Los Alamos Neutron Science Center

Activity Report 2011

Los Alamos
NATIONAL LABORATORY
EST. 1943

About the Cover

LANSCE's Science Spans the Globe

LANSCE's science and outreach span the globe. What we accomplish locally affects neutron science, and beyond, globally.

LANSCE is not only neutron science in all its diversity; LANSCE's people, in all our diversity, work together for a common goal in supporting and producing the world's greatest science.

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LANSCE Activity Report 2011

LANSCE: Supporting basic and applied research for national defense and civilian applications.

Abstract

The "LANSCE Activity Report 2011" describes scientific and technological progress and achievements at LANSCE during CY11. This report includes LANSCE research highlights, accelerator operations highlights, and user program accomplishments.

This report is available online at lansce.lanl.gov.

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Foreward

Welcome to the 2011 LANSCE Activity Report, where you will find facilities improvements and science highlights—all made possible by a coordinated effort involving technicians, instrument scientists, the user community, and administrators. Achievements of note are the record isotope production in support of cardiac care and the beam reliability to all facilities, which averaged above 85%: great team work focusing on science and user program deliverables.

From the radiofrequency system upgrades to instrumentation, control, and diagnostics, the LANSCE-LINAC Risk Mitigation project made great progress. The first klystron was received and tested on site here at LANSCE.

In honor of Louis Rosen and his contributions to science, the Rosenfest Lectures (Rosenfest 2011) were held at the historic Fuller Lodge in Los Alamos (May 18–20, 2011). Rosenfest 2011 covered Louis's early life, career, and influence at LANL. During the event we announced the creation of the LANSCE Rosen Scholar Fellowship, which is aimed at attracting visiting scholars to LANSCE in the fields of nuclear science, materials science, defense science, or accelerator technology.

In December, the LANSCE User Group (LUG) officially named June Matthews as the LUG Executive Committee Chair for 2012. June is a Professor of Nuclear Physics at MIT, has worked with LAMPF and LANSCE-WNR since 1996, and has been a member of the LUG EC since 2010.

Also, 2011 will be remembered as the year of the Las Conchas Fire. The fire burned 156,593 acres, which made it one of the largest fires in New Mexico history. LANSCE was essentially unharmed by the Las Conchas Fire, which burned near Los Alamos and on an outlying portion of LANL property. The town of Los Alamos was evacuated for a week, and LANL (including LANSCE) was on standdown for almost 2 weeks. Thanks to the hard work and dedication of many, LANSCE facilities were back in operation shortly thereafter.

Finally, 2011 was another successful year for LANSCE, as well as an intense, productive, and busy year for all of the five LANSCE facilities. The User Program continues to grow strong, with a record number of proposals received for the first FY11 call.

We hope you enjoy reading this report as much as we did preparing it.

Alex H. Lacerda
Deputy Director, LANSCE

Kurt F. Schoenberg
Director, LANSCE

Contents

Los Alamos National Laboratory (LANL)

Established in 1943, Los Alamos National Laboratory is a premier national security research institution, delivering scientific and engineering solutions for the nation's most crucial and complex problems. Our primary responsibility is ensuring the safety, security, and reliability of the nation's nuclear deterrent.

The LANL of today emphasizes worker safety, effective operational safeguards & security, and environmental stewardship, while outstanding science remains the foundation of the Laboratory.

In addition to supporting LANL's core national security mission, our work advances bioscience, chemistry, computer science, earth and environmental sciences, materials science, and physics disciplines.

LANL personnel play leading roles worldwide in basic and applied scientific research and technology. Whether it's conducting crucial experiments in space and at our linear accelerator in Northern New Mexico or developing breakthroughs in nanotechnology and determining how best to prevent the spread of HIV and avian flu, the men and women of LANL help lead the way.

From the proliferation of nuclear weapons, the spread of deadly diseases, inadequate supplies of energy, to the effects of climate change—LANL research and development helps curb a wide variety of threats to US interests.

Los Alamos Neutron Science Center (LANSCE)

Today, five state-of-the-art facilities operate simultaneously at LANSCE, contributing to national security, nuclear medicine, materials science and nanotechnology, biomedical research, electronics testing, fundamental physics, and many other areas. For 8 months of the year, while the accelerator is operational, scientists from around the world work at LANSCE to execute an extraordinarily broad program of defense and civilian research.

LANSCE is one of the major experimental science facilities at LANL, underpinning the Laboratory as a world-class scientific institution.

The core of LANSCE's facility is one of the nation's most powerful proton linear accelerators or LINAC. The 800-mega-electron-volt (800 MeV) LINAC provides beam current, simultaneously, with unique capabilities to its five major facilities.

The LINAC's capability to reliably deliver beam current is the key to the LANSCE's ability to do research–thus the key to meeting NNSA and DOE mission deliverables as well as providing the scientific community with intense sources of neutrons that can perform experiments supporting civilian and national security research.

LANSCE also provides solutions to national security problems. It serves a wide range of applications that helps the nation maintain its leadership role in many areas of science and technology. Research conducted at LANSCE helps to maintain the nation's nuclear deterrent, counter the spread of weapons of mass destruction, and lay the foundation for many of the products we use in our daily lives by supporting materials sciences and technology.

Isotope Production Facility (IPF)

Los Alamos National Laboratory produces radioactive isotopes for medical, environmental, industrial and research applications. The Isotope Production Facility (IPF) at LANSCE supplies a wide range of radioisotopes to researchers all over the world and has been a leader in developing and producing new and unique isotopes for research and development.

Lujan Neutron Scattering Center (Lujan Center)

The Lujan Neutron Scattering Center (Lujan Center) uses a pulsed spallation neutron source equipped with time-of-flight spectrometers for neutron scattering studies. Neutron scattering is a powerful technique for probing microscopic structure and dynamics and is used in materials science, engineering, condensed matter physics, chemistry, biology, and geology.

Proton Radiography Facility (pRad)

The Proton Radiography Facility (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.

Ultracold Neutrons Facility (UCN)

Researchers working at LANSCE and eight other member institutions of an international collaboration are constructing the most intense source of ultracold neutrons in the world, measuring ultracold neutron production in their new source 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 (WNR)

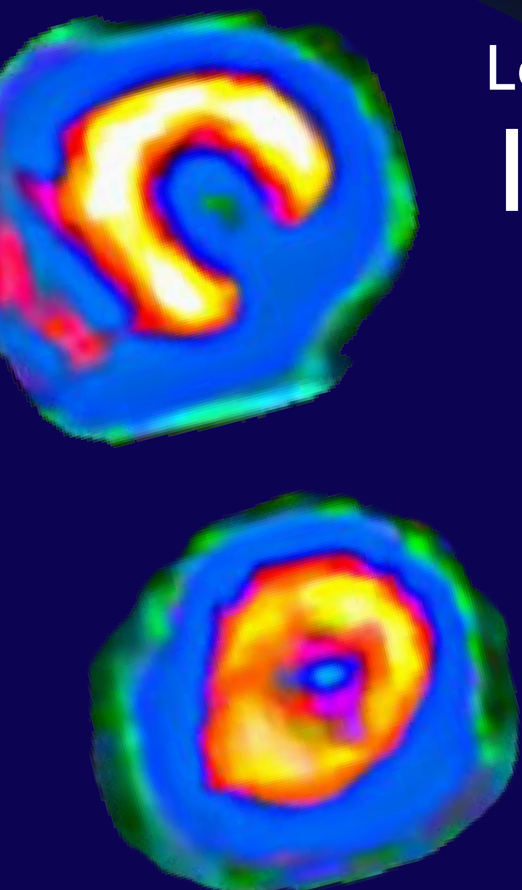
The Weapons Neutron Research Facility (WNR) provides neutron and proton beams for basic, applied, and defense-related research. Neutron beams with energies ranging from approximately 0.1 MeV to more than 600 MeV are produced in Target 4 (an unmoderated tungsten spallation source) using the 800-MeV proton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

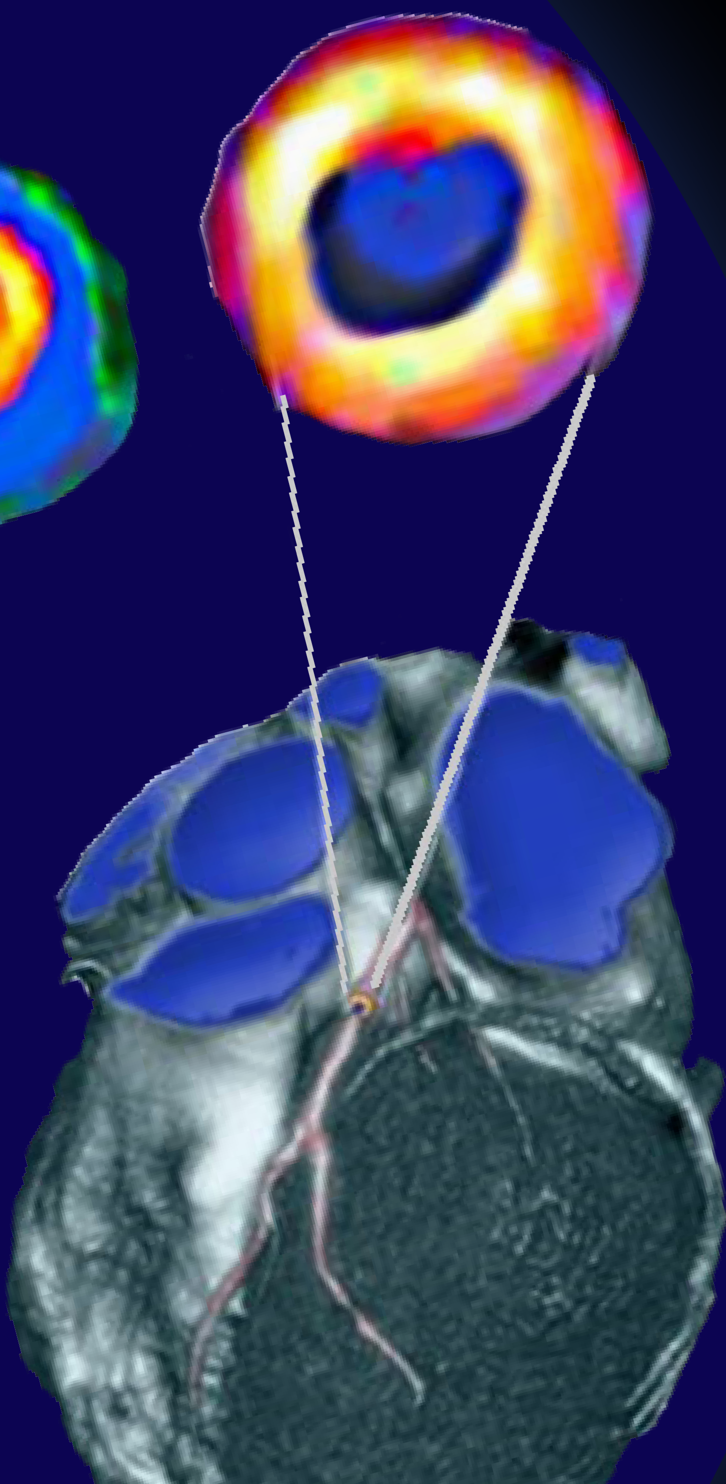
User Program

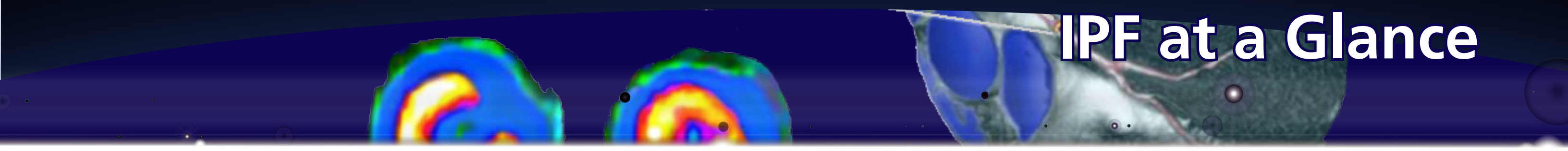
LANSCE's User Program enables the cutting edge of nuclear and materials science and technology. The User Program plays a key role in training the next generation of top scientists, attracting the best graduate students, postdoctoral researchers, and early-career scientists.

Los Alamos Neutron Science Center

Isotope Production Facility 2011

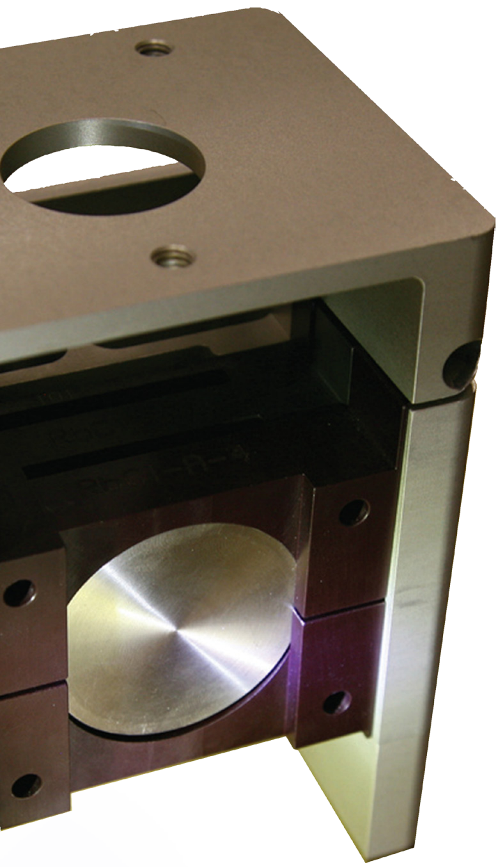




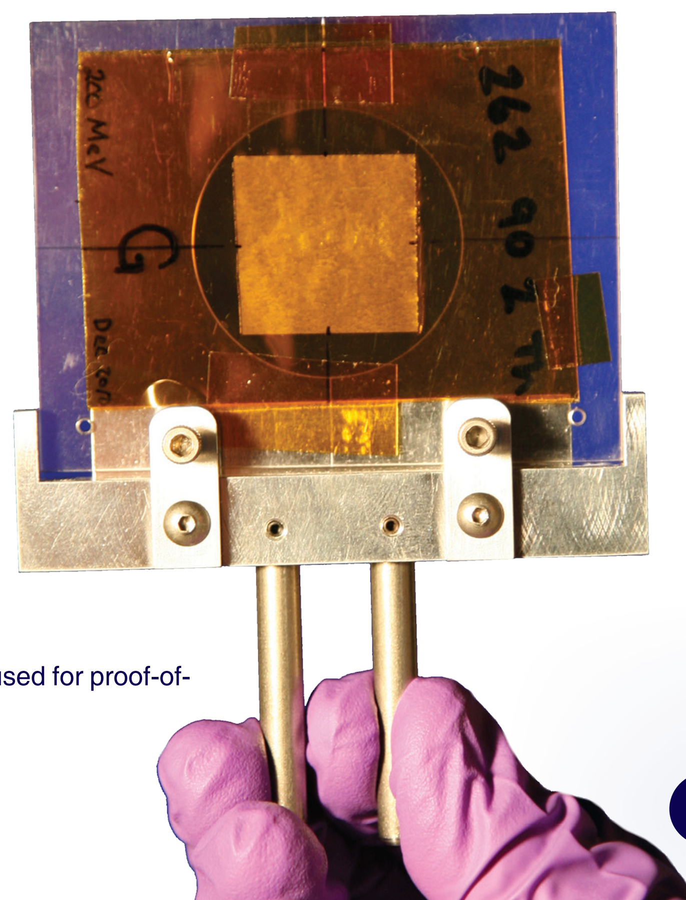


Isotope Production and Applications

A hot cell manipulator grips a target delivered from the IPF at LANSCE. After the proton beam strikes the target, scoring appears on the disc's center.



A target assembly loaded with discs is lowered 40 feet below the IPF for exposure to the proton beam. There, stable isotopes are converted to radioactive isotopes.



A thorium foil test target is used for proof-of-concept ^{225}Ac production.

The Making of a Radioisotope

For more than 20 years, LANL and Brookhaven National Laboratories have pioneered the production and supported the development of the clinical applications of two isotopes: strontium-82 (^{82}Sr) and germanium-68 (^{68}Ge).

