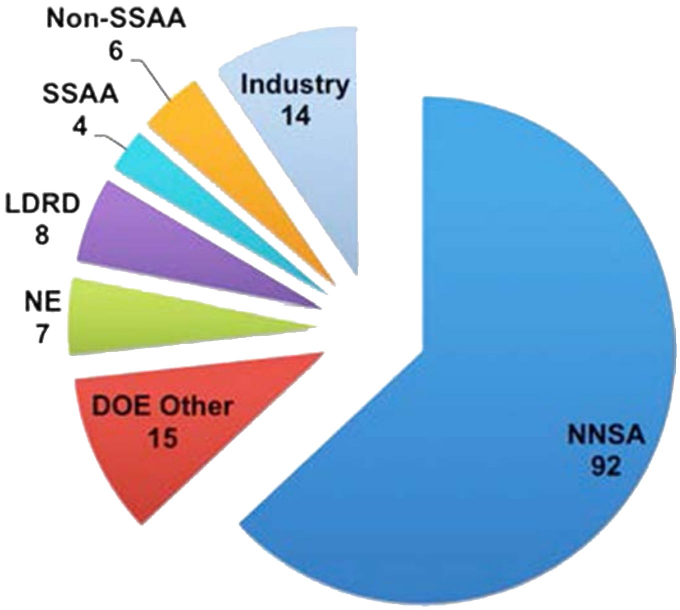
The User Program's demographics count user visits and unique-user visits.

User visits are the total number of visits made by all users.

A unique-user visit is defined as counting users only once—the first time they come to LANSCE during a calendar year.



Number of beam days provided per program during the 2015 run cycle.



Number of proposals run during the 2015 run cycle; data come from NNSA-designated national user facilities.

At left: LANSCE users at the Lujan Center.

Accelerator Operations Technology 2015

AOT at a Glance

Accelerator Operations and Technology (AOT) Division provides leadership in the Laboratory's core capability of accelerators and electrodynamics (A&E), which drives a wide range of LANL mission-relevant portfolios. A&E enables charged particle acceleration through controlled use of electromagnetic fields, supporting National Security missions involving radiographic imaging, remote measurements of electromagnetic signatures, sources of directed energy (for probes and defeat), and development of new capabilities such as radiation therapy and irradiation/sterilization of materials while furthering fundamental research in supporting key technologies.

In particular, AOT operates the LANSCE proton accelerator complex and conducts applied research and development in accelerator-focused technologies as they apply to FELs, National Security Science programs, and future accelerator missions.

AOT Division conducts fundamental and applied R&D needed to improve operations and operations support for LANSCE.

AOT's R&D efforts include the following:

- Plasma physics and ion beam generation
- Accelerator physics, engineering, and design
- High-space-charge proton-accumulator/compressor-ring physics
- Particle-beam-diagnostics physics and engineering
- High- and low-power radio-frequency (RF) system engineering
- Mechanical engineering and design
- High-vacuum engineering and technology
- Analog and digital control systems engineering and technology based on the experimental physics and industrial control system (EPICS)
- Specialized hydrogen-furnace brazing

Conduct of operations

A vital key to AOT's successful performance is our disciplined conduct of operations. Operations personnel undergo a rigorous technical and operational training program to ensure the highest standards of operational performance are met.

Accelerators and Electrodynamics (AOT-AE)

AOT-AE maintains a vigorous and robust technical base for addressing DOE and DoD needs by balancing its project portfolio between exploratory research, infrastructure development, and programmatic deliverables for sponsors. Funding is roughly 25% from the Laboratory's Directed Research and Development Program, 65% from DoD, and 10% from DOE.

Instrumentation and Controls (AOT-IC)

AOT-IC works with other AOT groups, as well as LANSCE and other Laboratory organizations on the incorporating new ideas, up-to-date knowledge, and cutting edge technology to make advancements in the control, instrumentation, and ion source disciplines. As parts of the process to provide continuous improvements, and maintain system viability, each of the five AOT-IC teams offers support for their deployed systems.

Mechanical Design Engineering (AOT-MDE)

AOT-MDE supports operations for the LANSCE beam-delivery complex, which includes the accelerator, Proton Storage Ring (PSR), and associated beam-transfer lines.

The group is responsible for the mechanical systems in the accelerator, the PSR, and the associated transfer lines. AOT-MDE teams with the other AOT groups to design and implement new capabilities throughout the machine.

Radio Frequency Engineering (AOT-RFE)

AOT-RFE maintains RF, pulsed-power, and magnet-power supply systems for accelerators and other related applications for the Laboratory.

At left: D. Bell performs critical system checkouts in the Central Control Room.

AOT

A new approach to trap atoms and molecules

Los Alamos researchers have demonstrated the feasibility of a new approach to the experimental technique of trapping cold atoms and molecules. Accumulator rings (i.e., storage rings and synchrotrons in the injection phase) are essential tools of high-energy physics (HEP) that build phase-space density in particle bunches by charge-exchange injection. The proton storage ring at LANSCE is an example. However, accumulator principles are not exclusive to HEP. The team found that accumulators may also be formed for the low-energy particles represented by laser-cooled neutral atoms and molecules. Excursions into low-temperature quantum chemistry could be enabled with an accumulator that gathers a variety of laser-cooled particles and causes them to collide with one another.

An accumulator uses a non-Hamiltonian process to build phase-space density. This circumvents Liouville's theorem, which states that phase-space density is preserved in processes governed by Hamilton's equations. In the case of HEP accumulator rings, the injected particles have one charge state, whereas the stored particles have another charge state. At LANSCE, negatively charge hydrogen atoms (protons cloaked in two electrons) are injected into the proton storage ring and pass through a stripper foil to remove the two electrons. The resultant bare protons join the protons already stored. Protons accumulate until a maximum number is reached against losses caused by space-charge forces, instabilities, etc. The non-Hamiltonian process is the change of the charge of the particles in the stripper foil.

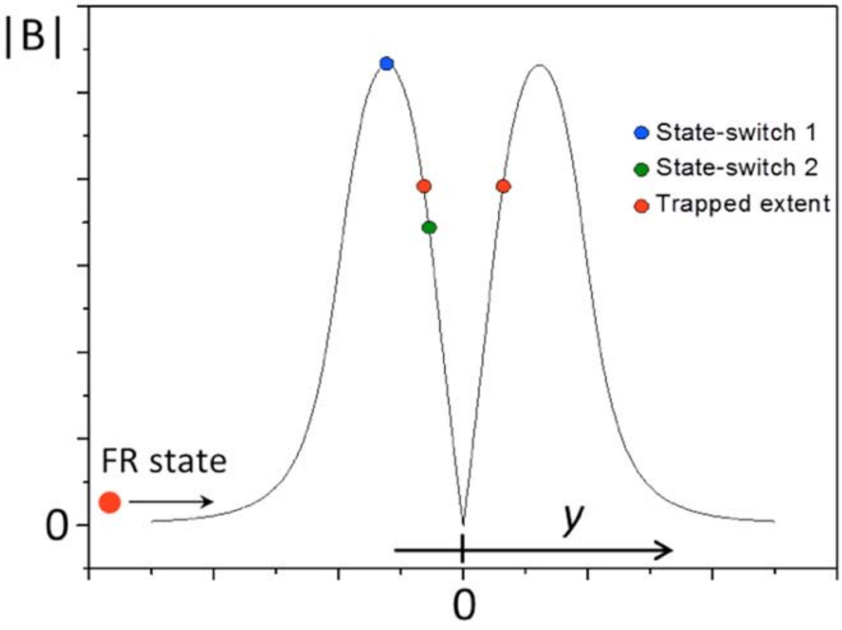
In the context of laser-cooled neutral atoms and molecules, the analogous non-Hamiltonian process is the change of quantum state the particles undergo during optical pumping. The accumulator need only be a simple magneto-static trap, appropriate for holding the great majority of laser-cooled particles, because they are paramagnetic. The top figure for this article shows a standard magnetic trap called a cusp solenoid that is suitable for these purposes. The arrows wrapping each cylinder depict the flow of electrical current. A cusp field could also be constructed from ring magnets.

The middle figure for this article depicts the variation of the axial magnetic field, $|B|$, by the solid line. In traps with a central minimum in $|B|$, like those depicted in the top and middle figures, the stored particles are in a field-repelled Zeeman state, pushed away by $|B|$ and oscillating about its minimum. Laser-cooled particles would likely approach the trap in the same field-repelled state. Between approach and storage must come the non-Hamiltonian process of optical pumping that changes the particle to a different state for injection. Through evidence in the literature and the team's own calculations, it appears that optical pumping can switch field-repelled particles quickly to their quantum opposite of a field-seeking Zeeman state. This sets the stage for an accumulator.

As indicated in the middle figure, a field-repelled particle (red dot) approaches the trap and climbs to the top of the confining potential with a finite velocity. There, it is switched (blue dot) to field-seeking. Because the switch does not change the velocity, the particle proceeds into the trap and continues to lose momentum. Now in the field-seeking state, the particle sees the decreasing field as a potential hill to climb. Before it comes to a halt, the particle is switched back (green dot) to field-repelled for storage. The process repeats, building the trapped number and density. The two red dots within the trap bracket the turning points of oscillation. A simple consideration of potential and kinetic energies shows that the trapped particles are cooler than those injected.

Beyond these notional considerations, researchers subjected the accumulator concept to the scrutiny of a sophisticated particle-tracking code drawn from the Laboratory's work spanning HEP to the storage of ultracold neutrons.

Solenoid arrangement for a cusp field.



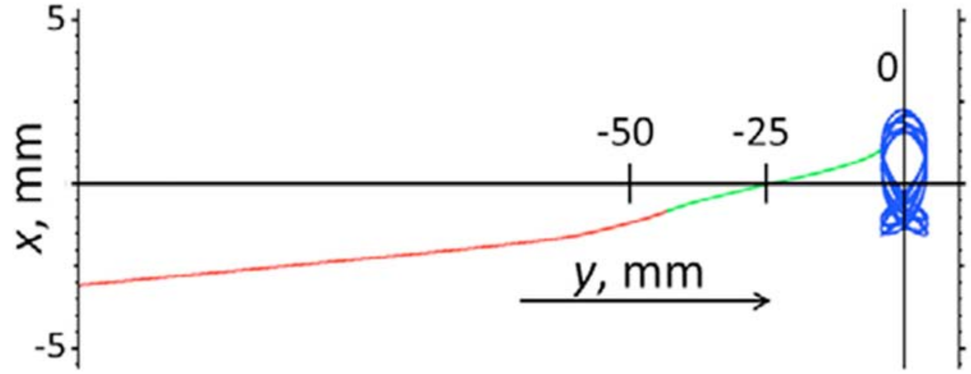
Axial variation of the cusp field (solid curve) and accumular concept by state switching. FR is field-repelled.

A new approach to trap atoms and molecules (continued)

The bottom figure for this article depicts the computed trajectory of a lithium atom injected into and trapped within a cusp-field accumulator fashioned from permanent magnets. The trajectory is colored red where the atom is in the field-repelled state and heading toward the trap, green when in the field-seeking state, and blue when returned to the field-repelled state for trapping. The loops of the blue-colored trajectory show the atom to be trapped near the field minimum. The models indicate that the cusp-field configuration offers a high acceptance of laser-cooled particles. Once inside the trap, the particles could be further cooled and made denser in phase space through known processes that dissipate kinetic energy. If proven, this accumulator concept could enable experiments in cold-particle quantum physics and chemistry that are outside the reach of current methods.

Researchers include the following: Principal Investigator M. Di Rosa (Physical Chemistry and Applied Spectroscopy, C-PCS), P. Walstrom (Accelerators and Electrodynamics, AOT-AE), and J. Velasquez (formerly C-PCS, now with W88 Systems Engineering, W-4).

The Laboratory's LDRD Program funded the initial work. Follow-on research to explore the next phase of this work is currently in the proposal stage. The work supports the Laboratory's Science of Signatures science pillar.



Trajectory of a lithium atom injected into the accumulator and subsequently trapped in stable orbits.