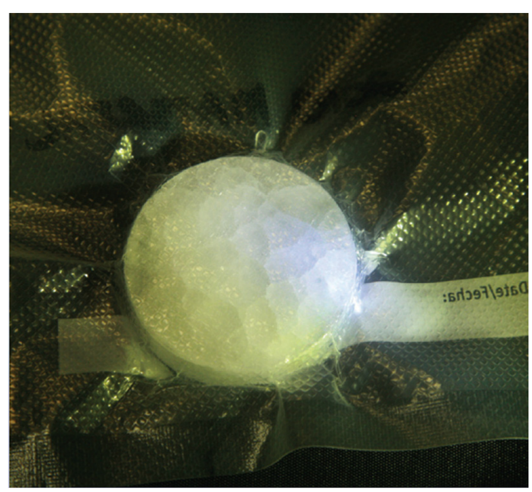
Today, the IPF supplies ^{82}Sr to companies in North America and Europe for the rubidium-82 (^{82}Rb) generator, which produces a radioactive drug on demand. Hospitals and medical laboratories purchase the generators to support cardiac imaging through positron emission tomography (PET). The LANL isotope program also manufactures silicon-32 (^{32}Si), which oceanographic researchers use to study the silicon cycle of marine organisms.

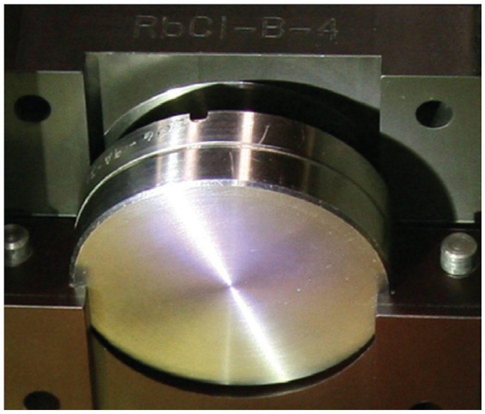
The DOE's Medical Radioisotope Program developed the generator technology during the 1970s and 1980s, and the technology was transferred to private industry in the late 1980s. The DOE isotope program continues to be one of the main suppliers of the ^{82}Sr for the generators.

Responding to the DOE's call for more ^{82}Sr, the Laboratory accelerated its overall production of the isotope by 350% in the past 5 years. With a team of 20, "I think that's a heck of an accomplishment," said Kevin John, who manages the LANL Isotope Production and Applications Program.

Excerpt from AOT and LANSCE - The Pulse, August 2011. LALP-11-017

1 Preparing the target: The process starts with a stable isotope. Rubidium-chloride granules (above), which look like salt, are melted and cast into a solid round shape. The raw material is sealed inside two metal lids, forming a puck-shaped target (below). Getting the production target qualified, with a certificate of analysis, takes several months.

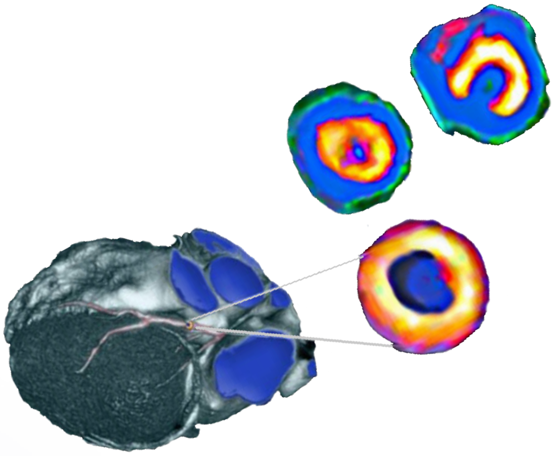




❷ Radiation: Three targets are horizontally stacked in a holder. Forty feet beneath the earth at the IPF, a beam irradiates the targets for 7-14 days. As protons from the LANSCE accelerator slam into the nuclei of the target's atoms, a stable bit of matter (Rb) is transformed into a radioactive substance (^{82}Sr).

❸ Purification: The cooled, irradiated targets are trucked in an 8,600-pound lead-shielded container the size of a small refrigerator to the hot cell facility, where the isotopes undergo a process of chemical separation and purification over three days. A crane lifts the container into the "warm corridor" that runs between two rows of hot cells. Only in these heavily shielded rooms with doors on the back and windows on the front can workers using telemanipulators safely view and handle the targets.

❹ Pharmaceutical delivery: Shipments vary based on the type of isotope and customer requirements, but in most cases the product is loaded into a sealed vial and placed in a heavy lead shield for transport. Customers will use the isotopes produced at IPF for generator technology. In a generator, the parent isotope is immobilized on a solid support and the daughter isotope is available on demand for imaging and therapy procedures. The customer, in turn, supplies the radionuclide generator to hospitals and imaging centers for clinical application.



❺ Patient impact: Inside the generator, long-lived ^{82}Sr converts to short-lived ^{82}Rb through radioactive decay. The Rb is eluted from the generator for PET scans. A patient's heart muscle absorbs the ^{82}Rb. The Rb decays by emitting positrons, which combine with electrons to produce gamma rays that are detected by the scanner. Cardiologists interpret that information to determine the condition of the patient's heart.

Record Isotope Production Supports US Cardiac Care

The LANL Isotope Program, through IPF at LANSCE and the hot cell processing facilities at the TA-48 radiochemistry complex (Inorganic, Isotope and Actinide Chemistry, C-IIAC), has a long history of supplying medical radioisotopes to the US healthcare industry for cardiac imaging and the calibration of medical devices that are critical to domestic healthcare. In recent years, the Isotope Program has been called to produce additional large amounts of the cardiac imaging isotope strontium-82 (^{82}Sr) used for cardiac imaging via PET at hospitals nationwide. Demand for this particular isotope is increasing because of the current shortage of molybdenum (Mo) used in single photon emission tomography (SPET) cardiac scans.

In mid-2009, the Lab generated what was then a record for the production of ^{82}Sr, shipped from LANL in the LANSCE FY2009 run cycle. Production in FY2010 increased by approximately 10% for ^{82}Sr product shipped from LANL – establishing an overall 350% production growth since 2005. In the current FY2011 run cycle, production of ^{82}Sr is occurring at over two times the rate of the 2010 production cycle. This increase is being achieved in part by operating IPF in dedicated mode for the month of January, in response to DOE's Office of Science - Nuclear Physics request that LANSCE and IPF postpone their scheduled shutdown and dedicate an additional 25 days of operation to produce the critical isotope. The radiochemistry team processed the material in the hot cell facility at TA-48, RC-1, and then sent the ^{82}Sr to customers for distribution.

IPF is one of only five production facilities worldwide capable of supplying the ^{82}Sr demand. Facilities such as the IPF, Brookhaven National Laboratory in New York, Institute of Nuclear Research in Russia, and iThemba in South Africa coordinate their production run cycles to optimize the ^{82}Sr supply. However, medical needs, the short half-life (25 days), and the ongoing ^{99}Mo shortage threaten a crisis in ^{82}Sr supply. Finding creative ways to produce additional ^{82}Sr could help defer this crisis. In principle, IPF could operate at higher beam currents to generate more ^{82}Sr, but present target materials cannot reliably withstand higher beam currents. The Isotope Program staff is developing new methods for target analysis and is engaging LANL experts in materials science and engineering to develop new production targets suitable for higher beam currents.

In addition to producing the present portfolio of isotopes, IPF enables research in the production of new isotopes, including actinium-225 (^{225}Ac), which provides unique and revolutionary cancer treatment opportunities. Ensuring a stable supply of these isotopes for medical research and clinical trials, while at the same time supplying record-breaking amounts of ^{82}Sr, requires unprecedented run-time reliability of both the LANSCE accelerator IPF, close coordination with upcoming LANSCE risk mitigation activities, and improved methods and apparatus for processing at LANL hot cell facilities. Kevin John is the LANL Program Manager, and Wolfgang Runde is the National Isotopes Program Manager. This work supports the Laboratory's Materials for the Future and the Science of Signatures capabilities.

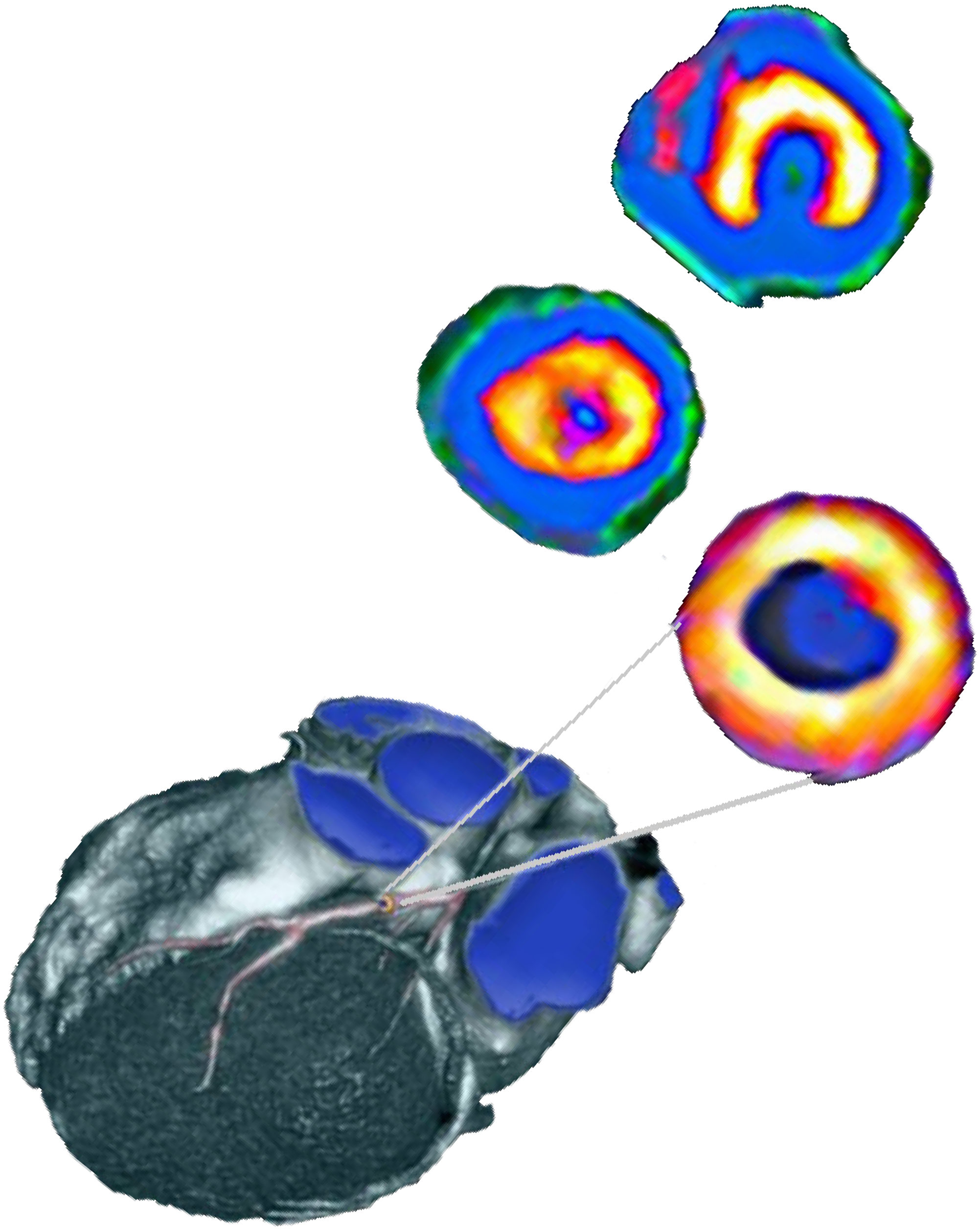


Image of a heart during a normal rest-stress myocardial perfusion PET study. Isotopes produced at IPF are critical for medical diagnosis and disease treatment. These positron emission tomography images were made possible using ^{82}Sr. Production of this critical isotope impacts approximately 23,000 domestic cardiac patients every month.

Keeping Ahead of Radiation Damage at IPF's Beam Window

IPF at LANSCE has a long history of isotope production for applications in medicine, industry, homeland defense, and weapons research. The IPF extracts the 100-MeV proton beam from the LANSCE accelerator and delivers it to isotope production targets inside a target chamber, which is a heavily shielded concrete and steel structure located in the IPF beam tunnel. The beam transport pipe ends with an Inconel 718 beam window that separates the beam pipe from the target chamber. This beam window is the sole separation between the high-vacuum beam line and the cooling water in the target chamber. Window failure would let cooling water (activated and contaminated) flood into the beam line, which would damage equipment and severely impact or even halt isotope production operations.

The beam window is subjected to stress by multiple factors, including the differential pressure across the beam window, thermal volume heating by energy deposition from the 100-MeV proton beam, and radiation damage. Under irradiation conditions, significant microstructural alterations are expected to occur because of atomic displacements induced by proton (primary) and neutron (secondary) irradiation. Defect structures, such as dislocation and vacancy loops, vacancy clusters, voids, and helium and hydrogen bubbles, form as a function of temperature of operation and proton and neutron fluencies that are quantified by displacement per atom (DPA). These cumulative factors may change the material properties of the window, causing it to become less ductile and more prone to failure in use. Since IPF started up in 2004, the beam window has accumulated approximately 20 DPAs based on Monte Carlo radiation transport MCNPX calculations, and by 2010 it had reached its estimated lifetime based on its design threshold limit. The beam window was replaced in March 2010 as part of the IPF preventive maintenance program. The window was placed in a shielded cask at TA-53 for several months to cool, and then the entire beam transport pipe (including the window at the end) was transferred in its shielded cask to the CMR Wing 9 hot cell facility in November 2010. Every activity required careful planning and coordination with experts from multiple LANL organizations.

Window analysis is now underway. Because no published data on the irradiation damage of Inconel 718 at 20 DPAs exist, this beam window presents a unique opportunity to understand how the beam window degrades under extreme irradiation conditions with a high-power proton beam. Examination will help scientists establish parameters for a failure mode and better inform replacement decisions. It will also provide insight into the development of new window materials with a longer operational lifetime. Because some of the factors listed above, as well as multiple additional factors, contribute to damage and occasional failure of target shells within the target chamber itself, study of the beam window will inform ongoing research in target shell design.

The window presents the research challenge of being literally "too hot to handle." The estimated dose rate from all gamma emitter isotopes produced inside the beam window was 100 R/h at 1 foot. A team comprising Inorganic, Isotope, and Actinide Chemistry (C-IIAC) Wing 9 hot cells and isotopes staff; Radiation Protection Operations (RP-1) radiation control technicians; Nuclear Materials Science (MST-16) scientists; and Waste Generator Services (WES-WGS) planned how to use the remote handling tools in the hot cells to remove the IPF beam pipe assembly from its shipping cask and cut the pipe into sections for analysis and characterization.

The activity was successfully executed on March 2. The unique capability of the machining, mechanical testing, and metallographic tools in the Wing 9 hot cells will be used to characterize the beam window. The team has found that in addition to the high dose rate expected for the Inconel window, the beam pipe itself and the graphite collimator within the pipe are showing unexpectedly high dose rates. Once the causes for these high dose rates are understood, they may suggest changes in the design of future window assemblies.

Meanwhile, the remaining pipe sections are being cut and segregated according to their dose rates, which will minimize the cost of disposal. The DOE Office of Science / Nuclear Physics supports the work. Kevin John is the LANL program manager.

(Left): A side view, taken through the 3-foot-thick lead-glass shielding window of the hot cell, of the end of the pipe containing the actual beam window.
(Right): The beam window itself with a ring-shaped proton beam pattern. The diagonal stripe is fixative remaining on the window that had been applied to control contamination during its removal.