2015 Production Delivery Summary

Area	Scheduled Hours	Delivered Hours	Reliability
IPF	2149.0	1807.0	84.0%
Lujan	2137 .0	1579.0	73.9%
pRad	378.0	336.0	88.9%
UCN	1162.0	1004.0	86.4%
WNR	2137.0	1652.0	77.3%
Total	**7963.0**	**6378.0**	**80.1%**

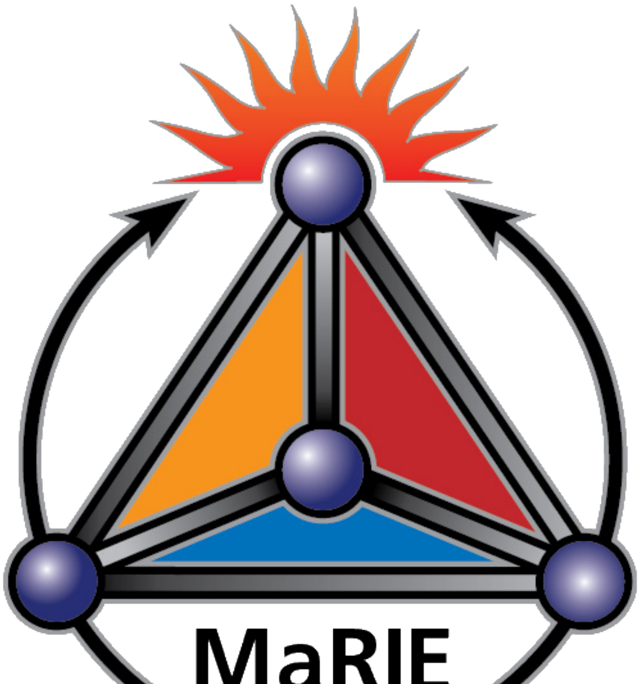
Long Range LANSCE Operating Schedule

31-Aug-16

~CY Operational Hours Available	FY	~FY Operational Hours Available
3744	2012	3696
3624	2013	3696
3624	2014	2256
1968	2015	1752
1992	2016	2784
2232	2017	3600
3720	2018	3744
3720	2019	3744
3720	2020	3744

Science on the Roadmap to MaRIE

2015



Science on the Roadmap to MaRIE

MaRIE at a Glance

MaRIE is designed to support key NNSA goals to understand the condition of the nuclear stockpile and to extend the life of U.S. nuclear warheads. When combined with the emerging computational capability to simulate materials at ultrahigh resolution, MaRIE will fill the gap in understanding of micro- and mesoscale materials phenomena and how they affect weapon performance.

Two new predictive capabilities
for weapons performance

1. Extreme conditions: The ability to predict how micro- and mesoscale materials properties evolve under weapons-relevant extreme conditions (including aging) and impact performance.
2. New materials: The ability to predict the microstructure of new materials (or those resulting from new manufacturing processes) and how that will affect weapons performance.

Six First Campaigns

These six representative experiments have been developed with colleagues from across the nuclear weapons complex and the broader scientific community to illustrate the mission impact and scientific potential of MaRIE.

Understand the condition of the nuclear stockpile
Dynamic materials performance

- Multiphase high explosive evolution
- Dynamic performance of plutonium and surrogate metals and alloys
- Turbulent material mixing in variable density flows

Extend the life of U.S. nuclear warheads
Process-aware manufacturing

- Controlled solidification and phase transformations
- Predicting interfacial microstructure and strain evolution
- High explosive functionality by design

These experiments collectively exemplify the broad scope of the facility and the titles speak to their mission relevance. This suite of experiments also enables detailed specification of MaRIE scientific and facility functional requirements.

MaRIE could be located at LANSCE to benefit from essential capability already existing LANSCE, particularly from its proton radiography capability that contributes extensively to resolving weapons issues. To realize the full capability of MaRIE, the facility at LANSCE will add the ability to accelerate the transition from today’s norm of observation and validation of materials performance to a future enabling prediction and control of materials functionality.

At left: The MaRIE logo "materials tetrahedron" is a representation of how structure and process combine with the properties of the materials to determine performance.

Science on the Roadmap to MaRIE

Neutron surface scattering used to study important characteristics of actinide surface chemistry

Actinides and actinide oxides exhibit some of the most intriguing and challenging chemistry known. Not only are their compositions frequently not stoichiometrically precise but also their oxide structures can change dramatically under various environmental conditions. Studies of actinide surfaces and surface-initiated chemical evolution of bulk materials are even more demanding. The scientific challenge is not to disturb their microstructures yet successfully identify, measure, and understand characteristics of their surface chemistry, which can depend on preparation methodology and aging conditions. For example, details related to the chemical evolution of ^{239}Pu surfaces, in particular the Pu valence state, play an important role in understanding stockpile aging, especially the reversible auto-reduction 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.

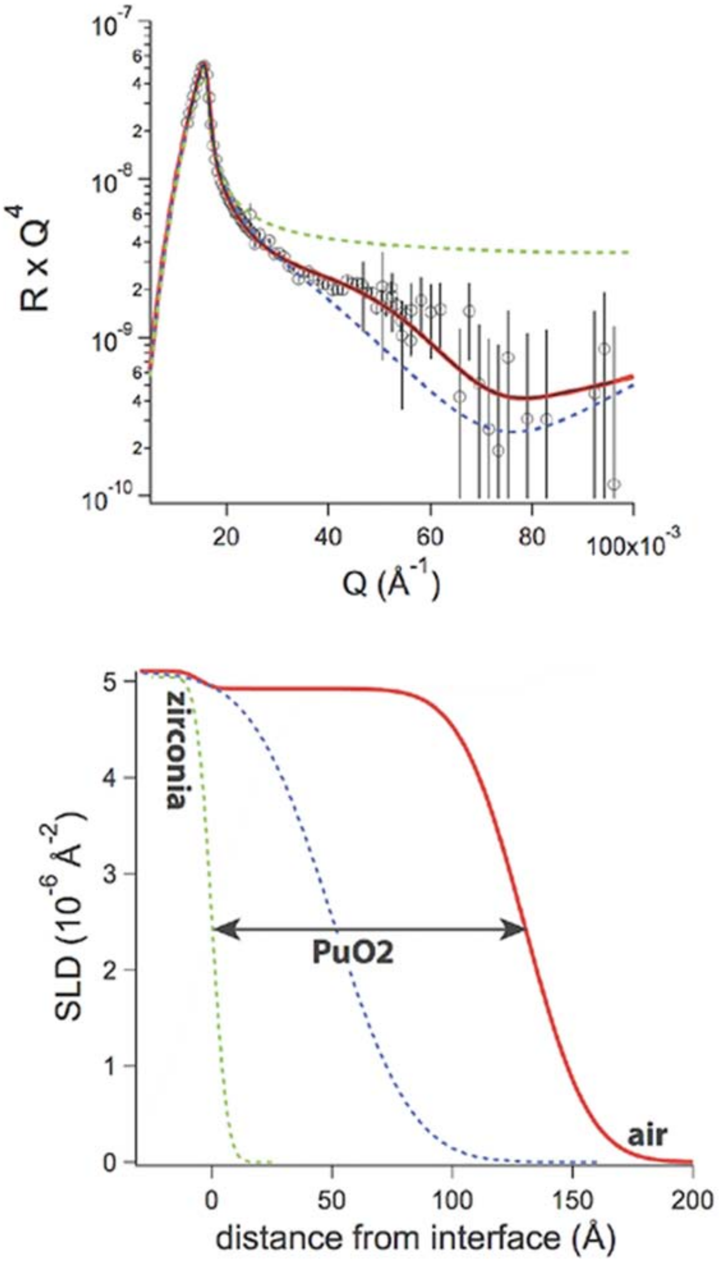
For the first time, neutron reflectometry (NR), via the ASTERIX and SPEAR neutron spectrometers in the Lujan Center at LANSCE, was used to measure films of plutonium oxide (PuO_x), uranium oxide (UO_x), and thorium (Th). The results indicate that neutron-surface-scattering techniques (with reflectometry, grazing incidence diffraction, and grazing incidence small-angle scattering) could give unique insight into these important systems from sub-nm to µm length scales. Studies of the surface chemistry and reactivity of actinides would benefit a broad spectrum of problems, from environmental remediation to stockpile stewardship.

Unlike x-rays, neutrons provide a distinct advantage in evaluating the structural characterization of lighter elements, as well as accessibility of buried interfaces. This advantage makes them an excellent probe for studying and mapping different hydride and oxide forms at surfaces and interfaces of heavy metals. Neutrons have excellent penetrability and comparable scattering cross sections for actinides and isotopes of interest (molecular oxygen, hydrogen, and deuterium). These characteristics are ideally suited to the study of change in Ångström (Å, 10^{-10} m) length scales in the chemistry of these materials.

The team conducted preliminary studies of NR of $^{239}PuO_x$, UO_x and Th thin films at LANSCE using ASTERIX and SPEAR. They used polymer-assisted deposition to grow nanometer-thick films of PuO_x on a zirconia substrate with approximately 1 cm^2 surface area (total mass of PuO_x less than 50 micrograms). DC-magnetron sputtering prepared the films of UO_x and Th. Researchers used NR and off-specular neutron scattering to determine the thickness and composition of the films.

Preliminary neutron-scattering data of the PuO_x film quantified the characteristics of a high-quality film (top figure on the next page). The scattering length density (SLD) distribution normal to the surface is homogenous and matches almost exactly the literature value for crystalline $^{239}PuO_2$. The team did not observe a lower density region between PuO_2 and zirconia substrate or other chemically different layers at the air interface. Researchers detected the air/PuO_2 and zirconia/chemically different layer at the air interface. The air/PuO_2 and zirconia/PuO_2 roughness were approximately 20 and 5 Å root mean square, respectively. Very small off-specular scattering indicates a high degree of in-plane order within the film.

In situ time-dependent neutron reflectivity measured changes in the SLD and thickness of the thorium films during a controlled oxidation process (bottom figure on the next page). As the oxidation progressed, several sub-stoichiometric thorium oxides, ThO_x ($x<1$), preferentially formed between the thorium metal and its dioxide layer. The SLD value of these new oxides increased until a constant value for ThO was reached.



The top graph shows PuO_x neutron reflectometry data (symbols with error bars) and fits (lines) correspond to the scattering-length-density models presented in the bottom graph. Green and blue depict pure zirconia interfaces with different roughness values. Inclusion of the PuO_2 layer (red) was essential to fit the data.

Science on the Roadmap to MaRIE

Neutron surface scattering used to study important characteristics of actinide surface chemistry (continued)

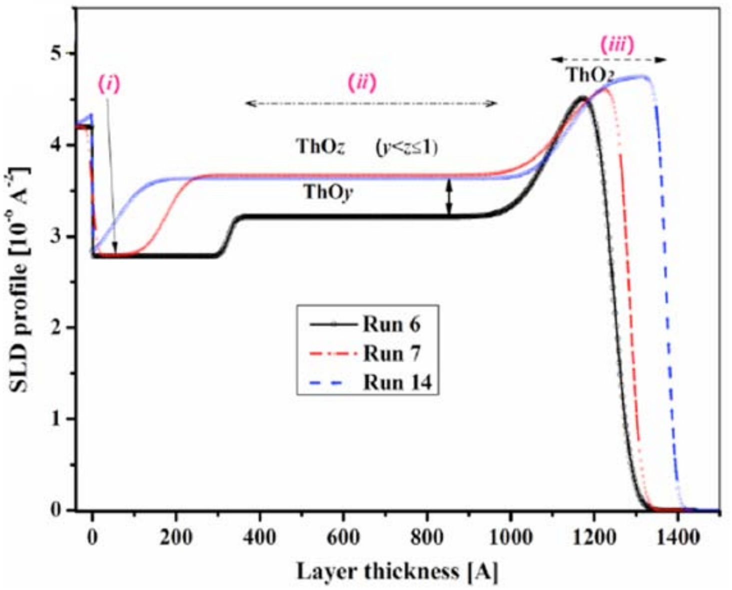
These NR experiments demonstrated that the kinetically favored ThO could be preferentially generated over the thermodynamically favored ThO_2. The near-perfect stoichiometric lattice and relative low oxygen solubility in the ThO_2 top layer limits the availability as well as diffusivity of oxygen species interacting with ThO. These limitations prevent or slow the successive further oxidation. The team concluded that solid-state thorium monoxide, measured for the first time, is produced at material interfaces. The material has potential practical applications. For example, it could provide an ideal combination of features between metal fuel and oxide fuels in nuclear fuel. These features include the thermophysical properties relative to metal fuel and chemical stabilities similar to oxide fuel. ThO fuel shows many advantages with enhanced performance compared with traditional oxide fuels: high fissile density (good breeding performance), high thermal conductivity, and high melting point with adequate chemical stability.