Los Alamos Neutron Science Center

Lujan Neutron Scattering Center 2011

LANSCE
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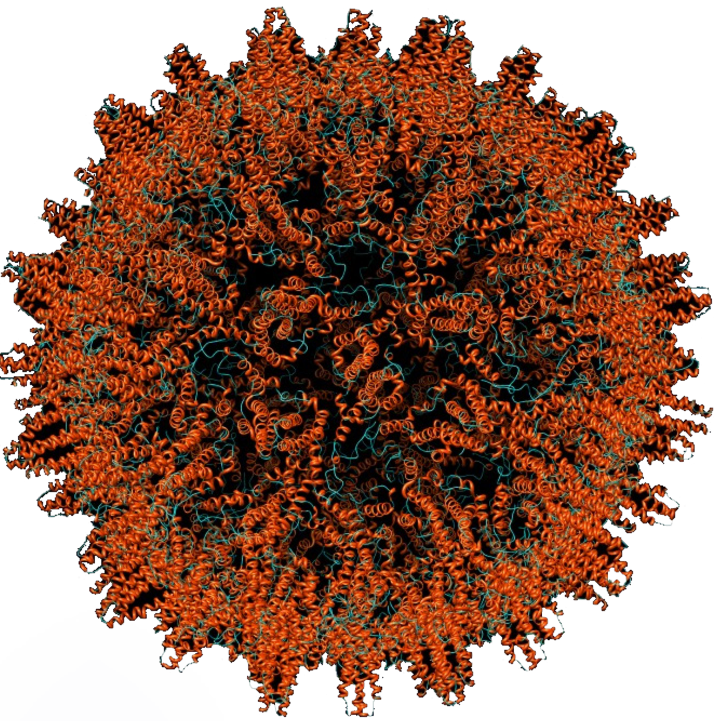
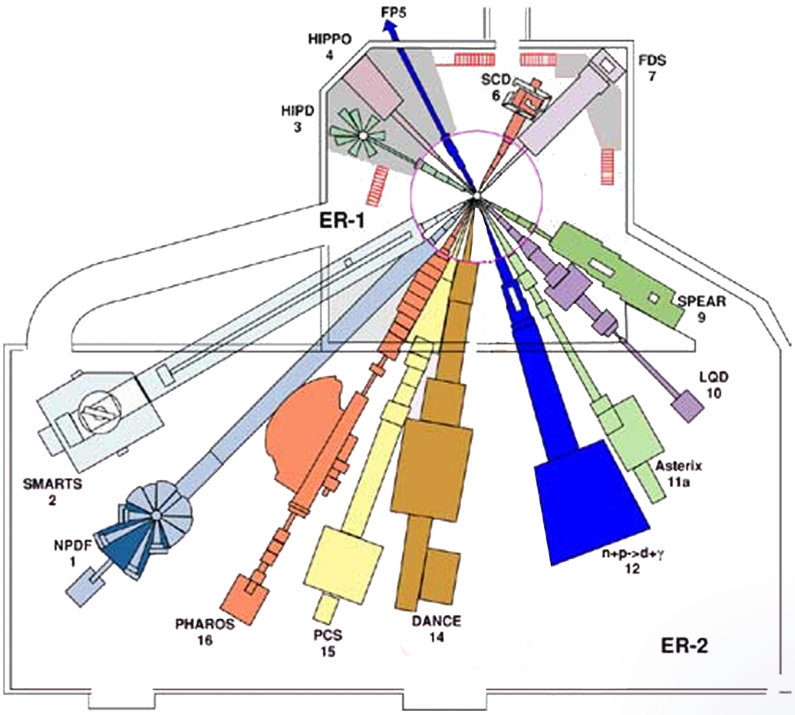
Instrumentation and Applications



Capsid structure of human hepatitis B virus derived from x-ray diffraction. The structure of the capsid, the distribution of DNA, and the distribution of a flexible protein segment of the capsid protein that directs the distribution of DNA in the mature nucleocapsid are being studied using the Lujan Center small-angle instrument Low-Q Diffractomert (LQD).

The Protrein Crystallography Station (PCS) is a high-performance beam line that forms the core of a capability for joint neutron and x-ray macromolecular stucture and functions determination. The beam-line exploits the pulsed nature of spallation neutrons and a large electronic detector in order to efficiently collect wavelength resolvesd Laue patterns using all available neturon in the white beam (0.7 - 7 Å wavelength band).



Lujan Center Experimental Hall flight paths. Most of the flight paths at the Lujan Center are equipped with spectrometers for determining the atomic, molecular, and magnetic structures, as well as the vibrational and magnetic excitations of materials.

Neutron Total Scattering Monitors Shifts in Valence States

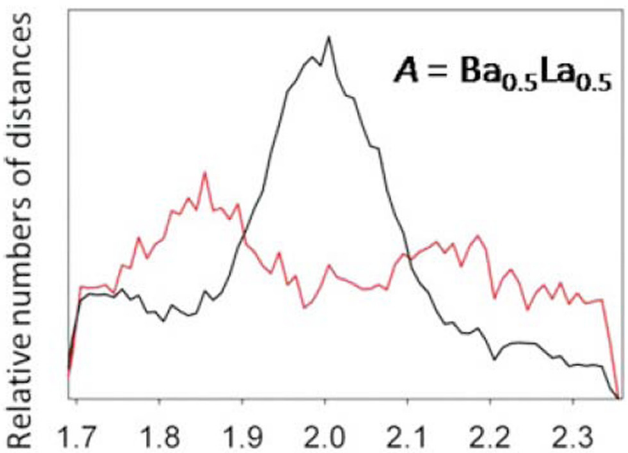
The interplay among electronic, lattice, and magnetic degrees of freedom is at the origin of the broad variety of emergent phenomena exhibited by mixed metal oxides. Perovskites are a type of ionic crystal structure with the general formula ABX_3, where A is a tetravalent cation, B is a heptavalent cation, and X is an anion—usually oxygen, as in $NaNbO_3$ and $BaTiO_3$. Many of these compounds are ferroelectric. The group also includes some superconductors, semiconductors, and compounds that display magnetic ordering. Perovskite compounds containing Manganese (Mn) or ruthenium (Ru) are among the most interesting of these systems because they possess many properties of technological importance, such as colossal magnetoresistance, multiferroic behavior, itinerant electron ferromagnetism, and superconductivity in closely related Ruddlesden Popper phases. (Ruddlesden-Popper phases are layered perovskites with the general formula $AO(ABO_3)n$.) The physical properties of perovskites, which contain both Mn and Ru, are primarily governed by the oxidation states of the Mn and Ru cations. These cations often exist in a state of mixed valency. The properties of these materials can be tuned by controlling the ratio of Mn to Ru and by manipulating the charge and/or size of the cations on the A site.

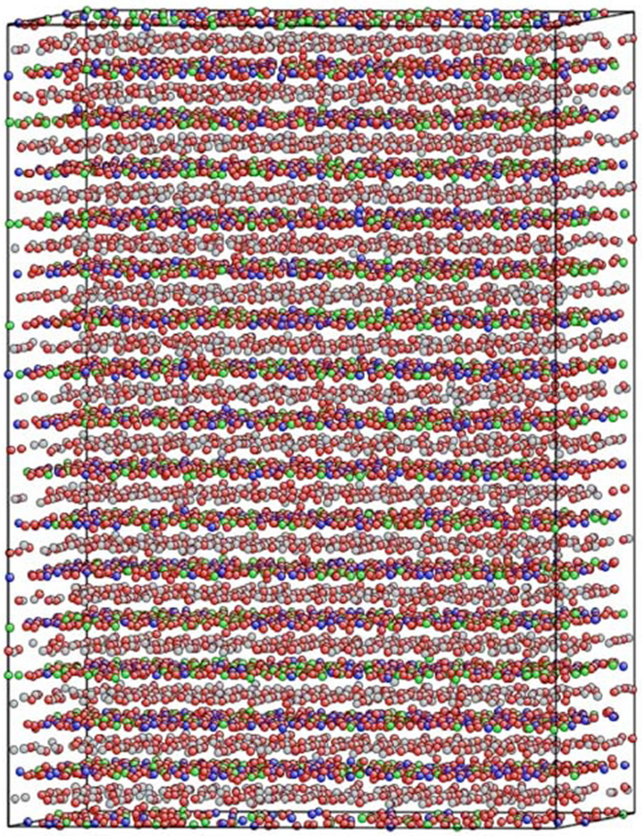
Lujan Center scientists Graham King and Anna Llobet and collaborators at Ohio State University used neutron scattering to monitor a shift in electron density between Mn and Ru cations in a series of $AMn_{0.5}Ru_{0.5}O_3$ perovskite compounds. In these compounds, the oxidation state of the Mn ions can vary between +3 and +4, and the oxidation state of the Ru ions can vary between +4 and +5. Because the Mn and Ru atoms are randomly distributed over the same crystallographic site, standard structure determination methods cannot distinguish between the coordination environments of the two atoms. The researchers used reverse Monte Carlo simulations, which involve large supercells containing approximately 10_4 atoms, to model the pair distribution functions of these materials. By modeling the distributions of Mn-O and Ru-O bond distances, the scientists showed that the relative concentrations of the various oxidation states of Mn and Ru depend on the size of the *A*-cation and that there is a shift in the B-site cation charge distribution from nearly equal amounts of Mn^{3+}, Ru^{5+}, Mn^{4+}, and Ru^{4+} for $SrMn_{0.5}Ru_{0.5}O_3$ to primarily Mn^{4+} and Ru^{4+} for $CaMn_{0.5}Ru_{0.5}O_3$. When smaller *A*-cations are used, the compounds reduce their concentrations of Mn^{3+} by shifting some of their electron density onto Ru. This study also found that the *A*-site cations lie closer to the Mn ions than to the Ru ions; this asymmetry appears to be correlated to the degree of octahedral tilting.

Reference: "Linking Local Structure and Properties in Perovskites Containing Equal Concentrations of Manganese and Ruthenium," by Graham King, Rebecca A. Ricciardo, Jennifer R. Soliz, Patrick M. Woodward, and Anna Llobet, *Physical Review B* 83, 134123 (2011); doi:10.1103/PhysRevB.83.134123.

This work benefited from the use of the High-Intensity Powder Diffractometer (HIPD) at the Lujan Center and the Advanced Photon Source at Argonne National Laboratory, which the DOE, Office of Science, supports. The work supports the Laboratory's Energy Security mission area and the Materials of the Future capability.

AOT and LANSCE - The Pulse, October 2011.
LALP-11-017





(Left): Distribution of Mn-O (red) and Ru-O (black) bond lengths in $BaLaMnRuO_6$.
(Right): Reverse Monte Carlo supercell of $Sr2MnRuO_6$, which contains 10,240 atoms.

First Neutron Data Collection from a Glycosyltransferase

Scientists from the University of Victoria (Canada) and LANL used the Lujan Center's Protein Crystallography Center to collect the first-ever neutron diffraction data of a glycosyltransferase (GT). GTs are extremely diverse and widespread enzymes that build complex carbohydrates. In humans, GTs are involved in many diseases, from viral to bacterial infections, to several types of cancer, and even in various genetic disorders, such as congenital muscular dystrophy. GTs catalyze the formation of glycosidic bonds through the transfer of a single sugar from a donor molecule to an acceptor for the biosynthesis of oligosaccharides and glycoconjugates. The stereochemistry around the anomeric carbon can be either inverted or retained. The mechanism for the "retained" stereospecificity as catalyzed by GT has not yet been resolved.

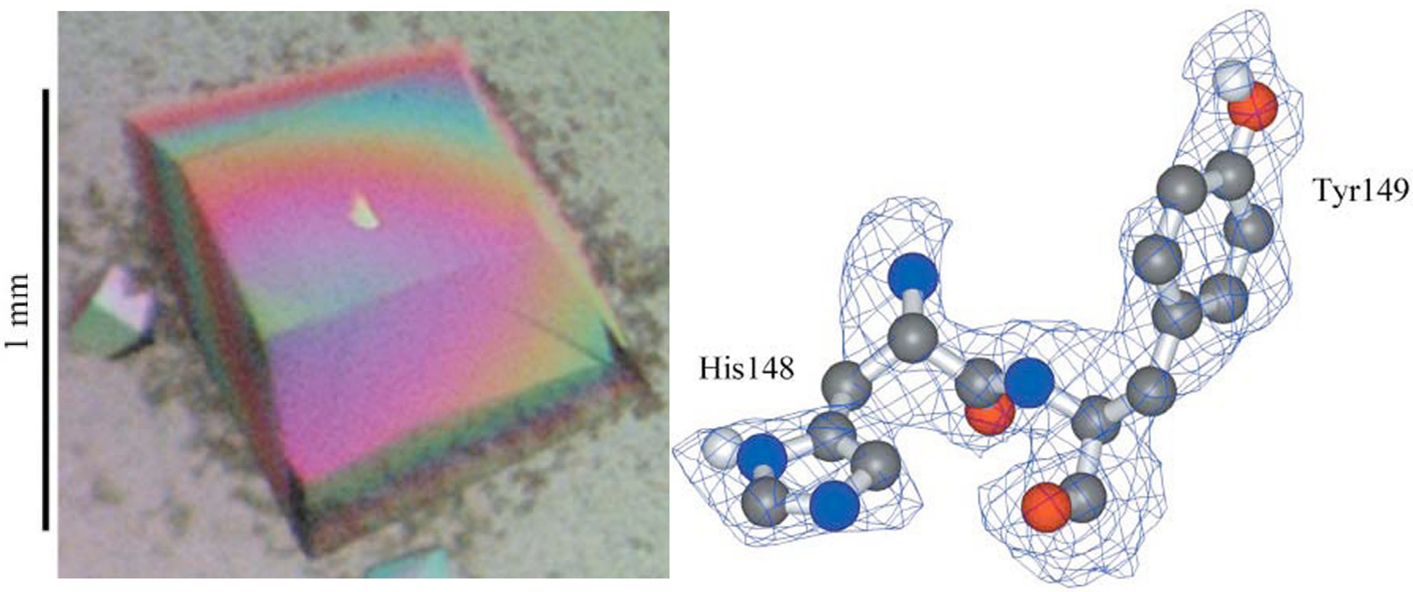
Knowledge of the fundamental structure-function relationships of GT enzymes is essential to determine the mechanisms of substrate recognition and catalysis. Evaluation of hydrogen bonding partners and amino-acid protonation states is critical for understanding the catalytic mechanisms of all retaining GTs. An understanding of these mechanisms can be used to develop biomedically therapeutic glycoconjugates and inhibitor drugs to treat diseases and genetic disorders. However, traditional structure-function studies with x-ray crystallographic techniques are limited because they cannot routinely reveal the protons and hydrogen bonds that mediate substrate recognition and binding in the active sites of these enzymes.

To overcome this issue and directly visualize hydrogen atoms in the active site of human GTA, researchers Steve Evans and Svetlana Borisova (University of Victoria) came to LANL to investigate the neutron structure of GTA. A detailed neutron structure of GTA will reveal many important aspects of catalysis, such as the role of protein residues involved in catalysis. Currently, there are two proposed mechanisms for how GTA works. Neutron studies of GTA will be instrumental in the investigation of which mechanism is more likely to be used by the enzyme and will pave the way for rational drug design. The diffraction data collected at the Protein Crystallography Center are a crucial first step in this process.

LANL scientists included S.Z. Fisher, A. Kovalevsky, and P. Langan (Bioenergy and Environmental Science, B-8). Collaborators from Oak Ridge National Laboratory and the Carlsberg Laboratory, Denmark, also participated in the research.

Reference: "Preliminary Joint Neutron Time-of-Flight and X-Ray Crystallographic Study of Human ABO(H) Blood Group A Glycosyltransferase," *Acta Crystallographica* **F67**, 258 (2011). doi:10.1107/S17443091 10051298.

The DOE Office of Biological and Environmental Research supports the Protein Crystallography Station, and Langan received partial support from the National Institute of General Medical Science.



(Left): Optical photograph of a large, single crystal of GTA.
(Right): Initial filled neutron maps of deuterium-exchanged residues after a single round of refinement showing the protonation of His148 and Tyr149.

Surprises from a "Hot" Metal

Strontium metal oxides exhibit a diverse range of electronic and magnetic properties. Strontium molybdate ($SrMoO_3$) is paramagnetic and has one of the highest conductivities of the metal oxides, while strontium ruthenate ($SrRuO_3$) is a metallic ferromagnet with a transition temperature around 160 K. Between molybdenum and ruthenium in the periodic table lies technetium (Tc). Strontium oxides based on this element should also exhibit interesting properties, but the absence of a stable Tc isotope has hampered the study of materials based on this fourth-row transition-metal element. To understand the solid-state chemistry and behavior of this largely unexplored element, scientists from The Lujan Center and collaborators have synthesized and characterized a series of new compounds containing Tc.

The researchers report the first comprehensive magnetic study of $SrTcO_3$, a compound that differs greatly from its Sr metal oxide cousins. Their results, featured in a *Physical Review Letters* Editor's Choice paper, reports the synthesis and characterization of $SrTcO_3$. Although it has a similar structure to $SrMoO_3$ and $SrRuO_3$, $SrTcO_3$ stands out both because it is antiferromagnetic and because it has the highest antiferromagnetic ordering temperature (roughly 1000 K) obtained in a material without a third-row transition metal. The scientists conclude that the comparatively greater hybridization that occurs between technetium and oxygen, the smaller energy splitting between the electronic orbitals on the Tc cation, and the suppression of competing antiferromagnetic states account for the higher-ordering temperature they observe for $SrTcO_3$.

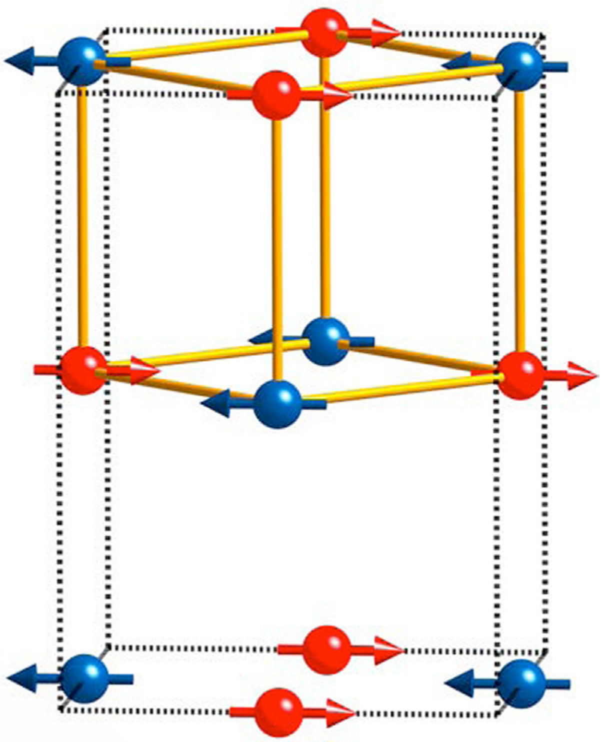
The team used a large set of scientific techniques, including neutron diffraction, synchrotron x-ray diffraction, and electronic structure calculations, to examine $SrTcO_3$.