Neutron reflectometry determined the chemical speciation signatures of a complex uranium oxide family. The method characterized both the surface and underlying layers of the uranium oxides with Å-level-resolution. This capacity cannot be achieved using x-ray scattering because it is not capable of distinguishing between U_3O_8 and α-U_3O_8 , especially at the nanometer scale. 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 of this method may also be applicable to a broad range of other scientific disciplines.

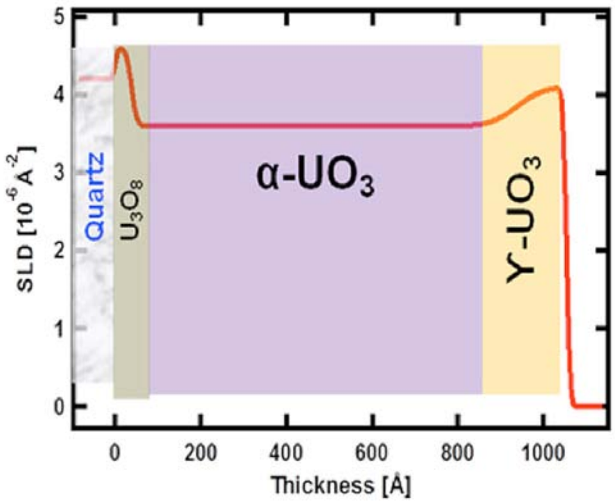
The work is an example of Science on the Roadmap to MaRIE, the Laboratory’s proposed experimental facility for control of time-dependent material performance. The combination of x-ray and neutron-surface-scattering methods at MaRIE could provide unprecedented, time-resolved access to structural properties of actinides and their surfaces from atomic scales to mesoscales. A complete picture of the chemical depth profiles and surface topography of hydrides and oxides formed at metal interfaces would be provided. The highly penetrative nature of neutrons, together with high-energy x-rays, could facilitate these studies over a range of chemical environments, pressures, and temperatures.

Researchers include the following: D. Schwartz, D. Moore, and J. Martz (MST-16); B. Scott, E. Bauer, and E. Watkins (MPA-11); A. Junghans (Polymers and Coatings, MST-7); P. Wang (formerly Lujan Center); K. Rector and H. He (C-PCS); D. Allred (Brigham Young University); and J. Majewski (MPA-CINT).

Sponsoring different aspects of this researcher were the NNSA Campaign 1: Primary Assessment Technologies, LDRD, and a G. T. Seaborg Institute postdoctoral fellowship sponsored different aspects of the research. This work benefited from the use of the time-of-flight neutron reflectometer SPEAR and ASTERIX at LANSCE’s Lujan Center, which the DOE's BES previously funded. The work supports the Laboratory’s Nuclear Deterrence and Energy Security mission areas and the Science of Signatures science pillar.



As shown in this graph, scattering-length-density distributions obtained from NR measurements correspond to various stages of controlled oxidation of Th film. Approximately 1200-Å-thick Th layer was deposited on α-quartz, exposed to ~100 ppm O_2 in Ar at 150° C, and investigated using neutron scattering in situ. Runs 6, 7, and 14 represent approximately 300, 350, and 700 minutes of O_2 exposure, respectively. The zero thickness is set at the quartz substrate/Th film interface. SLD profiles illustrate continuous growth of both ThO_2 and ThO_z regions with simultaneous swelling of the film. The final stage of oxidation corresponds with formation of ThO layer between the quartz substrate and ThO_2 capping layer.



This graphs shows the scattering-length-density distributions obtained from NR measurements of a uranium oxide film. Neutron reflectometry revealed that the film consisted of three distinctive sub-layers: (i) a film of α-U_3O_8 along the substrate interface, (ii) α-UO_3 (a uranium-deficient form of α-U_3O_8 with a large concentration of vacancies), and (iii) the top, atmosphere-exposed and thermodynamically most stable phase, of γ-UO_3.

Science on the Roadmap to MaRIE

Developing the 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 and other high-energy x-ray light sources, LANL researchers, in collaboration with BNL and the Advanced Photon Source (APS-ANL) at Argonne National Laboratory (ANL), successfully confirmed the possibility that new diffractive optics could efficiently focus high-energy photons (E > 50 keV).

MaRIE, the Laboratory's proposed facility for time-dependent materials science at the mesoscale, could ultimately provide a bright source of high-energy x-ray photons. 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, successfully demonstrated the use of silicon kinoform lenses and diamond solid refractive lenses to 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 want to probe these materials deeply with sub-millimeter x-ray beams, enabling micron-scale characterization. The combination of characterization with modeling would 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 – resulting in less probe heating. This weaker interaction with matter makes conventional focusing optics such as mirrors or zone plates either ineffective, inefficient, or expensive.

The top right photo on the following page [labeled (a)] shows a silicon wafer approximately 1 by 3 cm upon which are etched 10 kinoform lenses. The Center for Functional Nanomaterials at Brookhaven National Laboratory and the Cornell Center for Functional Nanomaterials used electron beam lithography and reactive ion etching to design and fabricate the lenses. The x-ray transmission image on the middle right image on the following page [labeled (b)] reveals some of the lens' microstructure. The bottom image on the following page [labeled (c)] shows as knife-edge scan of a spot six of 230 ± 20 nm at 51.2 keV.

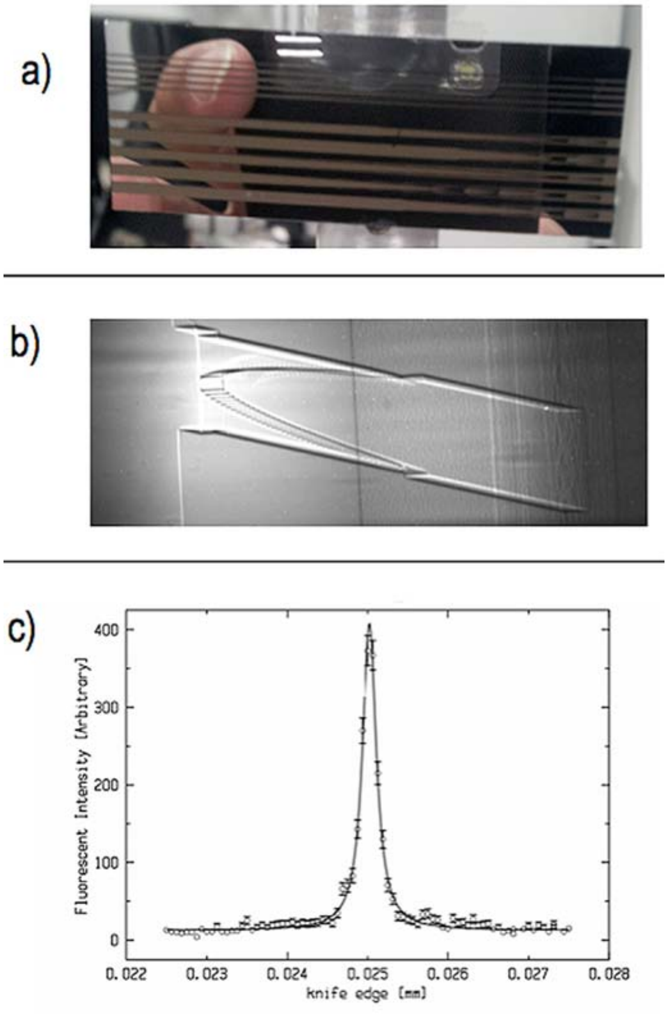
The gain was 87 ± 4, i.e., the resultant flux density on the sample is equivalent to increasing the light source ring current by a factor of 87. A 2-m lens had a gain of 181 and a spot size of 1.0 ± 0.1 microns. The first attempt to use a solid refractive diamond lens to focus hard x-rays demonstrated focusing functionality. Because diamond fabrication technology is not as advanced as silicon fabrication technologies, more research is needed to improve performance with this material.

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

Participants include the following: R. L. Sheffield (Associate Directorate, Experimental Physical Sciences, ADEPS), K. Evans-Lutterodt and A. Stein (BNL), S. D. Shastri and P. Kenesei (ANL), D. Brown (MST-8), and M. Metzler (Cornell University).

The MaRIE program (C. Barnes, LANL capture manager) supported these tests that established capability for the Laboratory's Nuclear Deterrence mission area and the Materials for the Future science pillar.

R. Sheffield checks distances for lens focal length and efficiency measurements at the APS 1-ID beamline.



The top optical image (a) shows a 1 × 3 cm silicon wafer upon which are etched 10 kinoform lenses. Designed focal lengths were 0.25 m, 1 m, 12 m, and 17 m. Design energies were 51.2 and 62.5 keV.

The middle image (b) is an x-ray "shadow image" of the f = 1 m, E = 51.2 KeV (absorption contrast).

The bottom graph (c) shows results from the APS beamline 1-ID, at 51.2 keV with F = 0.25m. Spot size: 230 nm; 1D gain: 87 ± 4, with an efficiency of 17%. The same lens was used to obtain a 1.5-micron spot size at 102.4 keV.

Science on the Roadmap to MaRIE

Using neutron diffraction to study high explosive powder during compaction

In work relevant to the Laboratory's role as the design agency for extending the reliability and safety of B61 bombs that have exceeded their life period, LANL researchers have obtained experimental results about the high explosive TATB (2,4,6-triamino-1,3,5-trinitrobenzene). By collecting the first data on a scale useful to developing constitutive mesoscale models, the team will aid in benchmarking and improving modeling efforts that incorporate how TATB responds to temperature fluctuations and compaction. Literature reports on thermal dependence of TATB lattice parameters and crystal structure do not always agree, and in situ measurements have never been made of texture evolution during a pressing process. Not only are these data critical in developing mesoscale models that can inform system-level models, such data can also be used to interpret and identify underlying mechanisms for other experimental findings.

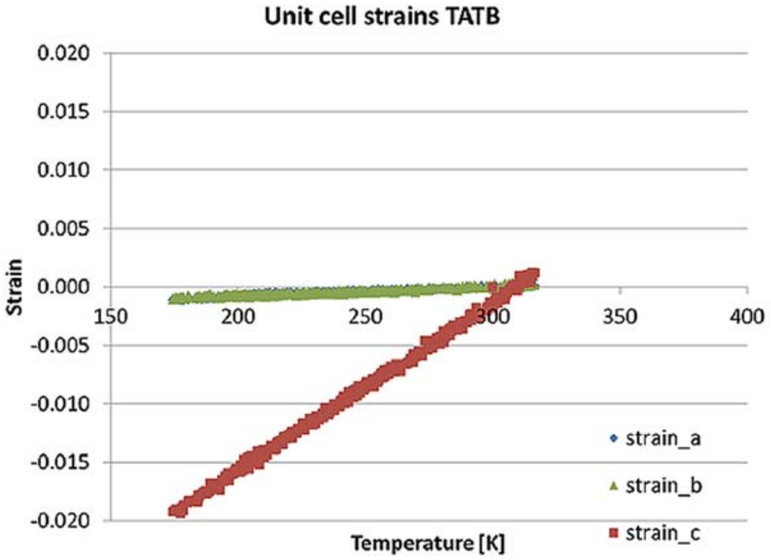
Many explosives detonate when exposed to fire of a shock; they may exhibit partial reaction or incur significant damage when a charge hits the ground. TATB is difficult to detonate by accident. Therefore, it is a prime choice for applications where extreme safety is required. However, TATB has undesirable properties; the most problematic is the anisotropy of the crystal. Mitigating or at least accommodating the problem requires a detailed understanding of TATB's response to temperature changes, as well as the compaction process.

The crystal structure of TATB is triclinic, the lowest possible crystal symmetry. It expands about 10 times more on its crystallographic c-axis than on the a- and b-axes. When a pellet of compacted TATB is heated and cooled a few times, this anisotropic thermal expansion leads to a permanent change in shape and size of the bulk material, an effect called ratchet growth. The temperature change experienced outdoors over the course of a year is sufficient for this effect to happen.