The researchers found that $SrTcO_3$ adopts a distorted perovskite structure with *G*-type antiferromagnetic ordering (all magnetic moments are antiferromagnetically coupled with respect to their nearest neighbors). The magnetic order persists up to an extraordinarily high Néel point, approximately 1000 K. Electronic structure calculations revealed extensive mixing between the Tc 4d states and oxygen states proximal to the Fermi level, which leads to a close relationship between magnetic ordering temperature and moment formation in $SrTcO_3$. These new findings add to previous publications as part of Efrain Rodriguez's [Lujan Center and University of California-Santa Barbara (UCSB)] thesis research at LANL. This research unveiled new families of Tc-based oxides and also established some fundamental properties of ^{99}Tc, such as its neutron scattering length.

Researchers include E.E. Rodriguez and A. Llobet (Lujan Center), F. Poineau (University of Nevada, Las Vegas), B.J. Kennedy (University of Sydney, Australia), M. Avdeev, G.J. Thorogood, and M. L. Carter (Australian Nuclear Science and Technology Organization); R. Seshadri (UCSB); D.J. Singh (Oak Ridge National Laboratory); and A.K. Cheetham (University of Cambridge).

Reference: "High Temperature Magnetic Ordering in the 4d Perovskite SrTcO3," *Physical Review Letters* **106**, 067201 (2011); doi:10.1103/PhysRevLett.106. 067201.

This work benefited from the use of the Neutron Powder Diffractometer (NPDF) and the High-Intensity Powder Diffractometer (HIPD) at the Lujan Center, which the DOE Office of Basic Energy Sciences funds.



(Left): The magnetic structure of $SrTcO_3$, which persists up to the highest temperature for any compound without a 3d metal.
(Right): Efrain Rodriguez performs radiochemistry on new Tc-based compounds at the Lujan Center chemistry laboratory.

Neutron Scattering Examines Dynamic Properties of Biomembranes

Lipid membranes play a critical role in all living systems, including humans. They define the outer boundary of cells, host transmembrane proteins, mediate transport, facilitate intercellular communication, and respond to changes in the surrounding environment. Because they participate in a multitude of tasks, lipid membranes are necessarily complex. Various experimental techniques have been used for the physical and chemical characterization of biomembranes. The sensitivity of neutrons to the light elements, carbon and hydrogen, makes neutron scattering one of best methods to study biomembranes.

In research accepted for publication in *Physical Review Letters*, scientists from the Lujan Center and collaborators from Ruhr-University and University of South Florida made the first successful demonstration that the Distorted Wave Born Approximation (DWBA) can be used to understand both the static and the dynamic structures of the model biomembranes. The researchers used the Surface Profile Analysis Reflectometer (SPEAR) at the Lujan Center for the measurements. SPEAR is a time-of-flight neutron reflectometer that measures chemical density profiles of thin layers (5 - 3000 Å) in a variety of different environments. The instrument uses an unpolarized neutron beam to study solid/solid, solid/liquid, solid/gas, and liquid/gas interfaces.

The scientists analyzed off-specular neutron scattering with DWBA from a thermoresponsive polymer-supported single 1,2-dipalmitoyl-sn-glycero-3-phosphocholine (DPPC) lipid bilayer in a liquid environment. Only the DWBA accurately models scattering near the total reflection region. The researchers measured interfacial fluctuations of the system and compared the data with theoretical calculations. Analysis of off-specular scattering can provide insight into a wide range of in-plane phenomena in situ to understand complex behavior of cellular membranes, protein transport and docking, lipid segregation into ordered domains, and modification of bulk membrane elastic properties due to membrane constituents and external stimuli. The researchers concluded that this model polymer-membrane system successfully mimics the complexity of cellular membrane morphology and offers opportunities to investigate how membrane composition and various external biological agents (toxins, viruses, and other pathogens) affect in- and out-of-plane membrane structure.

Reference: “In-Plane Correlations in a Polymer-Supported Lipid Membrane Measured by Off-Specular Neutron Scattering,” *Physical Review Letters*. 2011 Apr 1;106(13):138101. Epub 2011.

Researchers include Michael Jablin, Mikhail Zhernenkov, Manish Dubey, Hillary Smith, Alan Hurd, and Jaroslaw Majewski (Lujan Center), B. Toperverg and A. Vidyasagar (Ruhr-University, Germany), and R. Toomey (University of South Florida).

The DOE Office of Basic Energy Sciences funded the LANL researchers and the Lujan Center.

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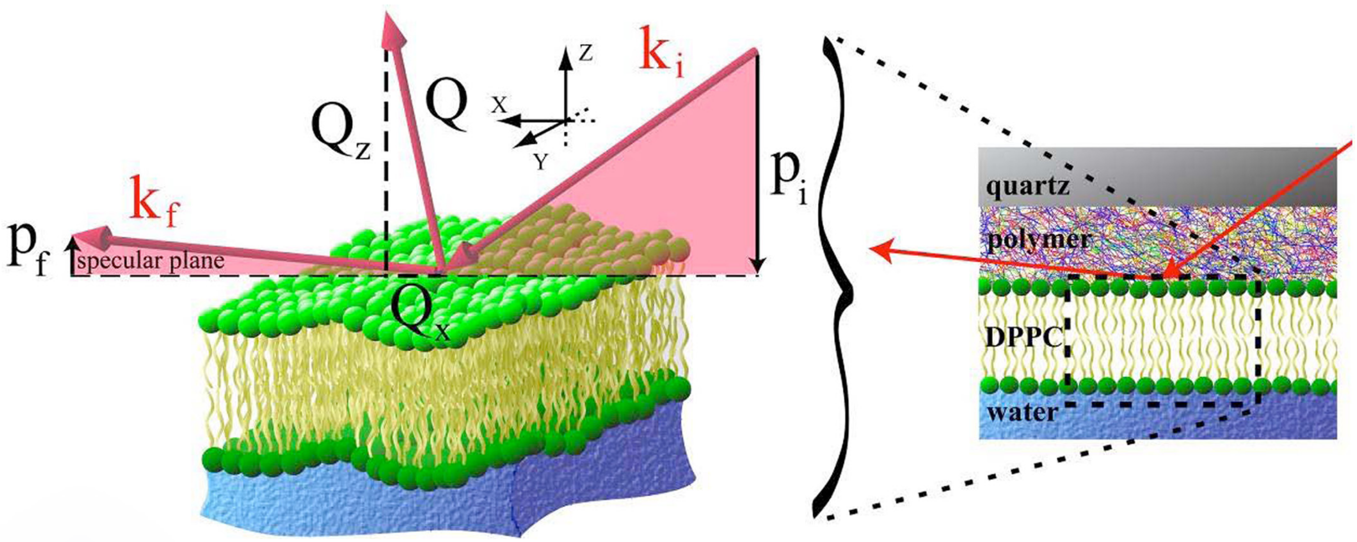
LALP-11-017



Geometry for an off-specular scattering event. The neutrons penetrate through the quartz substrate and polymer cushion to reach the buried membrane (shown on right). If the incident and outgoing angles are unequal, then the momentum transfer vector, Q (the difference of the reflected, kf, and incident, ki, wavevectors), has components perpendicular, Qz, and parallel, Qx, to the scattering interface. Qx probes the in-plane structure.

Cholera Toxin Binding to Model Membranes Reveals Potential Signaling Pathway

Biological membranes are complex, self-organized structures that define boundaries and compartmentalize space in living matter. Composed of a wide variety of lipid and protein molecules, these responsive surfaces mediate transmembrane signaling and material transport within the cell and with its environment. Interactions between proteins and the cell membrane are integral aspects of many biological processes. Diverse protein-lipid complexes exist, including transmembrane proteins, peripheral membrane proteins, and proteins bound to membrane-associated receptor molecules. The interplay between these biological components is multifaceted. Lipids can influence the structure and function of membrane proteins; at the same time, membrane proteins can impact lipid organization. These interactions can have an impact on the intake of toxins into cells.

Lujan Center scientist Jarek Majewski (Lujan Center), in collaboration with Professor Kuhl's group [University of California-Davis (UCSD)], used synchrotron x-ray scattering techniques to examine molecular level changes in lipid model membrane organization induced by multivalent binding of the cholera toxin B (CTB) subunit. The cholera toxin selectively binds to ganglioside glycolipids in the membrane. Therefore, the scientists studied structural changes to the model lipid membranes before and after specific binding of the cholera toxin to membrane-embedded ganglioside GM1 receptors. With unprecedented molecular details, the researchers showed how protein binding perturbed lipid packing, resulting in topological defects and the emergence of a new textured lipid phase. These altered packing arrangements are transmitted from the receptor-laden leaflet to the inner leaflet of the membrane, providing a means for outside-in signaling.

The generation of such new lipid phases in membranes may have broad biological implications if perturbations to lipid order can be appropriated as a signaling mechanism by the cell and allow for new types of lateral heterogeneity in membranes. The textured domains provide a means for protein-binding-induced changes in lipid order to be spread laterally by cooperative self-organization of adjacent lipids. Resulting alterations of membrane structure may facilitate lipid domain clustering and potentially influence protein function. The researchers suggest that the formation of textured lipid microdomains via the multivalent binding of cholera toxin and protein aggregation into clusters is important in triggering the endocytotic pathway to bring the cholera toxin into the cell.

Reference: "Membrane Texture Induced by Specific Protein Binding and Receptor Clustering: Active Roles for Lipids in Cellular Function," *Proceedings of the National Academy of Sciences of the United States of America*; doi:10.1073/pnas.1014579108.

This research benefited from the use of the Lujan Center at LANSCE, funded by the DOE Office of Basic Energy. The work supports the Laboratory's Science of Signatures capability.

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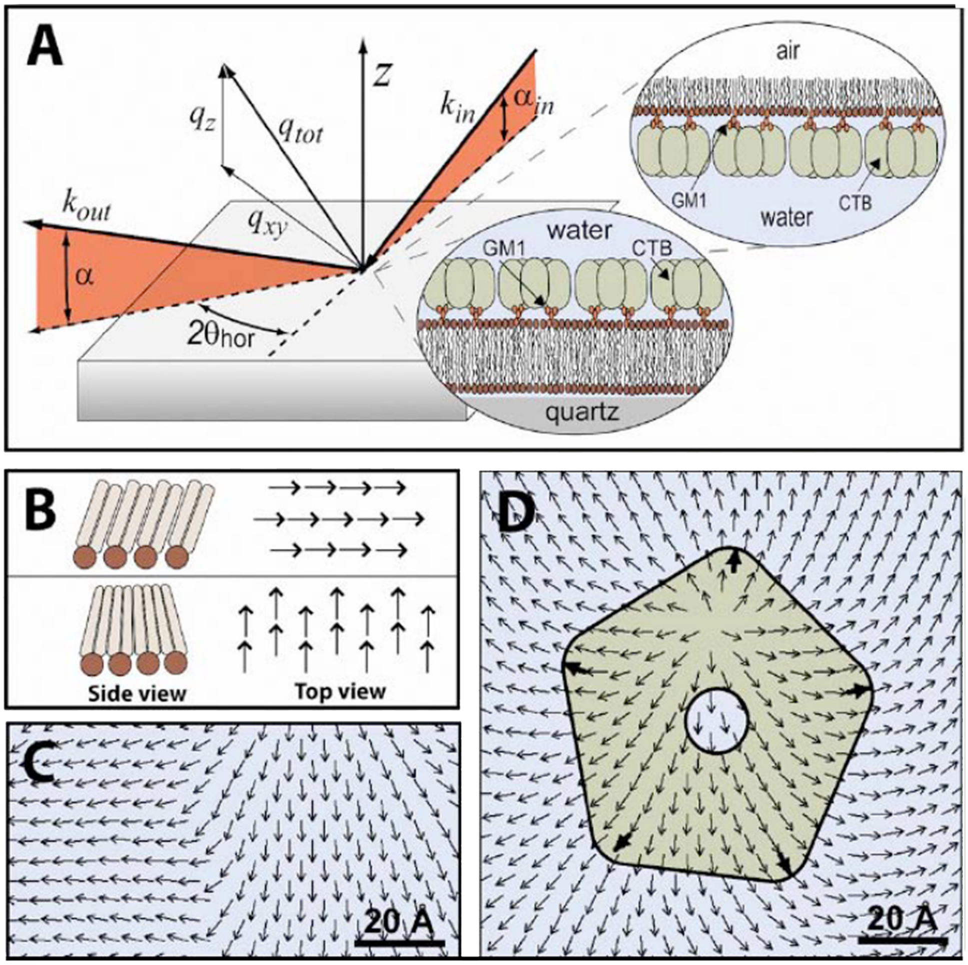

(A) The grazing incidence x-ray diffraction scattering geometry is shown with schematic insets representing the monolayer and bilayer lipid-CTB subunit systems studied. qz = $2\pi \sin \alpha$ is the momentum transfer of diffracted x-rays normal to the interface, and qxy = $4\pi \sin \theta$ is the momentum transfer perpendicular to the interface. (B) Tilt directors are vectors pointing along the lipids' alkyl chain backbones from the head group to the methyl end. (C) A boundary between two orientations of the lipid tilt director field. (D) Perturbation to the lipid tilt director field and associated topological defect induced by pentavalent binding of a single CTB protein.

Neutron Diffraction Study of γ-Chymotrypsin at the Protein Crystallography Station

Brandeis University graduate student Louis Lazar, his university colleagues, and researchers at the Protein Crystallography Station at LANSCE have collected the first complete neutron diffraction data set of γ-chymotrypsin at a spallation neutron source. Their goal is to develop methods for improving protein models with respect to hydrogen atom placement such that the models might be better used in various computational methods that critically depend on accurate and precise placement of hydrogen (H) atoms. In the field of rational drug design, significant improvements in the scoring functions of programs for computational ligand docking are possible when hydrogen sites can be explicitly assigned.

In a protein, hydrogen is perhaps the most important atom, being involved in all aspects of enzymatic catalysis, drug binding, protein folding, dynamics, and protein engineering. Computational methods – such as *in silico* drug design and docking, as well as quantum mechanics/molecular modeling (QM/MM) – depend on accurate H-atom position data. Little experimental data are available, and these methods rely on idealized geometry and standardized libraries to infer the location of the H atoms, which can lead to inaccurate modeling and incorrect drug binding docking studies. To address this critical knowledge gap, the scientists are generating neutron structures of γ-chymotrypsin prepared at various pHs to observe the changes in H bonding and H atom positions. Chymotrypsin is a biologically important molecule because it catalyzes the hydrolysis of proteins, degrading them into smaller molecules called peptides. Peptides are further split into free amino acids. The scientists subjected the γ-chymotrypsin crystal to hydrogen/deuterium exchange to enhance the neutron scattering imaging.

Initial data analysis reveals significant nuclear density for catalytically important residues. The researchers observed that the catalytic histidine is doubly protonated (deuterated). The serine and aspartate that make up the remainder of the catalytic triad do not show density for the presence of deuterium. The scientists also observed deuteration of backbone nitrogen hydrogen (NH) at terminal positions of beta sheets. Sample size and length of time to acquire neutron data are major impediments in the accessibility of neutrons to most structural biologists. However, these researchers obtained a complete neutron data set from a medium-sized crystal in under 2 weeks. These data will reveal many important details about the γ-chymotrypsin active site and ionization states of specific residues, as well as the hydrogen bonding patterns in the active site that support catalysis.

LANL participants include Zoë Fisher, Andrey Kovalevsky, and Paul Langan (Bioenergy and Environmental Science, B-8). Brandeis University participants include Lazar, Dagmar Ringe, Greg Petsko, Aaron Moulin, and Walter Novak.

The DOE Office of Science, Office of Biological and Environmental Research, funds the Protein Crystallography Center and the LANL scientists.

Reference: "Time-of-Flight Neutron Diffraction Study of Bovine γ-Chymotrypsin at the Protein Crystallography Station," *Acta Crystallographica* **F67**, 587 (2011). The work supports LANL's Science of Signatures capability.