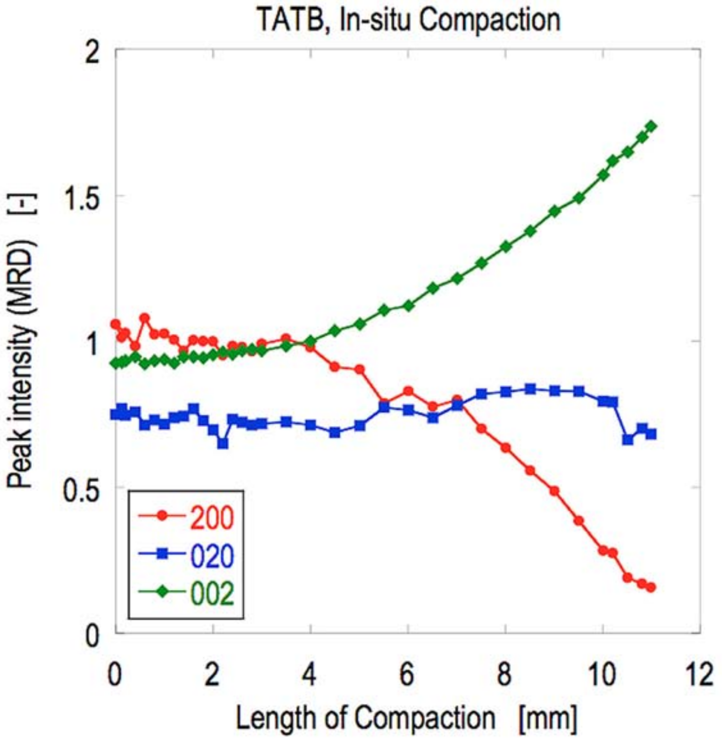
When the platelet-shaped crystals of TATB powder are compacted, the crystals become preferentially oriented due to their shape, similar to a deck of cards falling on the floor – it is very unlikely to see a card standing up. This preferred orientation, or texture, makes the thermal anisotropy even worse as more crystals are oriented with their c-axis parallel to the compaction direction, thus amplifying the effect of the thermal anisotropy.

Researchers D. Brown, B. Clausen, and S. Vogel (MST-8); J. Yeager (Shock and Detonation Physics, M-9); and D. J. Luscher (Fluid Dynamics and Solid Mechanics, T-3) designed and conducted experiments to probe these TATB crystal effects at an atomic and microstructural level. The team used instruments at the Lujan Center: HIPPO and SMARTS, to measure lattice parameters and orientations of the crystals as a function of temperature and compaction level. The work simulated the temperature changes and the compaction process experienced by a "real" component. The neutrons probed a large volume of crystals to enable diffraction on a quantity representative of the bulk material. Comparable experiments using a synchrotron x-ray source, for example, would have sampled a much smaller amount of material and so would require many more tests to gather equivalent information.

The HIPPO neutron diffractometer measurements revealed the relative change of the lattice parameters of TATB powder as a function of temperature (top figure on the following page). Results from multiple heating and cooling cycles indicate that the unit cell dimensions do not change with the number of cycles. The temperature dependence of the dimensions strongly agrees with one particular literature report and somewhat disagrees with another, enabling the model developers to identify the correct data to use. The martials pseudo-hexagonal construction causes an overlap of curves a and b.



The above graph shows relative change (strain) of the three crystallographic lattice parameters of TATB crystals as a function of temperature measured on the HIPPO neutron diffractometer.



The above graph shows the relative change of the peak intensity during compaction of a TATB powder measured on the SMARTS diffractometer. The (200), (020), (002) reflections correspond to the a, b, and c crystallographic axes, respectively. “Length of compaction” refers to the plunger location as it presses into TATB powder in a plunger-and-die setup. Higher length means a higher degree of compaction in the powder.

Science on the Roadmap to MaRIE

Using neutron diffraction to study high explosive powder during compaction (continued)

The bottom figure on the previous page shows the change of certain peak intensities as a function of compaction of TATB powder. During compaction, the grains gradually rotate such that the c-axis, as measured by the (002) reflection intensity, is increasingly aligned with the compaction axis. The platelet TATB crystals shift during compaction so that the largest face is perpendicular to the loading. This shift is confirmed with the full orientation data from a measurement after final compaction (the figure on the following page). Although this final configuration was generally known from previous experiments, the evolution of the texture during compaction had not been observed previously. The team determined that the c-orientation grows at the expense of the a-orientation, whereas the b-orientation remains approximately constant. Researchers expected a more balanced reduction of both axes. This surprising finding will have direct impact on the mesoscale model. Such experimental observations are uniquely provided by in situ diffraction measurements and can be compared to proposed deformation modes from TATB molecular dynamics simulations.

A material's crystal orientations are typically displayed as pole figures. Shown as a contour plot, a pole figure shows how likely a certain crystallographic direction (e.g., 100, 010, 001 on the labels of the three pole figures) takes a certain sample direction. The figure on the following page reveals that the powder has no measurable preferred orientation of the crystals, whereas the compacted pellet has a preferred orientation. The texture of the pellet proves that in addition to anisotropy at the single crystal scale, anisotropy at the mesoscale to macroscale exists.

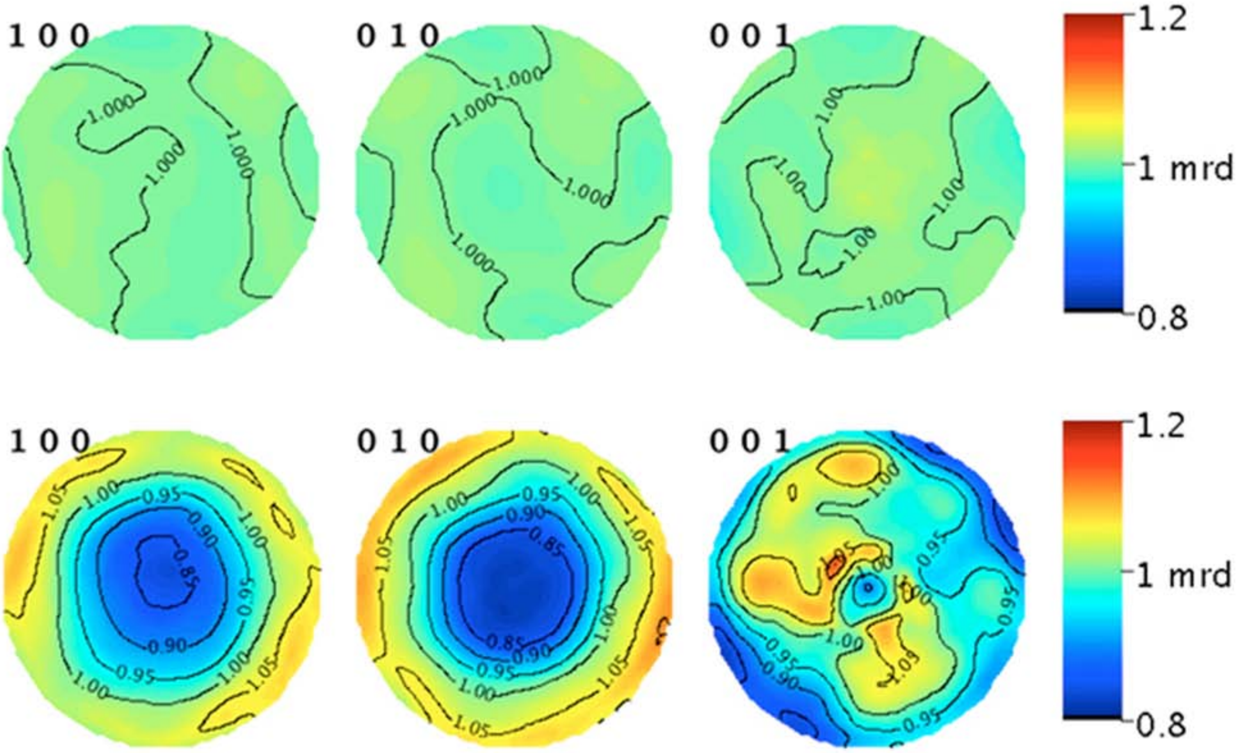
The data will inform a new mesoscale continuum model that a Laboratory team developed. The model relates the thermal expansion of polycrystal TATB specimens to their microstructural characteristics. LANL researchers will use the modified model to predict mesoscale effects in other geometries/experiments, which can be verified with further Lujan Center diffraction experiments in an iterative fashion.

Reference for the model: "Self-consistent Modeling of the Influence of Texture on Thermal Expansion in Polycrystalline TATB," *Modelling and Simulation in Materials Science and Engineering* **22,** 7 (2014).

Authors include the following: D. J. Luscher (T-3); M. A. Buechler and N. A. Miller (Advanced Engineering Analysis, W-13).

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. MaRIE's combination of x-ray and neutron-scattering methods would provide unprecedented, time-resolved access to structural properties of materials from atomic scales to mesoscales.

The B61 Life-Extension Program (Project Realization Team Lead D. Trujillo) and Campaign 1: Primary Assessment Technologies (Program Manager S. Sterbenz) funded the work, which supports the Laboratory's Nuclear Deterrence mission area and Science of Signatures and Materials for the Future science pillars through lifetime extension research on the explosives TATB and PBX 9502. LANL, SNL, the U.S. Air Force, and the Department of Defense use science-based R&D to certify the lifetime of each component and the functionality of the system as a whole. If a component is too old and cannot be recertified for a life extension, then it could be rebuilt as designed or completely redesigned.



Preferred orientation of TATB crystals for loose powder (top) and a compacted pellet (bottom), as measured on HIPPO and displayed as pole figures for the a (100), b (010), and c (001) axes. The sample cylinder axis is out of the paper's plane. The contours are in multiples of random orientation (mrd); i.e., a perfectly random orientation would be 1 in all directions. The powder shows completely random orientation, whereas the pellet shows strong (001) orientation.

Science on the Roadmap to MaRIE

Neutron scattering of pore morphology in shale reveals pore structure and gas behavior

In an effort to maximize unconventional oil and gas recovery, LANL researchers probed pore structure and water-methane fluid behavior in nanoporous shale rock at reservoir pressure and temperature conditions. To perform these studies, the team used LANSCE's LQD, the small-angle neutron scattering (SANS) Low-Q Diffractometer. Their results reveal information key to understanding how nanopore structure determines the distribution of fluids in reservoirs and its impact on oil and gas recovery.

To deliver fluid mixtures to the pressure cell, the team used a pressure sample environment capable of 414 MPa and 250 °C, as well as a gas-fluid mixing apparatus. The researchers performed in situ SANS measurements at various elevated pressures up to 172 MPa and at temperatures up to 66 °C with and without the presence of injected fluid. They discovered that the pores in shale are highly ramified interconnected sheets, accessible to water and methane, which flatten with increasing pressure. The hydraulic fracturing process is designed to open cracks so that fluid is allowed to flow. This result may give insight into the distribution of fluid in situ correlated with pore size and how this distribution would change with hydraulic fracture.

The researchers plan to develop an instrument to examine the hydrocarbon flow behavior in nanoporous shale rocks under uniaxial stress. This representation of in situ reservoir conditions would provide the first experimental results on hydrocarbon phase behavior and flow properties in shale formations where nanopore size, geometry, and connectivity are sensitive to pressure, strain, temperature, water content, and hydrocarbon species.

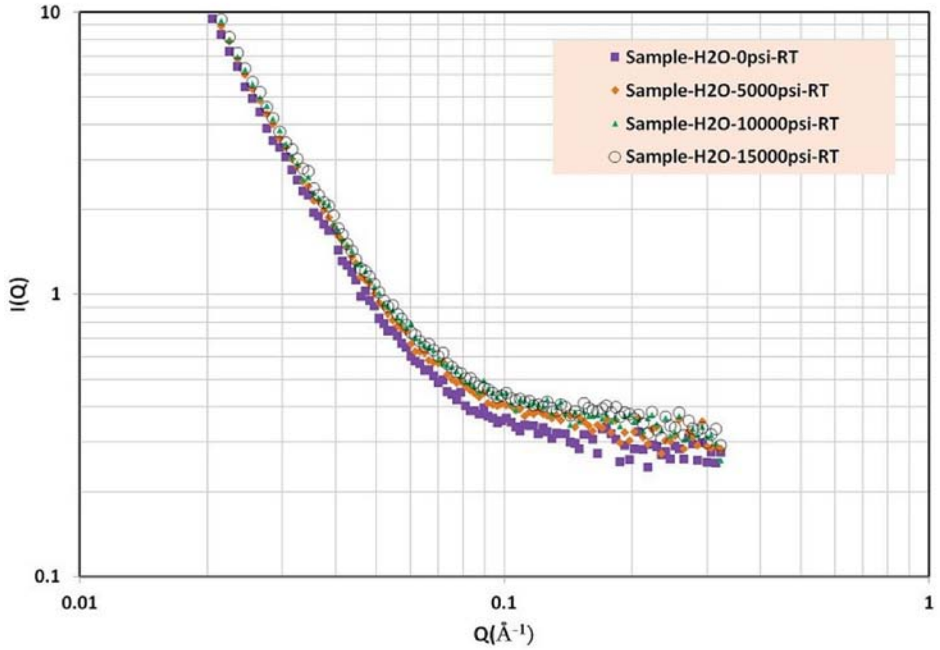
The study is preliminary to time-dependent nanoporous fluid flow studies, examples of Science on the Roadmap to MaRIE, the Laboratory's proposed facility for time-dependent materials science at the mesoscale. With MaRIE, studies on time dependent in situ geomechanical and fluid flow with extremely high time and spatial resolution would be possible to emulate gas and oil extraction procedures.