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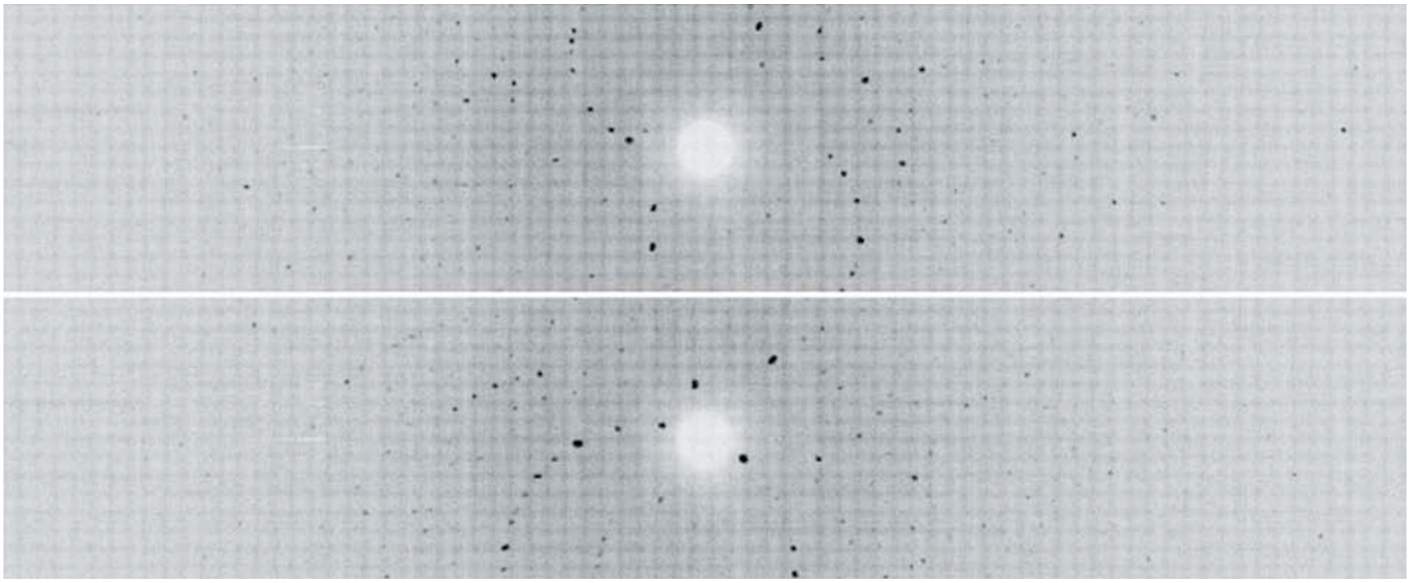

Neutron Laue time-of-flight diffraction images of γ-chymotrypsin collected at the Protein Crystallography Station at two different φ settings at k = 30° and 90°. For this representation, the time-of-flight data were overlaid to produce a conventional Laue pattern.

First Neutron Diffraction Study of a Stoichiometric Oxide Compound of Gold

Gold (Au) – traditionally regarded as one of the most inert elements in the periodic table – displays rich and various catalysis chemistries, many of which are still being discovered. Although the first report of carbon monoxide oxidation by gold was published in 1925, gold's catalytic action was noted in the 1820s during observations that it catalyzed the decomposition of ammonia. Because of gold's oxophobicity, its oxide crystal chemistry was relatively unknown until about 1960; it was another decade before crystal structure refinements were reported for most of its ternary phases and almost 10 additional years before the crystal structure of the binary gold oxide, Au_2O_3, was determined.

Anna Llobet (Lujan Center) and University of California-Santa Barbara (UCSB) collaborators have reported the first neutron diffraction study of any stoichiometric oxide compound of gold (La_4LiAuO_8). A previous single crystal x-ray diffraction showed the compound to adopt an ordered modification of the Nd_2CuO_4 structure, containing two-dimensional sheets in which AuO_4 square planes are separated from one another by LiO_4 square planes. However, in light of the meager x-ray scattering factors of lithium and oxygen relative to lanthanum and gold, the crystallographic description of this compound was questioned and the possible catalytic role of Au+3 required further analysis. Given the very large atomic number differences between Au and O, neutron scattering is required to draw reliable conclusions with regard to Au^{3+}– O distances.

In an excellent example of the strength of joint neutron and x-ray scattering techniques, Llobet and collaborators performed neutron and synchrotron x-ray powder diffraction experiments at the High-Intensity Powder Diffractometer (HIPD) instrument at the LANSCE Lujan Center and the Advanced Photon Source (Argonne National Laboratory) to examine the structure of La_4LiAuO_8. The team published the first neutron powder diffraction study of La_4LiAuO_8, definitively confirming the structure. X–N maps (which make use of nuclear positions obtained from Rietveld refinement of time-of-flight neutron diffraction data and electron densities obtained from synchrotron x-ray powder diffraction data) point to the highly covalent nature of the Au–O bonding in La_4LiAuO_8 which is in good agreement with charge densities and Bader charges obtained from full-density functional relaxation calculations of the structure. The strength of the Au^{3+} stabilization is related to the raising of O 2p states by the highly electropositive La^{3+} and Li^{+} counter cations, which enables improved orbital overlap between O 2p and Au 5d states.

Researchers include J. A. Kurzman, S. L. Moffitt, and R. Seshadri (UCSB); and A. Llobet (Lujan Center).

Reference: "Neutron Diffraction Study of La_4LiAuO_8: Understanding Au_{3+} in an Oxide Environment," *Journal of Solid State Chemistry* **184**, 1439 (2011); doi:10.1016/j.jssc.2011.04.021.

The DOE Office of Basic Energy Sciences funded the LANL portion of the research, which benefited from the use of the HIPD instrument at the Lujan Center. The work supports LANL's Materials for the Future science pillar.

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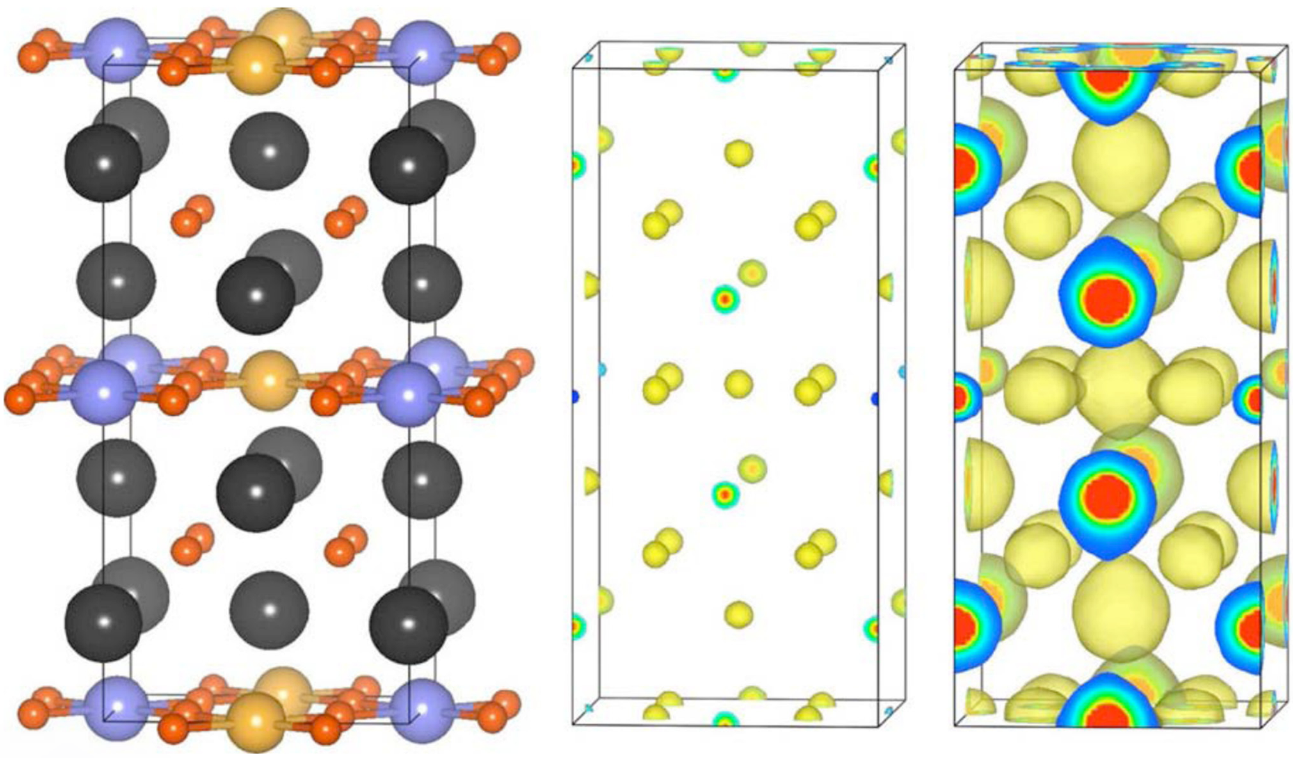

(Left). Unit cell depiction of La_4LiAuO_8. La is rendered black, Li blue, Au gold, and O orange. (Middle). Observed nuclear scattering densities (F_{obs}), shown at an isosurface level of ±0.3 fm $Å_{-3}$. (Right). X-N electron density isosurfaces at 1e$Å_{-3}$, determined by fixing the nuclear positions at those obtained from refinement of neutron data and then reconstructed by the MEM/Rietveld method using synchrotron x-ray data.

Neutron Scattering Provides Insight into Enzymatic Degradation of Cellulose

Growing interest in alternative and renewable energy sources has brought increasing attention to the use of cellulose materials to produce fuels and useful chemicals. Conversion of cellulose typically involves three steps: pretreatment of the biomass, enzymatic hydrolysis of cellulose and hemicellulose to fermentable sugars, and fermentation of the sugars to liquid fuels or other products. Improving the efficiency of enzymatic hydrolysis of cellulose is one of the key technological hurdles to overcome in reducing the cost of producing ethanol and other transportation fuels from lignocellulosic material. A better understanding of how soluble enzymes (cellulases) interact with insoluble cellulose could aid the design of more efficient enzyme systems.

A multidisciplinary group of scientists used complementary techniques of neutron reflectivity (NR) and quartz crystal microbalance with dissipation monitoring (QCM-D) to examine the effect of cellulase enzymes on the structure of cellulose films. NR shows the profile of water through the film at nanometer resolution. NR reveals whether an enzyme acts on the surface or throughout the bulk of the film and whether its activity results in removal of mass, increased water content, or changes in surface roughness. QCM-D provides changes in mass and film stiffness. The researchers used the Lujan Center time-of-flight surface profile analysis reflectometer (SPEAR) for the NR studies.

Comparison of cellulase action by a fungal enzyme extract with a single endoglucanase reveals important differences in the interactions of the enzymes with the films. The fungal enzyme extract initially digests cellulose at the surface, rapidly roughening the film/solution interface. Enzyme activity within the bulk of the film occurs after a significant fraction of the upper layer is degraded. On the same time scale, the single endoglucanase is active only at the surface. Because the fungal enzyme extract contains endoglucanases and exoglucanases, the scientists suggest that the interfacial roughening is due to the actions of the exoglucanases and possibly to the presence of cellulose-binding domains on the enzymes in the fungal extract. The single endoglucanase does not contain a cellulose binding domain.

Researchers include Michael Jablin, Manish Dubey, and Jaroslaw Majewski (Lujan Center); Gang Cheng, Ken Sale, Blake Simmons, Michael Kent (Joint BioEnergy Institute and Sandia National Laboratories); Zelin Liu, Chao Wang, and Alan R. Esker (Virginia Polytechnic Institute and State University); Jaclyn Murton (Sandia National Laboratories); Candice Halbert, James Browning, and John Ankner (Oak Ridge National Laboratory); and Bulent Akgun (National Institute of Standards and Technology and University of Maryland).

Reference: "Neutron Reflectometry and QCM-D Study of the Interaction of Cellulases with Films of Amorphous Cellulose," *Biomacromolecules* **12**, 2216 (2011); dx.doi.org/10.1021/bm200305u.

The DOE Office of Basic Energy Sciences, Scientific User Facilities Division, sponsors research at the LANSCE Lujan Center. The work supports the Lab's Energy Security mission area and the Materials for the Future science pillar.

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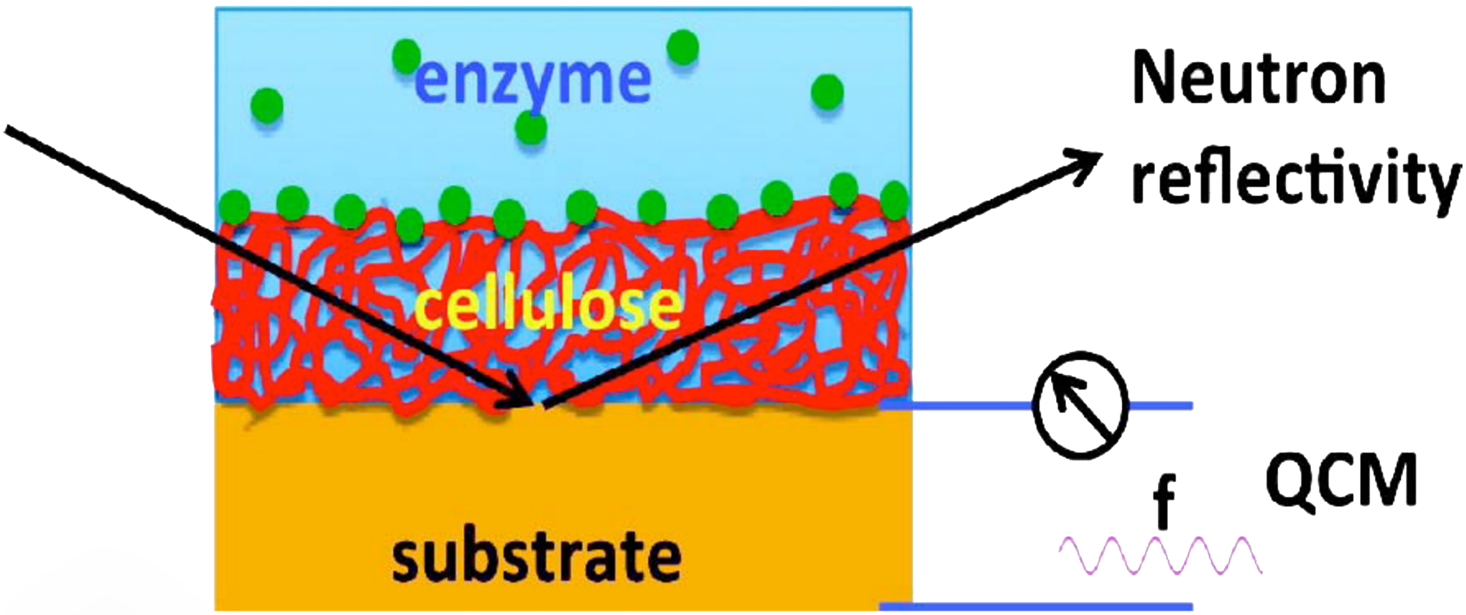


NR and QCM-D of the interaction of a fungal enzyme extract (T. viride) and an endoglucanase from A. niger with amorphous cellulose films.

Spatially Mapping Residual Stress in Finished Industrial Parts

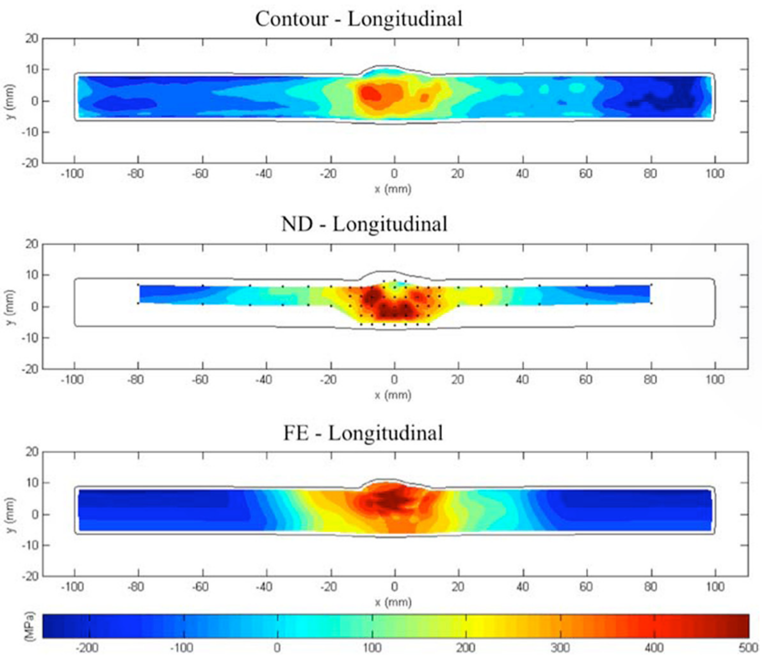
Approximately one-third of the beam time on the Lujan Center's Spectrometer for Materials Research at Temperature and Stress (SMARTS) is dedicated to spatial mapping of residual stresses in finished industrial parts. SMARTS is analogous to a bathroom scale. If one steps on a spring, measures the compression of the spring, and knows the spring constant, one can calculate the weight from Hooke's law. The atoms of a crystal may be considered as being connected by springs. By measuring the change in spacing of the atoms in the crystal, the internal strains ore, the stress is calculated from the generalized Hooke's law, if the spring constant (single crystal stiffness of the material) is known. Thus, SMARTS maps the stresses in the bulk of materials with a spatial resolution of approximately 2 mm. As part of the Lujan Center national user program, Thomas Sisneros and Don Brown (Structure/Property Relations, MST-8), Bjorn Clausen (Lujan Center), and Matthew Kerr (Nuclear Regulatory Commission, NRC) mapped the residual stresses in a model dissimilar metal weld. This weld type often joins nuclear reactor pressure vessels to relief valves.