Participants include the following: M. Ding and H. Xu (EES-14); E. Watkins (MPA-11); M. Borrego (P- 27); D. Olds and R. Hjelm (MST-8).

The DOE's Office of Fossil Energy through National Energy Technology Laboratory's Strategic Center for Natural Gas and Oil (LANL program manager G. Guthrie) sponsored the work. The research supports the Laboratory's Energy Security mission area and Materials for the Future science pillar through insight into how to optimize gas and oil extraction.

Science on the Roadmap to MaRIE

The photo above shows a sample of shale rock used for part of this research.



The graph above shows SANS measurements of shale at room temperature and various pressures, both of which reveal small-length-scale effects.

Science on the Roadmap to MaRIE

Using neutron scattering to study the response of polymer films to high mechanical stresses

Polymers serve as essential components for a variety of items, from cosmetics to the biocompatible surfaces to prosthetics to weapons components. However, the effect of fluid shear effect on the structure and properties of polymer thin films and mesoscopic assemblies has not been adequately investigated. Understanding such stresses plays a key role in expanding thin film applications in areas such as materials science to biology and medicine, where biomechanical forces are responsible for many critical processes.

In collaboration with the University of South Florida and Alcon/Vision Care Company, the Laboratory used the SPEAR beamline at the Lujan Center to investigate the effect of fluidic shear on polymer electrolytes thin films. The team utilized neutron reflectometry, one of the few physical probes with sufficient nanometer-scale resolution, penetrability, and sensitivity to address the properties of ultra-thin polymeric coatings in contact with flowing liquid and the stresses to which they are subjected.

The journal *Langmuir* published their research, which raised important questions regarding the behavior of water molecules hydrating polymeric chains and their response to external stresses, especially in non-equilibrium states. One of the most common substances on Earth, water is vital for many physico-chemical processes, including those essential for all known life forms. An enhanced understanding into its properties, especially in the nano- and meso-scales, is of great importance. To address such time-dependent, soft material problems, scientists are applying an experimental approach that aligns neutron surface scattering with the capabilities of MaRIE, the Laboratory's proposed facility for materials studies at the mesoscale.

Surface properties are very important for implantable biomaterials and tissue engineering. These properties influence tissue and cellular events such as protein adsorption, cell adhesion, and inflammatory response. Combining different poly-ions, nanoparticles, enzymes, proteins, and DNAs enables scientists to create new composite nanostructures, thereby increasing the applications in which such thin films can be used. Estimating the damages/changes within such devices induced by shear stresses is critical for their design and optimization. Fluidic shear stress can be significant: compared to ~500 s^{-1} shear rates in a fire hose, shear rates in the human body caused by blood flow reach up to ~1500 s^{-1} in capillaries and arterioles. In human ocular systems, shear rates can reach up to 30000 s^{-1}, depending on tear film thickness (usually in the µm range) and blink velocity (usually tens of cm/s).

Charged water-soluble polymers, poly-electrolytes are used to coat solid surfaces using a technique in which oppositely charged polymeric films are deposited consecutively deposited through appropriate polymer-water solutions. The team investigated the response of these mesoscale thick films, consisting of alternating polyethylene imine and polystyrene sulfonate layers coated on a quartz substrate, to fluid shear. The scientists used neutron surface scattering probes for the studies. The high penetrability of neutron reflectometry allows examination of buried solid-liquid interfaces, favorable scattering contrast (polymers are mostly built of carbons and hydrogen with which neutrons strongly interact), angstrom-scale resolution, and lack of beam damage. Thus neutrons present an ideal tool to study mesoscale structures in contact with fluids.

The neutron reflectometry results showed several unexpected results. For example, a monotonic decrease of the volume fraction of hydrating water inside the polymer film occurs with increasing shear rate, and an approximate 7% uniform water volume fraction decrease throughout the film for the highest shear rate applied (~7000 s^{-1}) occurs. The water content decrease does not cause any significant changes in the total polymer thickness. This phenomenon creates a significant negative osmotic pressure in the film. The polymers returned to their native state after the shear stress is relieved.

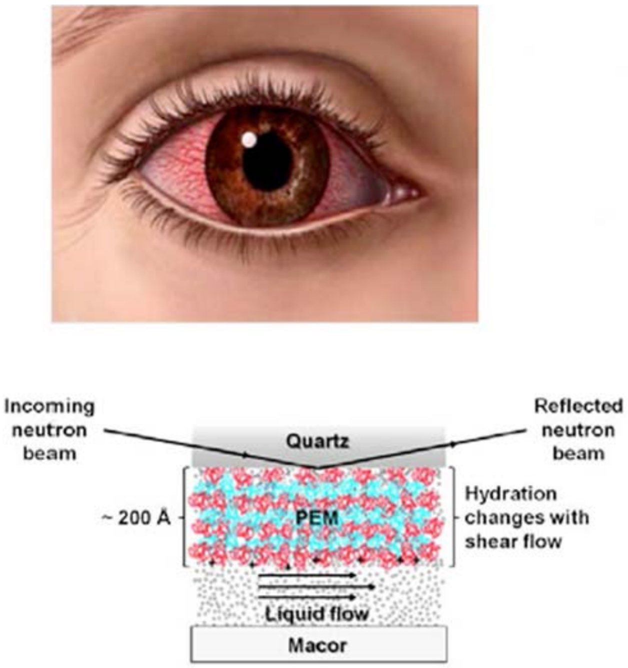
Science on the Roadmap to MaRIE

Reference: “Effects of Fluid Shear Stress on Polyelectrolyte Multilayers by Neutron Scattering Studies,” by *Langmuir* **31,** 2870 (2015).

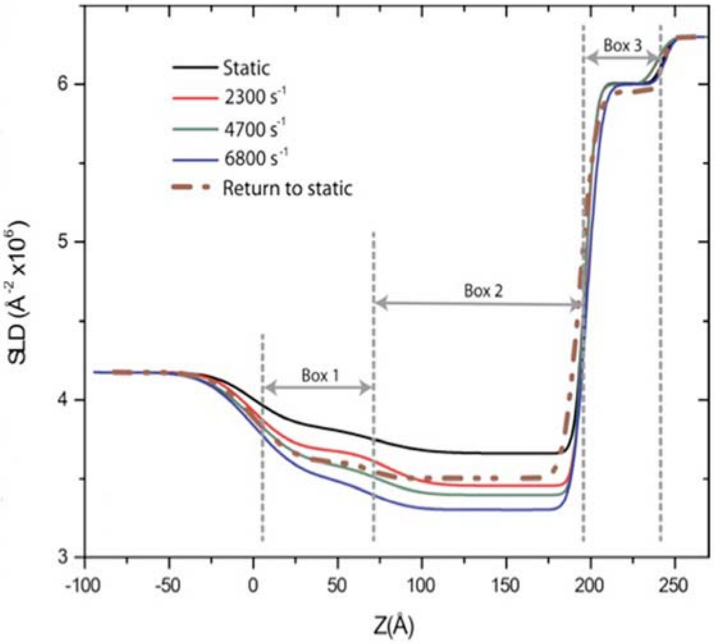
Authors include the following: A. Junghans (MST-7); S. Singh and J. Majewski (MPA-CINT); E. Watkins (MPA-11); Y. Kapoor (Alcon); and R. Toomey (University of South Florida).

This work benefited from the use of the Lujan Center at LANSCE funded by the DOE's BES and LANL under DOE Contract DE-AC52-06NA25396.

The research supports the Laboratory’s overall national security mission and Materials for the Future and Science of Signatures science pillars.



The ability of neutron reflectometry to probe fluidic shear effects on polymer electrolyte thin films benefits applications in which polymeric structures experience dramatic flow shear stresses. For example, the top image shows the surface of a contact lens, which can experience shear rates as strong as 30,000 s^{-1} as a result of a moving eyelid. Natural deficiencies in certain lubricating bio-molecules can lead to dry-eye syndrome and inflamed conjunctiva. The bottom graphic shows a model system that mimics the cornea’s surface as it undergoes shear stress.



The graph above shows neutron reflectometry results that record the response of the polymeric.

Science on the Roadmap to MaRIE

First in situ x-ray diffraction of explosives during impact at the Advanced Photon Source

Los Alamos researchers and their collaborators have used synchrotron radiation to capture for the first time in situ x-ray diffraction patterns of explosives during gas-gun-driven impact loading. As a result, they have demonstrated a crucial diagnostic that enables them to study how crystalline explosives deform under shock loading. This diagnostic represents one of the first experimental steps toward developing next-generation, physics-based mesoscale models. These model will have the predictive capability for high explosives, making them a critical part of supporting Science Campaign 2 milestones scheduled through FY 2023.

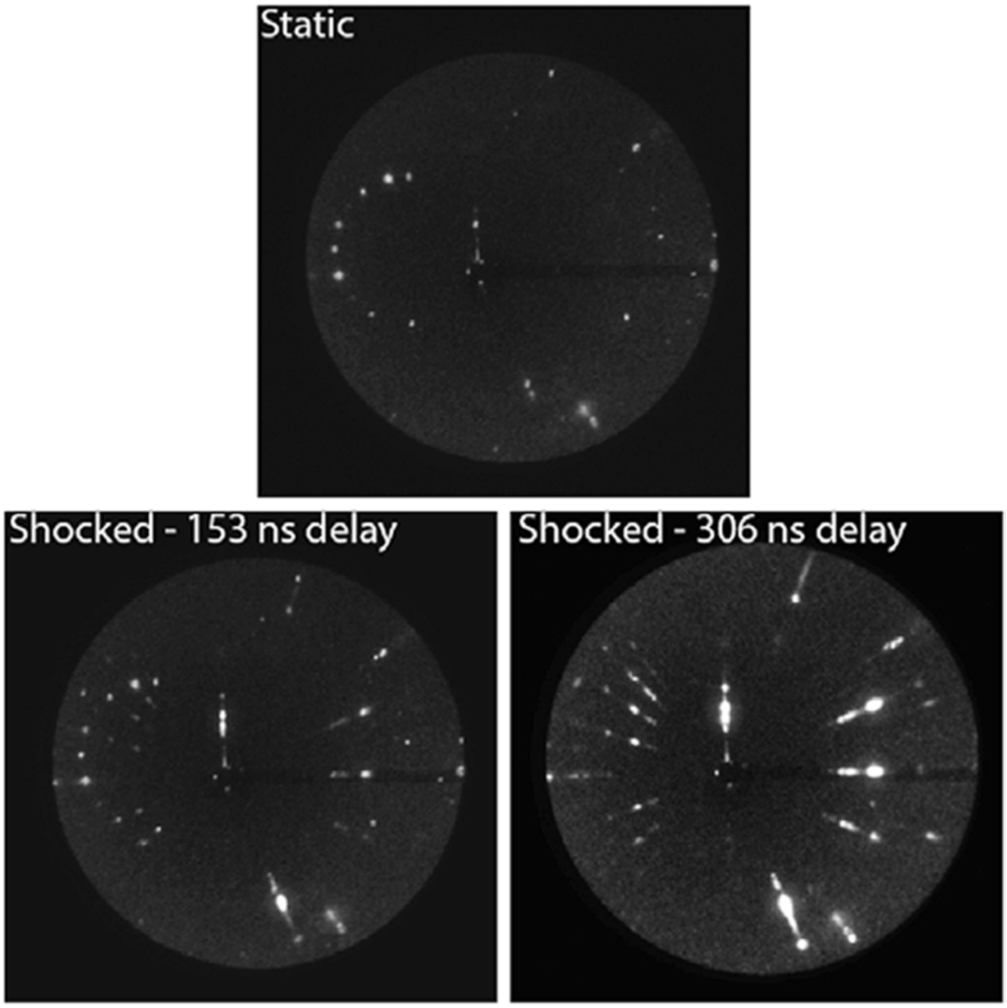
Scientists think that crystalline deformation in high explosives controls the size, temperature, and possibly also the spatial distribution of "hot spots," which lead to shock-induced reaction and detonation initiation. In this study, researchers used the synchrotron at APS-ANL to measure x-ray diffraction in situ during shock loading. The work involved investigating high-rate crystalline mechanics in single-crystal RDX (cyclotrimethylene trinitramine, an explosive).

Next steps include analyzing the x-ray diffraction patterns and comparing them to results from recently developed finite-element model simulations of the crystalline deformation during shock loading. The analysis will enable the extraction of previously unattainable equation-of-state information and the development and validation of an anisotropic plasticity model crucial for predicting thermomechanical localization of deformation and associated heating.

It is important and timely for the Laboratory to develop capabilities designed to make, measure, and model materials, as well as to demonstrate the extent of mission-relevant information that can be extracted from in situ experiments envisioned at the proposed MaRIE facility.

The research team includes the following: K. Ramos, B. Jensen, T. Pierce, V. Hamilton, C. Armenta, C. Owens (M-9); M. Cawkwell, J. Barber (T-1); D. J. Luscher, F. Addessio (T-3); A. Iverson (National Security Technologies LLC, NSTEC); and N. Sinclair and T. Gog (Dynamic Compression Sector, APS-ANL).

The Materials In Extremes exploratory research funding for this LDRD project enabled the experimental development of the x-ray diffraction and complimentary multi-scale modeling capabilities and benefited from the unique national resource for single-crystal growth at the Laboratory's High Explosives Crystal Lab. The x-ray diffraction capabilities created using LANL's IMPact system for ULtrafast Synchrotron Experiments (IMPULSE) and applied here to explosives will be used to study other materials, including metals, within the fiscal year. The research supports the Laboratory's Nuclear Deterrence mission area and the Materials for the Future and Science of Signatures science pillars through studies of materials in extreme environments for Stockpile Stewardship.



These x-ray diffraction patterns are from a {021}-oriented RDX sample.

Science on the Roadmap to MaRIE

Key development for implementing the next generation of high-brightness x-ray sources

Researchers have successfully designed, fabricated, and tested a new x-ray lens made from diamond. The material enables phase-preserving diamond optics. This is a promising advance in the development of the high-quality optics needed for MaRIE, the Laboratory's proposed facility for time-dependent materials science at the mesoscale, and other high-energy x-ray light sources.

MaRIE would provide a bright source of high-energy x-ray photons. To enable the full potential of the source to be realized requires focusing elements that concentrate x-rays on the region of interest. Beryllium (Be) is one of the best lens materials available for x-ray optical properties, and a large fraction of the existing refractive x-ray lenses in use around the world are made from beryllium. Unfortunately, Be has numerous drawbacks: it is usually produces as a polycrystalline material, it cannot handle high heat-loads, and it is hazardous. The polycrystallinity degrades the photon phase profile that is produced by the source, and the poorer thermal quality of Be precludes its routine use as the first optical element facing the source.

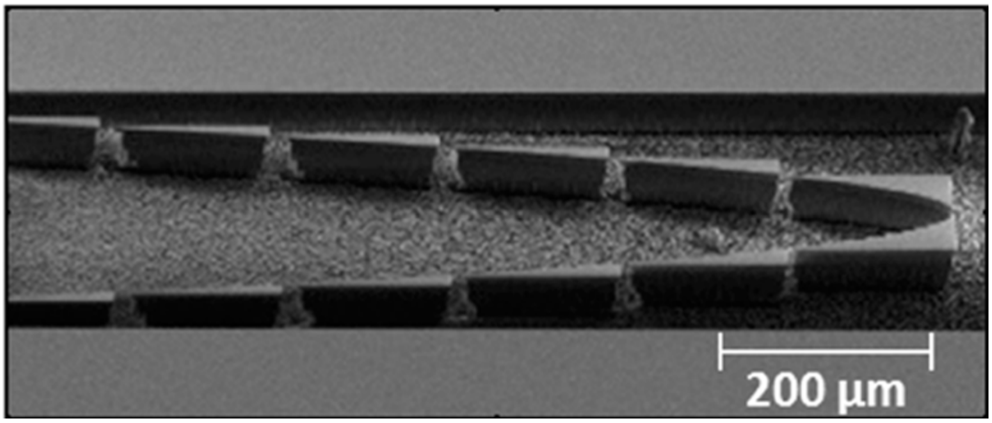
Diamond has long been realized as an excellent material for x-ray lenses due to its good optical properties for x-ray photons. More importantly, diamond has an order of magnitude higher thermal conductivity and lower thermal expansion compared with Be, and its excellent hardness would enable its use in the high heat-load present at new high brightness sources like the planned MaRIE.

Diamond solves most of the problems of Be, but it is difficult to fabricate the precise shapes needed to make high-quality x-ray lenses. This new research has successfully fabricated the complex shapes in diamond required for x-ray lenses. The top image on the following page shows a visible light image of a diamond kinoform lens, etched onto a diamond chip with a size thickness of 4.5 mm × 4.5 mm × 0.5 mm. This shape focuses in one direction and produces a line focus. The Center for Functional Nanomaterials at BNL performed the design and fabrication with electron beam lithography. Modern Microsystems conducted reactive ion etching. Researchers tested the lenses at the CHX beamline at NSLSII at BNL.

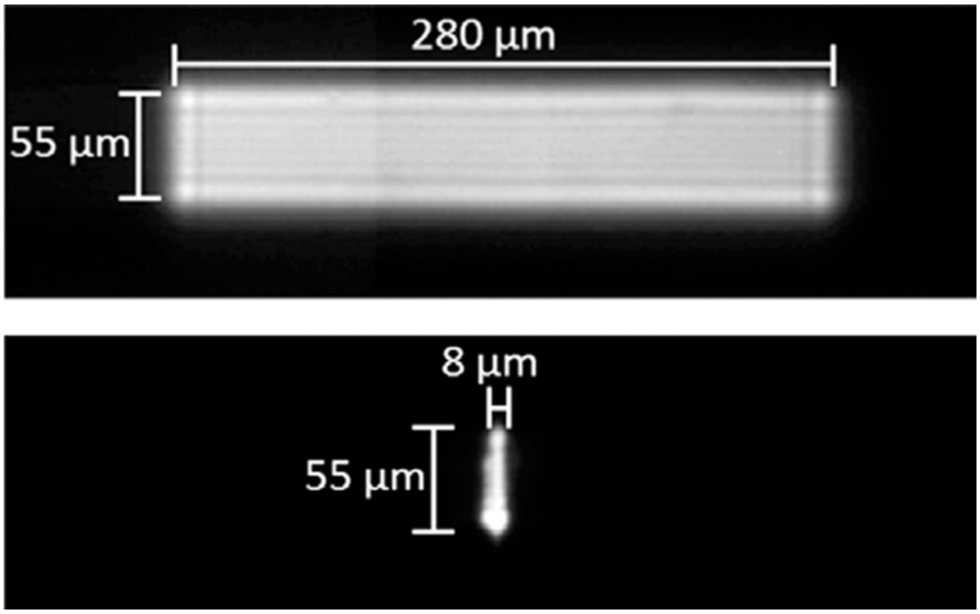
Researchers include the following: R. Sheffield (ADEPS), K. Evans-Lutterodt, A. Fluerasu, A. Stein, and L. Wiegart (BNL); and C. McGray (Modern Microsystems).

The MaRIE program (C. Barnes, LANL capture manager) supported these tests that established capability for the Laboratory's Nuclear Deterrence mission area and the Materials for the Future and Science of Signatures science pillars.

Science on the Roadmap to MaRIE



The image above shows a prototype kinoform x-ray optic formed into a single-crystal diamond by using deep reactive ion etching.



Experimental results on focusing performance of the prototype diamond kinoform x-ray optic. The transmittance of the optic was measured to be 75%±5%, at a photon energy of 12 keV.

Top: The 280-µm × 55-µm rectangle of x-ray illumination that is incident on the lens, as imaged by a YAG crystal. Dark fringes parallel to the aperture edges indicate the coherence of the beam.

Bottom: The one-dimensional focusing action of the lens reduced the 280-µm width of the beam to approximately 8 µm. The resulting line focus has dimensions of 8 µm × 55 µm. (Image brightness and contrast adjusted for clarity of presentation.)

Conferences and Workshops 2015

LANSCE
Los Alamos Neutron Science Center

Conference and Workshops at a Glance

Government, academic, and industrial researchers visit LANSCE to attend topical conferences and workshops. In conjunction with New Mexico State University (NMSU), LANSCE also runs the annual LANSCE School on Neutron Scattering, which is now in its ninth year. The Stewardship Science Academic Alliance Center of Excellence also meets at LANSCE once a year.

In addition to our conferences and workshops, throughout the year LANSCE hosts a variety of visitors, many of whom request tours of the accelerator, instruments, and laboratories. The US or foreign-citizen visitors come from academia, industry, other national laboratories, or representatives from local, tribal, state, or federal governments. As a National User Facility, LANSCE encourages visitors to schedule tours and fully supports educational outreach tours to higher education, K-12 schools, and youth organizations.

- Training the next generation through the Nuclear Safeguards and Security Summer School
- 2015 LANSCE User Group Meeting
- 11th LANSCE School on Neutron Scattering Materials at the Mesoscale

At left: Participants of the 11th LANSCE School on Neutron Scattering.

Conferences and Workshops

Training the next generation through the Nuclear Safeguards and Security Summer School

On August 3–12, The Nuclear Science and Security Consortium (NSSC), along with SNL and LANL, held a joint Nuclear Safeguards and Security Summer School. The school's purpose was to train the next generation of experts in nuclear security. The program features a five-day module at Los Alamos, followed by a three-day module at Sandia. Participating at this summer school were 24 students from seven universities.

The Los Alamos Nuclear Safeguards component of this summer school provided an introduction to the nondestructive assay (NSA) of uranium- (U) and plutonium- (Pu) bearing materials using gamma ray and neutron measurement techniques. Students had hands-on training using measurement techniques to quantify and characterize items containing Special Nuclear Materials, including uranium enrichment measurements, Pu isotopic measurements, active neutron coincidence counting of U, and passive neutron coincidence counting of Pu. Los Alamos presenters included M. Croce, D. Miko, K. Miller, P. Santi, and M. Swinhoe (Safeguards and Technology, NEN-1); R. Simpson (P-23); and P. Karplus.

In addition to hands-on exercises at Los Alamos, NSSC students worked on a mock material-verification exercise. The students discussed their ongoing research projects with LANL staff and NSSC campus-based faculty during a welcome event and poster session. Organizers designed the session to catalyze collaboration between LANL and university researchers and highlight the research of the students in radiochemistry, nuclear physics, nuclear engineering, instrumentation, and national security policy. LANL gave students tours of LANSCE, space-qualified flight hardware laboratory spaces, the high-explosive testing area, and the NHMFL.

The NSSC is a consortium of universities led by University of California, Berkeley. NNSA's Office of Defense Nuclear Nonproliferation R&D funds the consortium to support the nation's nuclear nonproliferation mission through the training and education of experts in the nuclear security field. Other NSSC universities: Michigan State University, University of California, Davis; University of California, Irvine; University of California, San Diego; University of Nevada, Las Vegas; and Washington University in St. Louis. Students in the consortium can collaborate with researchers at four DOE national laboratories: LANL, Lawrence Berkeley, LLNL, and SNL. M. Rabin (Space and Remote Sensing, ISR-2) is the LANL point of contact for the NSSC.

The work supports LANL's Global Security mission area and the Science of Signatures science pillar through LANL's nuclear nonproliferation activities.

Conferences and Workshops

R. Simpson and other participants discuss their research during the poster session.

P. Santi, far left, teaches active neutron nondestructive assay measurement techniques for uranium items to (from left to right) S. Queern, J. Richards, and A. Gallardo.