Mike Prime (Advanced Engineering Analysis, W-13) completed mechanical relaxation (contour method) measurements of the residual stress in the same part for cross validation. The color map (next page) shows a cross-sectional map of the longitudinal stress in the model weld measured by neutron diffraction and mechanical relaxation; the agreement is satisfactory. The part is under a large tensile stress (greater than 500 MPa) parallel to the weld near the boundary between the weld and the base metal due to the differential heating experienced during welding. The tensile stress on the weld is troublesome because weld metals necessarily lack the "working" that most metals receive to enhance their mechanical properties. Therefore, welds are susceptible to stress corrosion under tensile stresses.

Scientists use these results to validate predictive finite element models developed by the NRC. The plot also shows the finite element calculations of the residual stress. Although the model captures the correct magnitude of the longitudinal stress, the position of the maximum is not correct. Once validated, these models will be used to qualify welds for in-reactor service.

DOE Basic Energy Sciences funds the Lujan Center user program. The work supports the Lab's Energy Security mission area and the Materials for the Future science pillar.

Cross section of the weldment. The yellow diamond indicates the integration area of the neutron diffraction measurement. The base metal is ferritic steel, and the weldment is a nickel alloy. The change in chemistry complicates the measurement considerably.



Mechanical relaxation and longitudinal stress in the model weld.

Neutron Reflectometry Examines the Performance of Radiation-Resistant Materials

Precipitation of implanted helium (He) is a major concern for the performance and survivability of plasma-facing components in future nuclear fusion reactors. The deleterious effects of He may be minimized if it can be trapped at special microstructural features. LANL scientists and collaborators investigated metallic copper/niobium (Cu/Nb) multilayers and discovered that a remarkably high concentration of He can be trapped at certain heterophase interfaces before nanometer-scale bubbles are resolved via transmission electron microscopy (TEM). Atomistic modeling suggests that excess atomic volume leads to a high He "solubility" at these interfaces. Because TEM cannot resolve He clusters smaller than 1-2 nm in diameter, other techniques are needed to characterize He concentration profiles across interfaces.

An interdisciplinary group of scientists used neutron reflectometry (NR) to determine the changes in the transverse chemical profile of Cu/Nb-layered nanocomposites due to He ion migration, absorption, and storage after ion implantation. The researchers performed the NR experiments on the surface profile analysis reflectometer (SPEAR) at LANSCE. NR involves the specular reflection of a neutron beam from a surface or film and provides sub-angstrom-level resolution where the He-enriched interfaces. NR provides a nuclear (chemical)-scattering length density (NSLD) depth profile of the sample, with Angstrom resolution averaged over the coherent area of the neutron beam on the sample surface – typically microns. NSLD is the product of the number density of atoms and their nuclear coherent scattering lengths. From NR measurements, layer parameters such as thickness, density, chemical composition, and interface and surface roughnesses can be determined with sub-angstrom precision, regardless of the crystallinity of the sample.

Neutron scattering is a unique tool to study such nanolayered composites because the scattering strength is a non-monotonic function of the Z number of a material. Therefore, elements such as Cu and Nb provide the necessary neutron scattering contrast, even though their x-ray scattering contrast is low. Additionally, unlike electron microscopy, which yields local structure information, NR provides data averaged over a large sample area.

NR characterized [Cu/Nb]x-layered nanocomposites that had been exposed to extreme helium ion doses at the Ion Beam Materials Laboratory. Measurement of the effects of He ions on the interfacial roughness, layer swelling, and chemical mixing revealed that regions of high He concentration localize at Cu/Nb interfaces, whereas bulk Cu and Nb layers remain intact. The interfaces in [Cu/Nb] x systems irradiated with high He ion doses absorbed and stored He without distorting the planar structure of the layers. Because of the He irradiation, the Cu/Nb interfacial regions broadened approximately ten-fold and most of the He ions were segregated into these regions, thus swelling both the Cu and Nb layers. The scientists attribute this remarkable behavior to the efficient trapping and storage of He at interfaces as compared with bulk. Analysis of NR data from these samples provides insight into the behavior of interfaces in layered nanocomposites under an extreme environment such as may be expected in the first wall of a fusion reactor.

Researchers include M. Zhernenkov, M. Jablin, and J. Majewski (Lujan Center); A. Misra, M. Nastasi, and J. K. Baldwin (Center for Integrated Nanotechnologies, MPA-CINT); Y. Wang (Structure/Property Relations, MST-8); and M. Demkowicz (Massachusetts Institute of Technology).

Reference: "Trapping of Implanted He at Cu/Nb Interfaces Measured by Neutron Reflectometry," *Applied Physics Letters* **98**, 241913 (2011).

The research benefited from the use of the Lujan Center at LANSCE funded by the DOE Office of Basic Energy Sciences. LANL's Laboratory Directed Research and Development (LDRD) program sponsors the work on He ion implantation in multilayers. The research supports the Lab's Energy Security mission area and the Materials for the Future science pillar.

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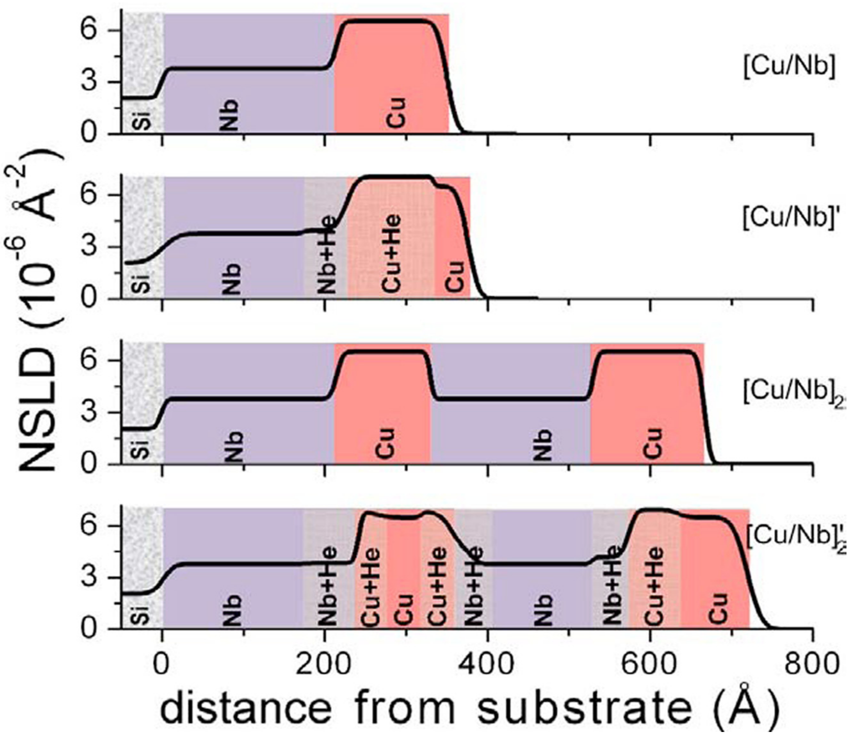


Nuclear-scattering length density (NSLD) profiles obtained from the NR fits and schematics of the real-space interpretations used to model the experimental data. A prime after a sample name indicates that the curve corresponds to a measurement after He ion implantation.

First Proof of Hydronium Ion's Role in an Enzymatic Process

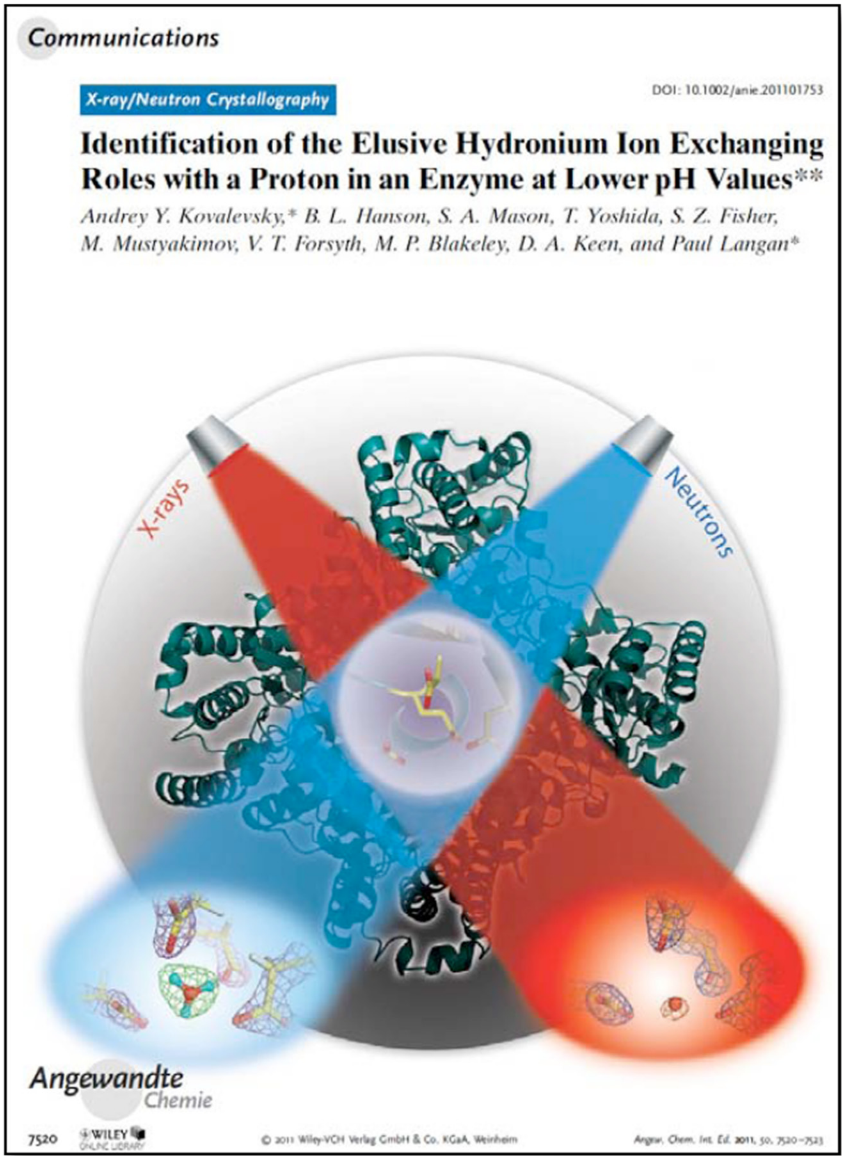
LANL researchers and collaborators have used neutrons for an unprecedented view of the critical role that the elusive hydronium ion plays in the transfer of protons during enzyme-catalyzed reactions. Before this work was done, no one had ever directly witnessed the role of the hydronium ion, a water molecule bound to an additional hydrogen ion, in the catalytic mechanisms of enzymes. Scientists took an interest in an enzyme that has the potential to allow the conversion of sugars in woody biomass into alcohol, a potential alternative fuel, because the enzyme loses its effectiveness when the pH value of the milieu is lowered — a common occurrence in the interior of industrial yeast cells fermenting alcohol.

The scientists used neutrons from the LANSCE to examine the mechanism of the biological reactions. The hydronium ion appears as a pyramid-shaped mass in the enzyme's active site, where the chemical reaction occurs. The researchers discovered a crucial change as the system fell into the acidic range of the pH scale (below 6). The hydronium ion facilitating the binding of a metal ion cofactor crucial to the conversion of the sugar molecule into its fermentable form suddenly becomes dehydrated. The space occupied by the relatively large hydronium ion collapses into a tiny volume occupied by the remaining proton (a positively charged hydrogen ion). The spatial change in the molecular structure prevents the enzyme from attacking the sugar, which explains why pH has such an important role in the process and renders the enzyme inactive under acidic conditions. The hydronium ion has a key role in the transport of protons in these types of biochemical systems. The research provides insight for the role of hydronium ions in biological systems and could aid in the treatment of peptic ulcers or acid reflux disease or enable more efficient conversion of woody waste into biofuels.

LANL scientists include Andrey Kovalevsky, Suzanne Fisher, and Marat Mustyakimov (Bioenergy and Environmental Science, B-8); Thomas Yoshida (Chemical Diagnostics and Engineering, C-CDE); and Paul Langan (B-8, currently at Oak Ridge National Laboratory). Collaborating institutions are the University of Toledo, Ohio; the Institut Laue Langevin, France; Keele University, England; and the ISIS facility in Oxfordshire, England.

Reference: "Identification of the Elusive Hydronium Ion Exchanging Roles with a Proton in an Enzyme at Lower pH Values," *Angewandte Chemie International Edition* **50**, 7520 (2011); doi: 10.1002/anie.201101753.

Laboratory's Directed Research and Development Program (LDRD), the DOE Office of Biological and Environmental Research, and the National Institutes of Health supported different aspects of the LANL research. The work supports the Lab's Energy Security mission area and the Materials for the Future science pillar.


Communications

X-ray/Neutron Crystallography

DOI: 10.1002/anie.201101753

Identification of the Elusive Hydronium Ion Exchanging Roles with a Proton in an Enzyme at Lower pH Values**

Andrey Y. Kovalevsky, B. L. Hanson, S. A. Mason, T. Yoshida, S. Z. Fisher, M. Mustyakimov, V. T. Forsyth, M. P. Blakeley, D. A. Keen, and Paul Langan**

Angewandte Chemie

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Angew. Chem. Int. Ed. 2011, 50, 7520–7523

A hydronium ion has been found to interchange with metal cofactors in the active site of an enzyme. Under more acidic conditions, the hydronium ion is dehydrated to a proton, and the binding site collapses.

From Pharmaceutical Tablets to Plastic-Bonded Explosives

The mechanical behavior of compacted granules is of importance for both pharmaceutical compacts and plastic-bonded explosives (PBX). Because tablet durability and mechanical failure are serious issues with many pharmaceutical drugs, determining the processing-structure-properties relationship for these powders is important. Many pharmaceutical powders used in medicine display poor compaction behavior. Therefore, the tablets are coated with a binder to improve tablet formation properties. PBX and compacted pharmaceutical tablets are analogous composite materials. A typical PBX composite consists of micron-sized explosive molecular organic crystals coated with a polymer binder. The mechanical properties of PBX and pharmaceutical compacts are defined similarly and display similar failure pathways. Cracking and de-bonding of the crystals from the binder results in anisotropy within the composite. Such brittle failure can cause processing and stability problems in these materials. In explosives, such cracks could have serious implications for safety and sensitivity or for the ease of accidental burning or detonation of the explosive. Detonative properties in intentional use might also be affected, and the effect of such cracks is poorly understood in this regime. Therefore, characterization of the interface between the binder and the crystal is necessary.

LANL scientists and a collaborator used a variety of techniques, including neutron scattering at the Lujan Center, to investigate the chemistry and structure of the model composite acetaminophen – Estane® interface with and without the addition of a nitroplasticizer. The ability of neutron scattering to probe interfaces and phase segregation makes it a particularly appropriate analytical technique for the research. Scientists chose to study the pharmaceutical acetaminophen due to its poor compaction properties, even in the presence of a binder and a similar crystal structure to the HMX explosive crystals. The PBX 9501 binder is a mixture of Estane 5703 (a commercially available poly(ester urethane) and a nitroplasticizer.

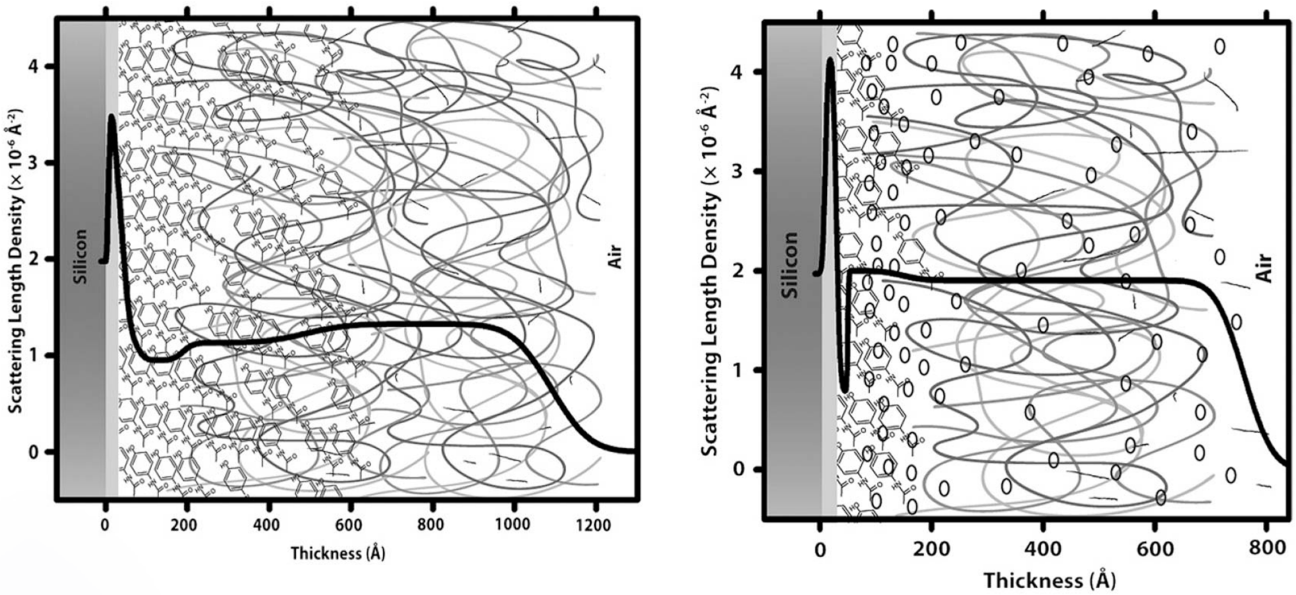
The research showed that a complex interphase region occurs in the non-plasticized and plasticized layered samples. The roughness and solubility of the acetaminophen film contribute to the formation of an interphase region when coated with the Estane® polymer (see left figure). The plasticizing agent concentrates at the interface, altering its structure and properties (see right figure). The observation of this interphase region is important for relating microstructure to mechanical properties. Grain-scale models can use this type of information to reproduce experimentally observed PBX failure more accurately. Neutron scattering provides a tool to study the relationship between processing and structure, exemplified here by the difference between Estane® and nitroplasticizer/ Estane® at the acetaminophen interface. This procedure for measuring interfacial properties of molecular composites provides a path for analyzing mechanical behavior and a link between processing and structure. These results have important ramifications for the mechanical behavior and damage propagation models currently used by the explosives community and for similar organic crystal – polymer composites of pharmaceutical interest.

Reference: "Interfacial Structural and Chemical Characteristics Between a Copolymer Binder and an Organic Crystal," *Polymer* **52**, 3762 (2011); doi:10.1016/j polymer.2011.06.031.

Researchers include J.D. Yeager and D.E. Hooks (Shock and Detonation Physics, WX-9), M. Dubey, M. Wolverton, M.S. Jablin, and J. Majewski (Lujan Center); and D.F. Bahr (Washington State University).

The DOE/DoD Joint Munitions Project sponsored the work, which benefited from the use of the Lujan Center at LANSCE (funded by the DOE Office of Basic Energy Sciences).

The work was performed, in part, at the Center for Integrated Nanotechnologies, a DOE Office of Basic Energy Sciences user facility. The work supports the Lab's Nuclear Deterrence and Global Security mission areas and the Materials for the Future science pillar.



(Left). Scattering length density profile for the Estane® – acetaminophen layered sample, showing a thin layer of acetaminophen (seen as drawings of acetaminophen molecules) intermixing with the polymer (shown as curved lines). Schematic depicts variations in chemistry as a function of thickness.

(Right). Scattering length density profile for the nitroplasticizer/ Estane® – acetaminophen layered sample, showing a thin layer of acetaminophen (shown as drawings of acetaminophen molecules) intermixing with the plasticizer (depicted as ovals) at the interface. The polymer is shown as curved lines. Schematic depicts variations in chemistry as a function of thickness.

Unveiling the Superconducting Pairing Mechanism in Iron Chalcogenides

According to the Bardeen-Cooper-Schreiffer theory of superconductivity, the superconducting state and magnetism are thought to be incompatible. However, the proximity of magnetism is crucial to the development of the superconducting state in some systems. This phenomenon was observed in the cuprate superconductor and in the recently discovered superconducting iron pnictides [pnictides contain phosphorus (P), arsenic (As), or antimony (Sb)] and chalcogenides [chalcogenides contain sulfur (S), selenium (Se), tellurium (Te), or oxygen (O)]. Although the origin of the pairing mechanism leading to the superconductivity is still debated, extensive experimental and theoretical work on the iron pnictides and chalcogenides have revealed important traits that make them uniquely different from those of superconducting cuprates. Iron pnictides and chalcogenides do not require charge doping to increase the superconducting temperature (TC), and magnetic ion doping does not suppress TC. Magnetic fluctuations persist in the superconducting phase, such as $FeTe_{1-x}T_{ex}$, or even increase with TC as in FeSe.

Despina Louca (University of Virginia) led a team from LANSCE's Lujan Center, Ames Laboratory, and the University of Tokyo to investigate the mechanisms affecting superconductivity in $FeTe_{1-x}S_{ex}$. The scientists examined how the crystal structure and properties change when the material is annealed without introducing foreign atoms or applying pressure. In many related systems, annealing increases the superconducting or magnetic transition by reducing inhomogeneities and thus improves sample quality. Annealing has the opposite effect for $FeTe_{1-x}S_{ex}$ – it reduces TC.

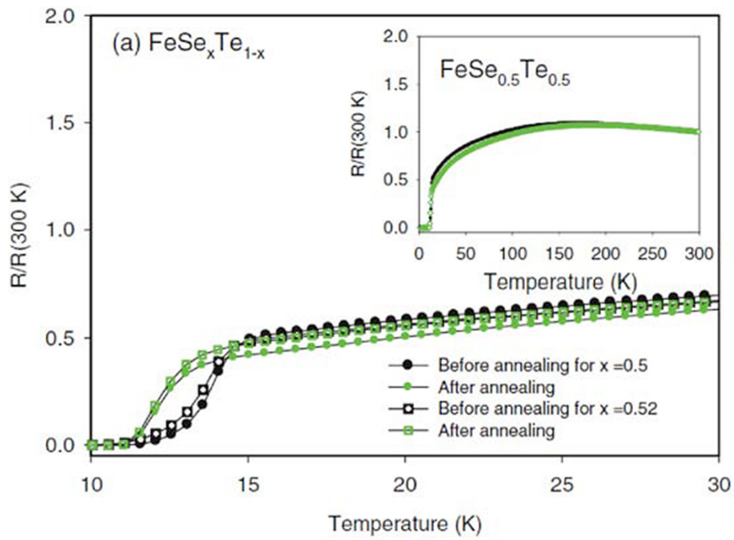
The scientists used the capabilities of the High-Intensity Powder Diffractometer (HIPD) at the Lujan Center to show that Tc depends on the atomic configurations of the Te and Se ions. The data enabled the study of the long-range crystallographic order, potential magnetism, and local structure analysis using the pair distribution function.

These results show how low-temperature annealing homogenizes the Te and Se ion distribution and suppresses TC due to changes in the chalcogen ion's z parameter. This subtle change in the local structure arrangement of the atoms creates a different local environment for Se and Te that allows them to have random occupation of unequivalent sites. Local structure analysis reveals that upon low-temperature annealing, the height of Te from the Fe basal plane is much reduced, whereas that for Se shows a modest increase. The structural changes that are caused by annealing are markedly different from the effects induced under pressure. Pressure changes the volume by a significant amount and decreases the Se z parameter or anion height significantly. Annealing mainly changes the Te z parameter. Therefore, annealing decreases the bond length between Te and Fe and simultaneously increases the bond angle between them. The bond length between Fe and Se decreases upon annealing, and the bond angle between them is reduced. Under pressure, the Se height decreases, while the angle approaches the optimal 109°. This study shows how the local atomic configuration of the chalcogen ions, in particular the height of Te, is the dominant factor suppressing TC and that this effect does not occur through application of external pressure or introduction of foreign atoms into the lattice.

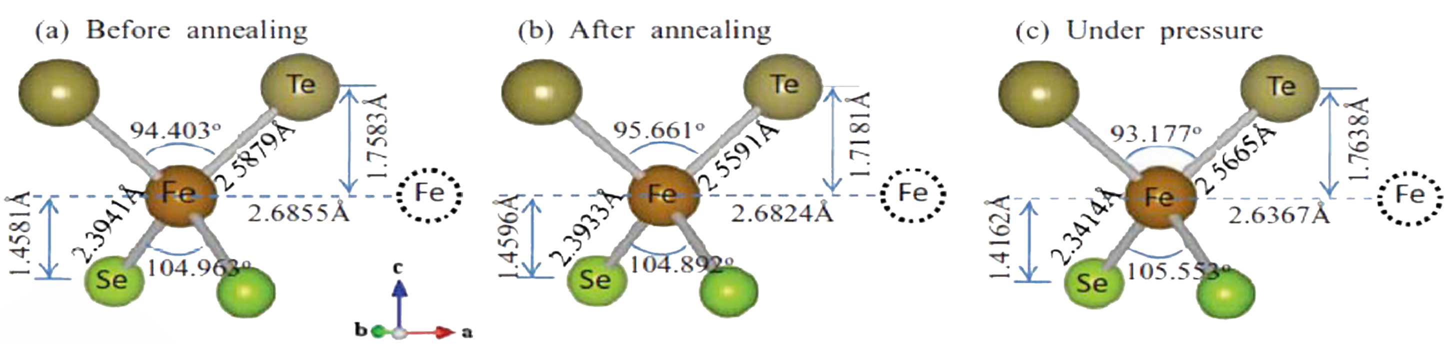
Researchers include Despina Louca (University of Virginia), Jiaquiang Yan (Ames Laboratory), Anna Llobet (Lujan Center), and Ryotaro Arita (University of Tokyo).

Reference: "Suppression of Superconductivity in Fe Chalcogenides by Annealing: A Reverse Effect to Pressure," *Physical Review B* **84,** 054522 (2011); doi:10.1103/PhysRevB.84.054522.

The DOE Basic Energy Sciences sponsored Llobet's research at the Lujan Center on the high-intensity powder diffractometer. The Lujan Center is a DOE Office of Science user facility. The work supports the Laboratory's Energy Security mission area and the Materials for the Future science pillar.



A plot of the resistance normalized to the room temperature value for two samples: $x = 0.5$ and 0.52. A reduction in TC occurs in both samples.



The bond angles, bond lengths, and Te and Se ion heights from the basal plane are compared in the crystal structures (A) before annealing, (B) after annealing, and (C) under pressure. The height of the Te ion changes dramatically with annealing, but less so under pressure. The reverse happens with Se.

Characterizing Functional Piezoelectric Materials Under Extreme Conditions

Piezoelectric (PZT) materials have two unique properties that are interrelated. The materials produce a voltage in response to an applied force, and applying voltage induces a change in dimension. These materials are usually ceramics with a perovskite structure and the general formula ABO_3. PZT materials are used in electromechanical devices as actuators in micromotors, pumps, and cell phones. In PZT ceramics, the response to external stress or electric field consists of intrinsic (single crystal response) and extrinsic (grain boundaries, preferred orientation or texture of the grains, and changes in crystal phase fractions) contributions. The chemical composition is chosen such that two phases coexist near a first-order phase transition. An example is the morphotropic phase boundary in the classical PZT lead zirconate titanate ($Pb(Zr_xTi_{1-x})O_3$). A morphotrophic boundary consists of adjacent phases with equal Gibbs free energy in a phase diagram. LANL scientists and collaborators used neutron scattering to characterize PZToxides in the quest to develop improved, lead-free PZT materials.

Neutron scattering is an excellent tool for studying the complex changes occurring in oxides in response to pressure, heat, or compositional modification. This characterization method has the unique ability to determine the oxygen and cation positions, phase fractions, and magnetic ordering in materials. LANL scientists and collaborators conducted neutron diffraction experiments to investigate two perovskite oxides: ferroelectric lead titanate ($PbTiO_3$) and manganese-modified strontium titanate ($Sr(Ti_xMn_{1-x})O_3$). Lead titanate and ($Sr(Ti_xMn_{1-x})$ are classical perovskite oxides. High-pressure (up to 8 GPa) neutron powder diffraction experiments and density functional theory computations show that the competition between two factors determines the morphotropic phase boundary for $PbTiO_3$.

Oxygen octahedral tilting favors the rhombohedral *R3 c* phase, and entropy favors the tetragonal phase above 130 K near the morphotropic phase boundary. If the two factors are in balance over a large temperature range, a steep phase boundary causes a pressure-temperature plane that is desirable for applications. The advantageous feature of the *R3 c* phase is its ability to be compressed efficiently by tilting the oxygen octahedra, in contrast to symmetries prohibiting oxygen octahedral tilting.

The predicted oxygen octahedral tilting under high pressure in $PbTiO_3$ motivated the scientists to investigate crystal symmetries of magnetic-ion-modified $SrTiO_3$, a lead-free material. A small substitution (2 at.% manganese for titanium) in the perovskite $SrTiO_3$ decreases the symmetry from cubic to orthorhombic, which exists at room temperature (see bottom figure). Orthorhombic symmetry remains down to the lowest temperatures measured (11 K). The figure at left (top) shows the corresponding oxygen octahedral tilting. The small amount of manganese doping causes a magnetic anomaly between 70 and 80 K, accompanied by an anomalous behavior in lattice parameters at 50 K.

These results show that novel multiferroic materials, being PZT and magnetic, can be found in systems possessing octahedral tilting and magnetic ions, such as manganese. The research at LANSCE is dedicated to high-pressure neutron studies of PZT with a morphotropic phase boundary at which two phases, *R3c* and *Cm* co-exist. At the morphotropic phase boundary, the electromechanical coupling coefficient, the most important figure of merit of a PZT material, peaks. The scientists' goal is to determine the temperature- and pressure-dependent changes in phase fractions and atomic scale structures. The experiments test the ab-initio computational studies, which predict that the rhombohedral phase is favored above 9-GPa pressures.

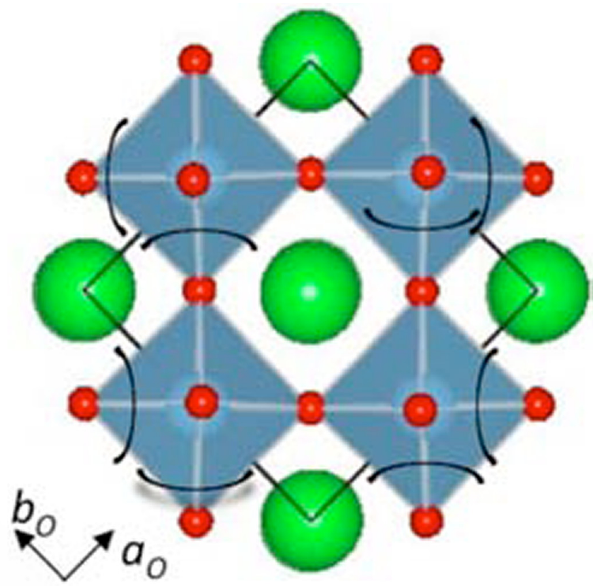
References: “The Factors behind the Morphotropic Phase Boundary in Piezoelectric Perovskites,” *Journal of Physical Chemistry B* (in press); “Neutron Powder Diffraction Study of the Effect of Mn-Doping on SrTiO,” *Materials Science Forum* **700**, 28 (2012); online at www.scientific.net; doi:10.4028/www.scientific.net/MSF.700.28.

Researchers include Johannes Frantti, Yukari Fujioka, and Risto Nieminen (Aalto University, Finland), Jianzhong Zhang, Sven Vogel, Yusheng Zhao, Luke Daemen, Zhijun Lin, Helmut Reiche, and Adrian Losko (Lujan Center).

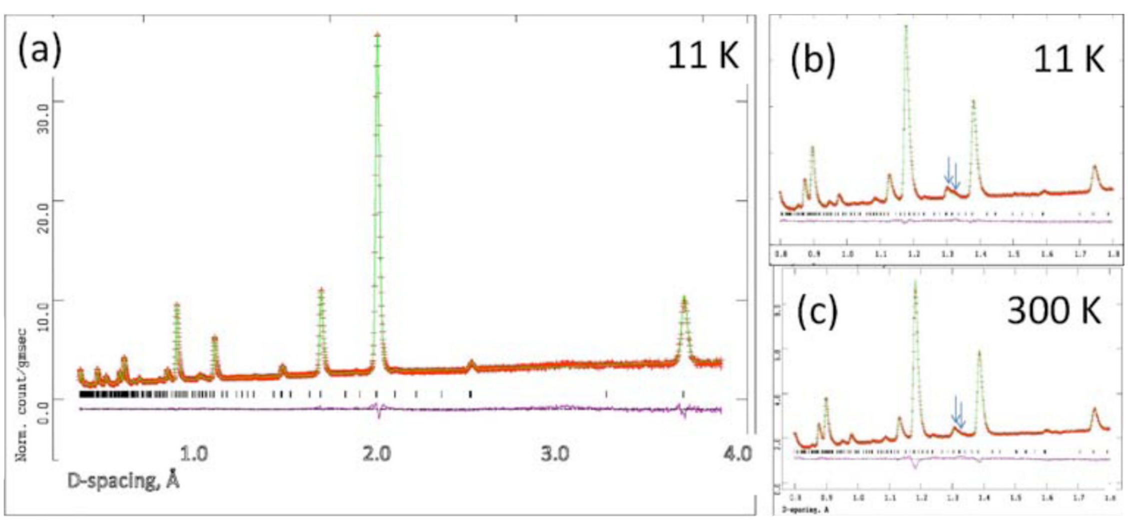
The work benefited from the use of the High-Pressure Preferred Orientation (HIPPO) diffractometer at the Lujan Center.