Conferences and Workshops

2015 LANSCE User Group Meeting

On November 2–3, 2015, the LANSCE User Group Meeting (LUG) was held at La Posada in Santa Fe, New Mexico. This year's topic was LANSCE Futures. Members of the LANSCE scientific community and user program members, provided feedback on capabilities needed at LANSCE over the next five years. LANSCE as a national user facility continues to provide the scientific community with intense sources of neutrons and protons for experiments supporting civilian and national security research.

The meeting included presentations and discussions covering the main areas of research at LANSCE: imaging, proton and neutron radiography, materials science, nuclear science supporting national security, fundamental nuclear and particle physics, and industrial applications. Presenters from the LANSCE user community showcased the current status of the facility, the needs of the scientific community, and the future of LANSCE with respect to MaRIE, the proposed Matter-Radiation Interactions in Extremes experimental facility. MaRIE is LANL's proposed facility for time-dependent control of dynamic properties of materials designed to address national security science missions.

A. Young (North Carolina State University), chair of the LUG Executive Committee, is working with LANSCE management to help invigorate and increase user community involvement.

The DOE, NNSA, Office of Science, and Office of Nuclear Energy, Science, and Technology are the principal sponsors of LANSCE, which supports the Laboratory's national security missions and the Materials for the Future, Nuclear and Particle Futures, and the Science of Signatures science pillars.

Poster from the 2015 LANSCE User Group Meeting: LANSCE Futures.

11th LANSCE School on Neutron Scattering-Materials at the Mesoscale

Spanning nine days, the 11th LANSCE School on Neutron Scattering addressed how neutron scattering benefits studies related to materials at the mesoscale (from nanometers to millimeters—between the atomic and macroscopic scales). School instructors examined the influence of surfaces, interfaces, and microstructure on the properties of materials and functionalities. Laboratory staff and 36 selected applicants from 28 universities participated in lectures, tutorials, tours, and hands-on experiments at the LANSCE Center for Integrated Nanotechnologies. The majority of the participants did not have prior exposure to neutron-scattering techniques.

The purpose of the LANSCE school is to develop a strong, diverse neutron-scattering community by introducing early-career scientists to a variety of neutron-scattering techniques and demonstrating how they complement other materials analysis techniques in a selected topical area. This year's topic, mesoscale science, has the potential to revolutionize the discovery, design, and application of materials by revealing properties that can be tailored to create new functionality. Students became familiar with several neutron and x-ray scattering approaches (powder diffraction, small-angle neutron scattering, local structure determination, and neutron reflectometry) and their use in addressing important materials science questions at the mesoscale realm. The mesoscale is often difficult to probe using other techniques.

A Llobet of P-27 and H. Nakotte of New Mexico State University (NMSU) co-directed the school. E. Fohtung (NMSU), G. King (MST-8), and J. Majewski (CINT) served as organizing committee co-chairs. Presenting lectures were experts from LANL (MST, MPA, and C), ORNL (SNS), UC – Berkeley and Santa Barbara, Columbia University, Princeton University, Queen's University, NMSU, and Colorado School of Mines. Overview presentations addressed the importance of mesoscale science. J. Sarrao (Associate Director of Theory, Simulations & Computation, ADTSC) discussed opportunities to design architectures and interactions among nanoscale units to create new macroscopic behavior and functionality. C. Barnes (Capture Manager for MaRIE) described the challenge of dynamic mesoscale imaging and new scientific opportunities that would be available with MaRIE, the Laboratory's proposed experimental facility for the time-dependent control of dynamic material performance.

The school introduced participants to the capabilities of a NNSA-funded national user facility. The facility has become a bridge for many who return as LANSCE users, helping to foster the next generation of LANSCE staff scientists, building new collaborations with university researchers, and strengthening the community of neutron science in all its diversity.

The NSF sponsored the students. LANL, the Laboratory's Institute for Materials Science, and the MaRIE project funded instructor and local expenses. LANSCE and NMSU provided planning and logistics; CINT supplied special experiment support.

Students in the LANSCE School on Neutron Scattering learn about SPEAR capabilities with staff scientist E. Watkins.

News
and
Celebrations
2015

News and Celebrations at a Glance

The remarkable men and women of LANSCE go above and beyond in their service to our facility—the stories featured here are some of the newsmakers for 2015.

LANSCE celebrates and applauds the outstanding accomplishments of our users, staff, students, researchers, and contributors.

- Kurt Schoenberg
- Ellen Cerreta
- Edwin Fohtung
- Kathy Prestridge
- Dinh Nguyen
- Andy Saunders
- Benno Schoenborn
- Elena Fernandez
- Eric Brown

At left: Louis Rosen and colleagues celebrate as the LAMPF accelerator achieves 800-million-electron-volt beam of protons.

News and Celebrations

Farewell, Kurt Schoenberg

On October 1, 2015, Kurt Schoenberg, LANSCE user facility director and deputy associate director, retired from Los Alamos National Laboratory.

Over the past decade, Kurt has steered the facility through funding and programmatic challenges, but more importantly, he has been integral in creating opportunities for LANSCE and the neutron community through the LANSCE User Program, as well as open collaboration and outreach endeavors. He has striven to honor the vision of our founder, Louis Rosen, and worked as a steward of Louis' belief that LANSCE as an interdisciplinary facility would keep Los Alamos as the world leader in nuclear technology through international scientific excellence and "deterrence through competence." Not only has Kurt met Louis's iconic vision, he has also served LANSCE as an innovator in future concept facilities, creating a vision of the future of LANSCE on the path toward MaRIE.

As LANSCE User Facility Director, Kurt had overall operational responsibility for LANSCE and oversaw the basic, applied, and national security research performed at the five facilities that comprise LANSCE, including neutron-scattering research at the Lujan Center, nuclear science and technology at the WNR Facility, and national security research at the Proton Radiography Facility.

Kurt received his BS in engineering physics with high honors from the University of Illinois in 1972. In 1979, he was awarded a PhD in physics from the University of California, Berkeley, and joined the Los Alamos National Laboratory's research staff. Kurt's research expertise and accomplishments, as documented by over 100 publications, include the experimental and theoretical investigation of magnetically and inertially confined plasmas for controlled thermonuclear fusion, intense particle accelerators, plasma accelerators, plasma-based space propulsion, missile interceptor systems, and high-energy-density-physics.

Kurt plans to spend significant time in Europe as an EMMI (Extreme Matter Institute) visiting professor of physics at the Technische Universität Darmstadt and as a senior scientific advisor. He leaves LANSCE on a positive trajectory, and we thank him for his dedication and leadership. We are a stronger facility thanks to Kurt's efforts and positive presence.

Thank you, Kurt.

News and Celebrations

Kurt Schoenberg

News and Celebrations

Ellen Cerreta joins ASM Board of Trustees

In June 2015, MST-8 Group Leader Ellen Cerreta began a three-year term as an ASM International Trustee. The ASM Board of Trustees guides the course of the society by defining its ideals and activities, approving budgets, choosing the managing director, and advising ASM's top leadership. The board includes four officers and nine trustees.

Ellen Cerreta

Ellen received a PhD in materials science and engineering from Carnegie Mellon University, and then joined the Laboratory in 2001 as a postdoctoral research associate. She became a full-time staff member in 2003, MST-8 deputy group leader in 2013, and MST-8 group leader in March 2014. At Los Alamos, she studies dynamic damage caused by to shock loading and shear deformation of metals. She leads research into the deterministic features of dynamic failure with the goal of developing damage-tolerant materials for aerospace, defense, automotive, and manufacturing applications. She has held leadership roles at Los Alamos, ASM, and The Minerals, Metals & Materials Society (TMS). Ellen has served on the board of directors for TMS from 2009 to 2012.

ASM International is the world's largest association of metals-centric materials engineers and scientists. Through publications, databases, and events, the organization informs, educates, and connects the materials community to solve problems and stimulate innovation around the world. Jim Foley (Metallurgy, MST-6) was the previous trustee from the Laboratory, serving from 2012 to 2015.

News and Celebrations

Edwin Fohtung named 2015 Rosen Scholar

Edwin Fohtung is the 2015 Rosen Scholar at LANSCE. The Rosen Scholar is a fellowship that honors the memory or renowned LANL physicist Louis Rosen for his accomplishments and dedication to a broad range of science performed at LANSCE.

A materials physicist, Edwin is the LANSCE professor in conjunction with the Department of Physics at NMSU. He received a PhD from the University of Freiburg in Germany. He uses experimental and numerical modeling to explore neutron and coherent scattering techniques, laser-based pump-probe experimental techniques, and pulsed electric and magnetic fields to probe emergent soft and condensed matter systems. He investigates multiferroics, magnetoelectric, electronic, straintronics, and magnetic phases arising from competing and/or coupled charge, spin, orbital ordering and lattice interactions. Edwin also provides scientific consultation for MaRIE, the Laboratory's proposed experimental facility. He guest edited the *Journal of Optics* special issue on coherent diffractive imaging, serves as a member on the ORNL Neutron Sciences Review Committee, and received a Department of Defense Air Force Office of Scientific Research award.

Louis Rosen originally came to Los Alamos to work on the Manhattan Project. From there, he built the foundation of what would become a prestigious scientific career spanning more than six decades. As a result of his scientific acumen and tireless dedication for work at LANSCE, he is now known as the "father of LANSCE." His outstanding leadership and scientific career at LANL included conception of the Los Alamos Meson Physics Facility (LAMPF) during 1960, which culminated with its commissioning in 1972. LAMPF was a unique nuclear science research tool through the 1990s. Now called LANSCE, the facility continues to play a paramount role in basic sciences and national security needs for the country. The Laboratory hosted "Rosenfest" to honor his legacy in May 2011. LANSCE provides the scientific community with intense sources of neutrons for experiments supporting civilian and national security research. The DOE, NNSA, Office of Science and Office of Nuclear Energy, Science and Technology – the principal sponsors of LANSCE – have synergistic long-term needs for the accelerator and neutron science that is the heart of LANSCE.

Edwin Fohtung

News and Celebrations

Kathy Prestridge expands APS diversity goals for women in physics

In her role as chair of the APS Committee on the Status of Women in Physics (CSWP), Kathy Prestridge, (P-23) recently briefed the Society's Council, including CEO K. Kirby and President S. Aronson, on CSWP goals and activities, many of which have been expanded under her leadership. The following updated goals are designed to focus the committee's activities and increase the benefits of diversity in physics:

- Increase the number of women involved in physics by increasing the number who enroll in and complete undergraduate degrees in physics.
- Understand and implement solutions for gender-specific issues such as stereotype threat, subconscious bias, and impostor syndrome that affect the careers of all physicists.
- Provide workshops that enhance professional development opportunities for women in physics. Workshops would cover topics such as mentoring, mentor training, and negotiation skills.
- Remedy issues that impact gender inequality in physics by encouraging research into fundamental causes, assessing policies, and advocating good practices.

Programs designed to advance these goals include the following: the Conferences for Undergraduate Women in Physics, Professional Skills Development Workshops, and Climate Site Visits to physics departments and collaborations. One of the most successful, the Professional Skills Development Workshops, will continue under a new five-year National Science Foundation grant. Principal investigators T. Hodapp (APS), S. Yennello (Texas A&M University), and Kathy are developing Train the Trainer, a new program addressing subconscious bias and teaching negotiation skills to graduate students, postdoctoral researchers, and early-career job seekers pursuing positions in academia, industry, or national labs.

Nine established leaders in physics who are representative of diverse technical and geographical areas attended the April 10 inaugural workshop in Baltimore, Maryland. These women will give workshops on negotiation and career skills at their home organizations. If your group would like to hold a workshop, contact Prestridge at kpp@lanl.gov.

Election to the CSWP occurs through nominations to the APS, with final approval made by the council and invitations extended by the CEO. Questions regarding the CSWP should be addressed to kpp@lanl.gov.

Participants in the first Train the Trainer Workshop: K. Prestridge (LANL, Chair CSWP, fluid dynamics), D. Stokes (University of Houston, solid state physics), A. Opper (Jefferson Laboratory, NSF, nuclear physics), P. Sandick (University of Utah, cosmology), S. Blessing (Florida State University, high energy physics), N. Houfek (Professional Trainer), K. Hafidi (ANL, nuclear physics), S. Yennello (Texas A&M University, nuclear physics), J. Vedrine-Pauleus (University of Puerto Rico – Humacao, condensed matter physics), and K. Daniels (North Carolina State University, soft matter physics).

American Physical Society names new Fellows

Los Alamos scientists have been elected as Fellows to the APS for 2015. Selection as a Fellow recognizes exceptional contributions to the physics enterprise, such as outstanding physics research, important applications of physics, leadership in or service to physics, or significant contributions to physics education. Fellowship is a distinct honor signifying recognition by one's professional peers. The following website provides more information regarding APS Fellows:
www.aps.org/programs/honors/fellowships/

Dinh Nguyen (AOT-AE) was cited "For an outstanding record of innovation and contribution to the initial development of high-brightness photo-injectors, early experimental validation of self-amplified spontaneous-emission theory, and high average current injectors."

The APS Division of Physics of Beams nominated him. Dinh received a PhD in chemistry from the University of Wisconsin–Madison. Since joining the Laboratory in 1984, he has performed pioneering work in single-molecule detection, up-conversion solid-state lasers, RF photoinjectors, advanced photocathodes, and high-gain amplifier free electron laser (FEL) concepts such as the self-amplified spontaneous emission (SASE) and regenerative amplifier. His high-gain SASE experiments in 1997 were the first in a series of experiments that have culminated in the first x-ray FEL at SLAC. His current research includes the development of high-power FEL, high-average-current RF injectors, rugged photocathodes, and new ideas of hard x-ray FEL.

Andy Saunders (P-25) was cited "For contributions in developing proton radiography and the LANL ultra cold neutron source, enabling new applications of nuclear science and an improved understanding of the decay of the free neutron."

The APS Division of Nuclear Physics nominated him. Andy received a PhD in physics from the University of Colorado and joined the Laboratory as a postdoctoral researcher in 1998. He has participated in the development of pRad since the early demonstration experiments conducted at BNL in 1997. He has led the Los Alamos pRad imaging capability since 2013 and served as the radiographer in charge of executing more than 150 explosively driven dynamic experiments at LANSCE for the weapons program, for which he is now developing new techniques in charged particle radiography. Andy also participated in the design and construction of LANL's UCN, which uses the LANSCE proton beam to produce ultracold, slow-moving neutrons that enable fundamental physics measurements of unprecedented precision. He is co-spokesperson of a project measuring the average lifetime of the free neutron. Andy has been honored with nine NNSA Defense Program Awards of Excellence and five LANL Distinguished Performance Awards.

Dinh Nguyen

Andy Saunders

News and Celebrations

Benno Schoenborn chosen for Bau Neutron Award

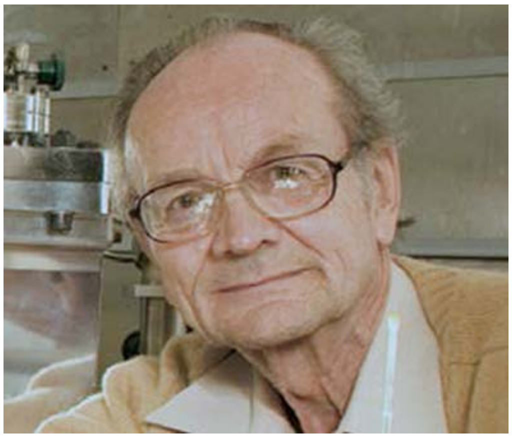
The American Crystallographic Association (ACA) has selected Benno Schoenborn (formerly B-11) to receive the 2016 Bau Neutron Award. The award recognizes exceptional research achievement in neutron diffraction. Benno is the second recipient of this triennial award, which honors his pioneering research in macromolecular neutron crystallography and the design and development of the neutron crystallography beamline PCS at LANSCE.

A Laboratory Senior Fellow, Benno retired from Los Alamos in 2013. Before coming to Los Alamos, he worked at BNL, where he conducted innovative work in macromolecular neutron crystallography, beginning with the very first neutron structure of myoglobin in 1969. Neutron crystallography uses neutron diffraction to elucidate protein structures: when a beam of neutrons hits a crystallized protein, they are scattered by the crystal and their diffraction pattern recorded. Using this approach, scientists can determine the location of hydrogen atoms; such information enables them to gain a better understanding of enzyme mechanisms, hydrogen bonding, and water structure in macromolecules.

Known as the "father of neutron crystallography," Benno first demonstrated this technique at a time when few scientists believed the process was even possible. He performed his first demonstration of this technique at a time when few scientists believed that it was even possible. Benno persevered and proved that neutron diffraction of macromolecular crystals was not only possible but that the information gleaned was unique and extremely useful. Upon arrival at LANL in 1993, Benno began work on designing and building the first neutron PCS at a spallation neutron source at LANSCE. Working with colleagues E. Pitcher, P. Ferguson, and later P. Langan, Benno designed every component of the PCS to maximize neutron intensity while reducing background scattering.

With PCS, scientists could no collect excellent data during 15 to 30 days of beam time by using small protein crystals. The big payoff was that the larger proteins, for which large crystals are nearly impossible to grow, now were amenable to neutron crystallography.

Once completed in 2002, the PCS was the first macromolecular crystallography beamline at the spallation neutron source until 2008, at which time Tokai, Japan, completed its iBIX station.



Benno Schoenborn

The PCS remained the only macromolecular crystallography station in North America until 2010, at which time ORNL commissioned the TOPAZ/MaNDi/IMAGINE instruments. The PCS has been used as an example for this type of instrument in construction of similar beamlines at the Australian Nuclear Science and Technology Organisation and ORNL. Over the last 14 years, research at LANL's PCS has revealed unexpected and critical data on enzyme mechanisms and highlighted the unique characteristics and chemistry of enzyme active sites. The data have proved to be critical for drug design and protein engineering.

The award is given in memory of Professor Robert Bau, University of Southern California (1969–2008) and president of the ACA in 2006. Professor Bau made major contributions to the development of the technique of single-crystal neutron diffraction and to its applications in chemical and biomacromolecular crystallography. This award recognizes exceptional research achievement in neutron diffraction.

The American Crystallographic Association, Inc. is a nonprofit, scientific organization of over 2,200 members in more than 60 countries. Founded in 1949, the Association promotes interactions among scientists who study the structure of matter at atomic (or near atomic) resolution. These interactions advance experimental and computational characteristics of crystallography and diffraction. Understanding the nature of the forces that both control and result from the molecular and atomic arrangements in matter will provide insight into chemical interactions in nature and could lead to treatments for disease.

Elena Fernandez Receives 2015 APEX Award of Excellence

Elena Fernandez, senior public information specialist (NMSU), received the 2015 APEX Award of Excellence for the 11th LANSCE School on Neutron Scattering. The school's outreach and marketing and meeting materials were entered in the Campaigns, Programs & Plans - Education & Training category.

The APEX Awards is an annual competition for publishers, writers, and designers who create print, Web, electronic, and social media.

“The twenty-seventh annual awards program recognized excellence in publications work by professional communicators. APEX Awards are based on excellence in graphic design, editorial content and the ability to achieve overall communications excellence. With close to 1,900 entries, competition was exceptionally intense.” - John De Lellis Editor and Publisher

The meeting and its materials also received high marks from the attendees.

Elena is deployed from NMSU on a special contract with LANSCE and has worked with LANSCE since December 2010. Her work with LANSCE has already resulted in 2011–2014 APEX Awards of Excellence for the 2011, 2012, and 10th LANSCE Schools on Neutron Scattering, as well as the 2010 LANSCE Activity Report.

Elena has received past APEX Awards for her work with NMSU in a variety of categories, such as web design, poster design, and special programs and campaigns such as the American Physical Society Four Corners and Texas Sections joint meeting.

This is Elena's ninth APEX Award of Excellence.

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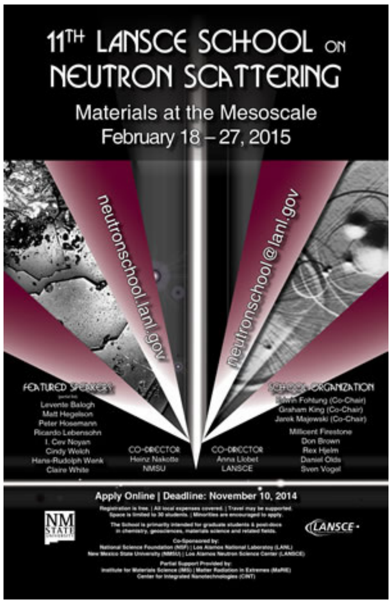


11th LANSCE School on Neutron Scattering promotional poster.

News and Celebrations

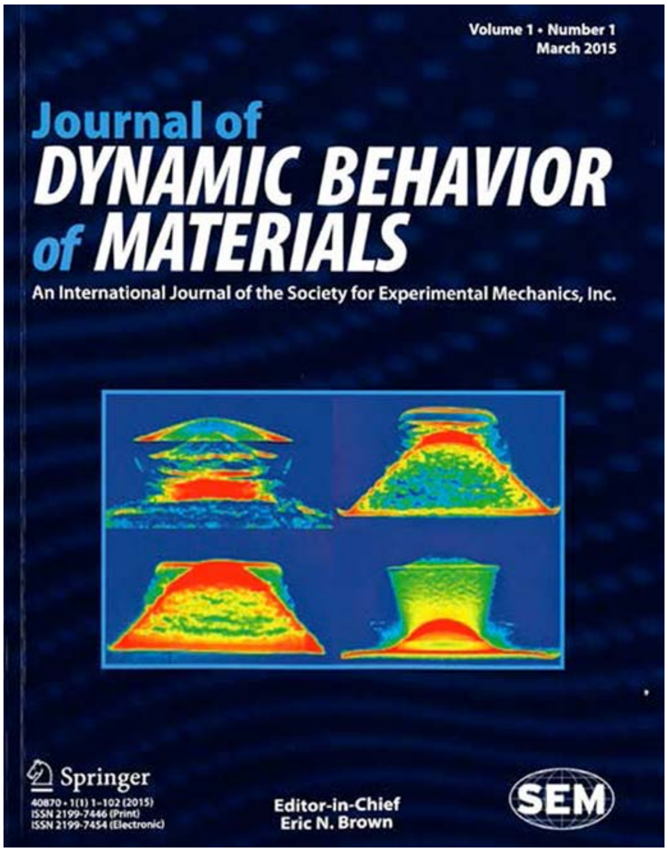
Inaugural issue of *Journal of Dynamic Behavior of Materials* published

The Society for Experimental Mechanics (SEM) and Springer have published the first issue of the *Journal of Dynamic Behavior of Materials*. Current and retired Laboratory researchers have major roles in the journal. E. N. Brown (previously P-23, now M-DO) is editor-in-chief, E. Cerreta (MST-8) and R. S. Hixson (retired from WX Division, now with NSTec LLC) serve as associate technical editors, and D. Dattelbaum (previously M-9, now Campaign 2 Program Manager) serves on the international advisory board. Eric has worked closely with SEM and its board of directors and staff over the past two years to launch the new journal.

The peer-reviewed archival journal focuses on the response of materials to dynamic loading, particularly in cases that involve extreme conditions, such as high strain rate, impact, blast, penetration, and shock response. Over the past decade there has been a dramatic increase in research on the science and engineering of the dynamic behavior of materials. The journal was created to give the community a scientific outlet focused on both materials science/engineering and dynamic-loading aspects of such work. The journal publishes experimental, theoretical, modeling and simulation, and interdisciplinary papers. The content also includes articles regarding the development of new methods, diagnostics, and techniques to study the dynamic response of materials.

The cover of the first issue of the *Journal of Dynamic Behavior of Materials* features a series of proton radiographs of disks taken at LANSCE's pRad facility. The images reveal the internal structure of explosively shocked aluminum, copper, tantalum, and tin. The Laboratory is an international center of excellence for research in the field of dynamic behavior of materials and materials in extremes.

Articles can be submitted at the following website: www.editorialmanager.com/jdbm/. The *Journal of Dynamic Behavior of Materials* web page: www.springer.com/materials/special+types/journal/40870



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Eric N. Brown

SEM

The journal's cover image depicts a series of proton radiographs of disks (left to right, top to bottom) of 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, and the tin sample displays characteristics of melting.

Image courtesy of D. Holtkamp and the pRad Team.

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This is the fourteenth report in this series.

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