The DOE Office of Basic Energy Sciences funded the LANL scientists and the Lujan Center at LANSCE. The work supports LANL’s Energy Security mission area and the Materials for the Future science pillar.

AOT and LANSCE - The Pulse, November 2011.
LALP-11-017



(Top). Oxygen octahedral tilting in $Sr(Mn_{0.02}Ti_{0.98})O_3$ sample. *Pbnm* symmetry corresponds to the three-tilt system ($a^+b^-b^-$ in Glazer’s notation). Arrows indicate the octahedral antiphase tilts (b^-b^- tilts) in the orthorhombic *ab*-plane. Blue spheres are oxygen, light blue ones are B-cations, and green ones are Sr ions.



(Bottom). Neutron powder diffraction patterns for $Sr(Mn_{0.02}Ti_{0.98})O_3$. Panel (A) shows a large region diffraction pattern measured at 11 K. Panels (B) and (C) show a detailed picture of the diffraction pattern at 11 K and 300 K. The arrows point to reflections that are the clearest indication of a symmetry lowering.

Local Iron Displacements and Magnetoelastic Coupling in a Spin-Ladder Compound

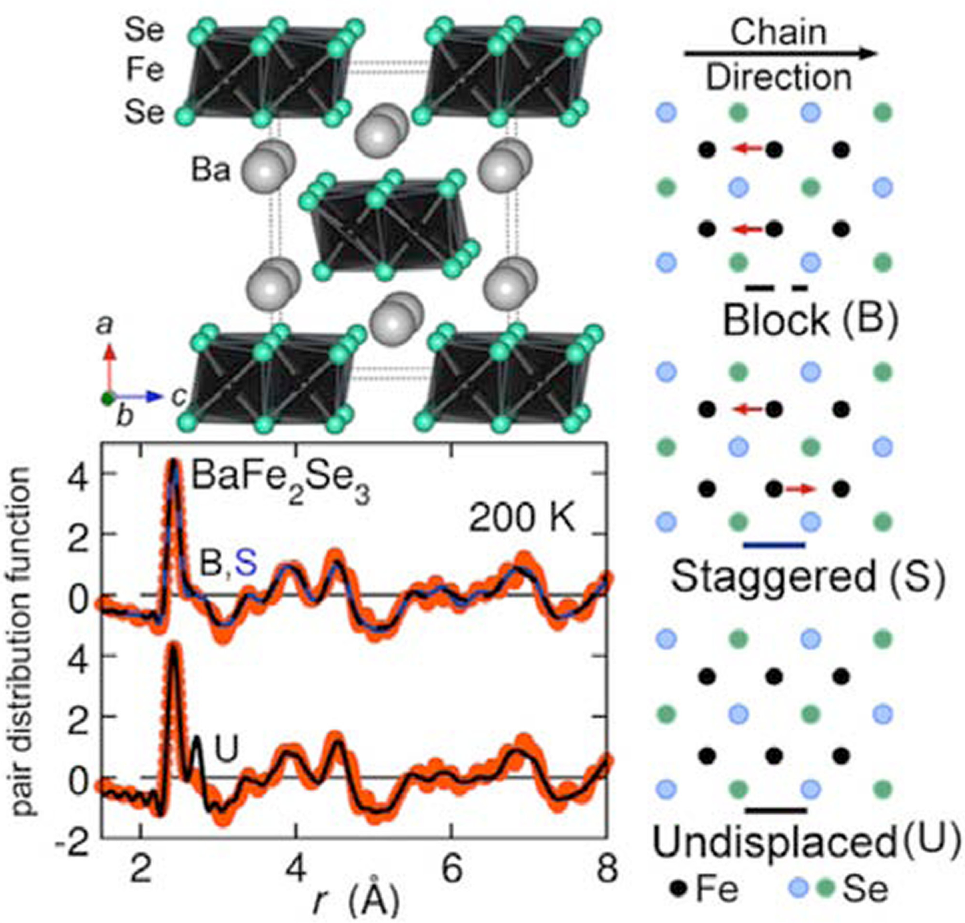
Scientists from John Hopkins University, in collaboration with Anna Llobet (Lujan Center), have revealed the existence of highly correlated local iron (Fe) displacements in the spin-ladder iron chalcogenide $BaFe_2Se_3$. Their study of structural and magnetic properties confirms significant magnetoelastic coupling in $[FeX_4]$-based materials, an ingredient hypothesized to be important in the emergence of superconductivity. The research shows that knowledge of these local displacements is essential for understanding the electronic structure of these systems.

The researchers performed neutron diffraction experiments on the chalcogenide with the LANSCE High-Intensity Powder Diffractometer (HIPD) and Neutron Powder Diffractometer (NPDF) instruments. They discovered that short-range magnetic correlations (approximately 35-Å at room temperature) develop into long-range antiferromagnetic order below TN = 256 K, with no superconductivity down to 1.8 K. The magnetic ground state, which is built of ferromagnetic Fe_4 plaquettes, correlates with local displacements of the Fe atoms as determined from neutron pair-distribution function analysis of the same data. The spins align perpendicular to the plane of the ladders, with an alternating spin direction between adjacent plaquettes. The HIPD enabled this finding. Although the experiment was performed to determine the nature of magnetism in the double chains, analysis of the total scattering profile revealed these iron displacements. An additional experiment performed on NPDF confirmed the presence and magnitude of these displacements.

Their results highlight the importance of reduced dimensionality in spin-ladder compounds, but also show that local metal atom displacements are ubiquitous in $[FeX_4]$-based materials and must be included when trying to understand the resulting magnetism and superconductivity. Llobet and collaborators observed similar local offsets in FeSe and $FeSe_{1-x}Te_x$, (*Science Highlights*, 9/21/2011), in which the presence or absence of superconductivity is very sensitive to their pattern.

Reference: “Iron Displacements and Magnetoelastic Coupling in the Antiferromagnetic Spin-Ladder Compound $BaFe_2Se_3$,” *Physical Review B* **84**, 180409(R) (2011); doi:10.1103/PhysRevB.84.180409. Researchers include J.M. Caron, J.R. Neilson, D.C. Miller, and T.M. McQueen (The Johns Hopkins University, Maryland); and Anna Llobet (Lujan Center).

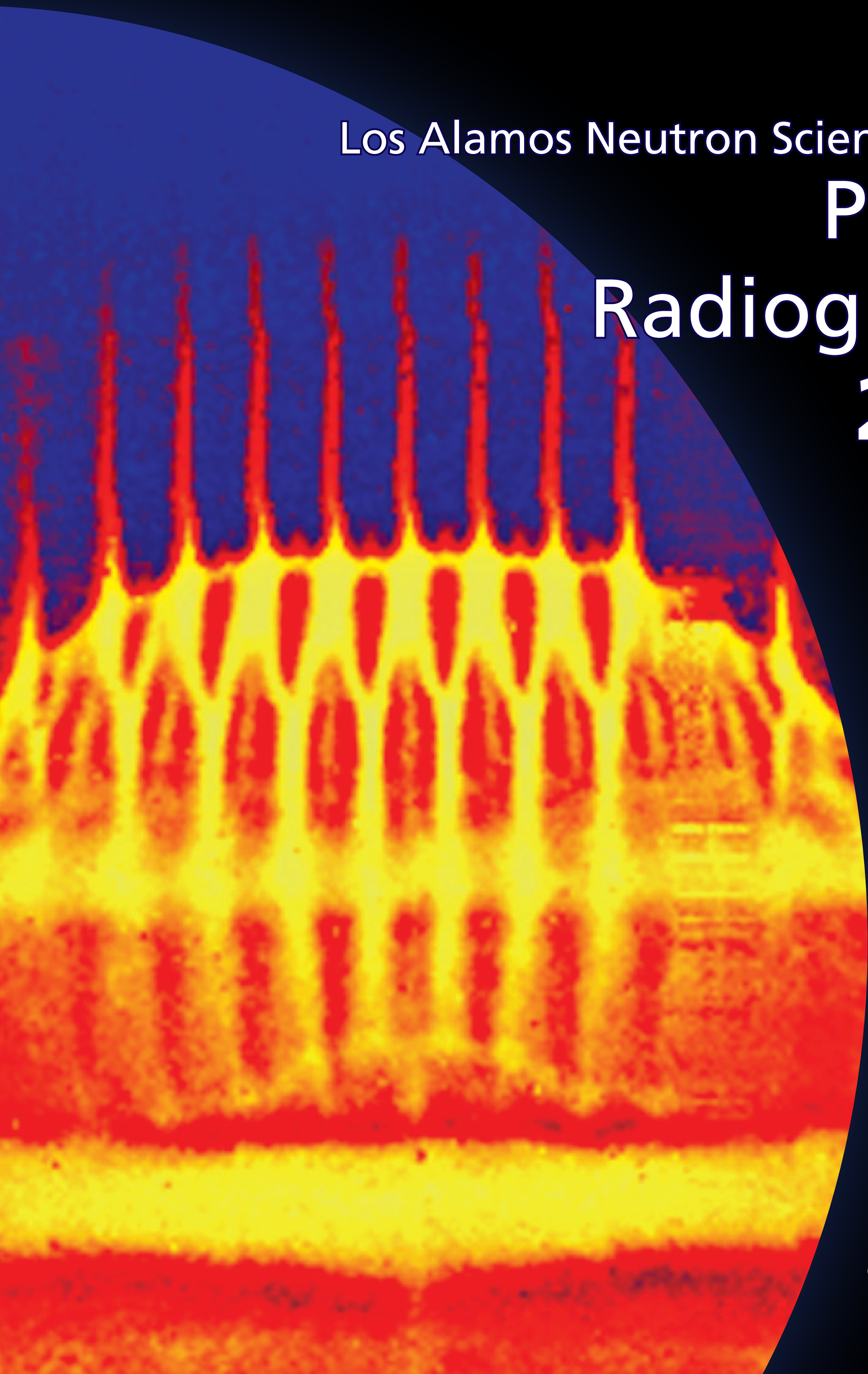
The DOE Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, funded the LANL research. This research benefited from the use of the HIPD and NPDF instruments at the Lujan Center at LANSCE, funded by DOE Office of Basic Energy Sciences. The work supports the Lab’s Energy Security mission area and the Materials for the Future science pillar.



The structure of $BaFe_2Se_3$ consists of double chains of edge-sharing $FeSe_4$ tetrahedra, which extend in and out of the page. The chains are well separated from each other by Ba ions. The spin-ladder $BaFe_2Se_3$ exhibits local Fe-Fe displacements from their ideal positions along the chain direction. The magnitude of the displacements is magnetoelastically coupled.

Los Alamos Neutron Science Center

Proton Radiography 2011



LANSCE
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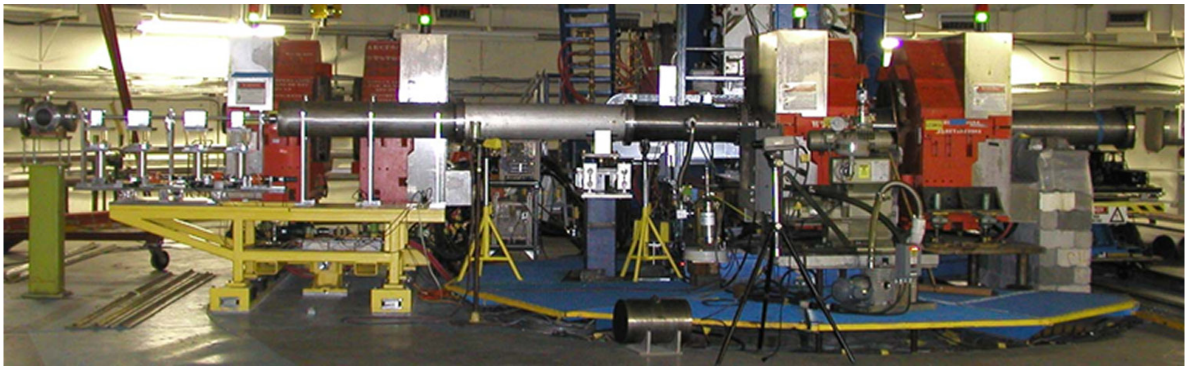
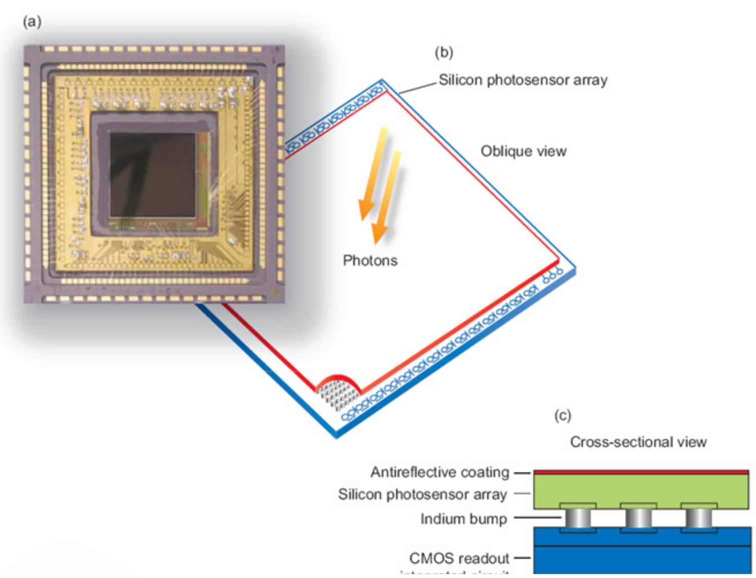
Instrumentation and Applications



The magnifier provides approximately 60-micron resolution over a 40-mm field of view and is used for over half of the dynamic radiography. The identity lens system is used for the other experiments, providing 200-micron resolution over a 120-mm field of view. These two systems allow the flexibility to study a large range of experiments designed to understand materials in extreme environments.



The camera system was developed by LANL and fabricated by Teledyne, providing 15 frames of high-quantum-efficiency images. This camera system won an R&D 100 award, and the technology developed to build these cameras is being further developed for other applications.

This 6-ft-diameter vessel is made of 2-in.-thick steel and is capable of containing dynamics experiments that use up to 10 lb of high explosives. This vessel is used to perform ~50 dynamic experiments per year without maintenance, enabling the pRad project to fully use the available beam time.

Proton Radiography Granular Flow Experiments for a 2D Mesoscale Model

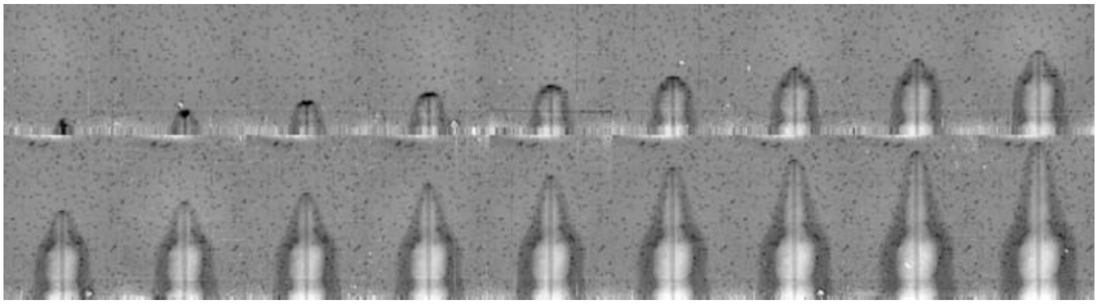
The use of granular materials is vital to industries, ranging from mining to ballistic mitigation in the commercial and military sectors. Macroscopic solid grains under dynamic load have different physical properties from either a bulk solid or a liquid. Until recently, the study of shock compression of granular materials such as sand has been limited due to lack of in situ diagnostic techniques at such high pressures and high velocities. Proton radiography, a technique developed at LANL, has the unique ability to generate a time series of many radiographs of a single dynamic experiment. LANL researchers collaborated with the Institute of Shock Physics at Imperial College London and Cambridge University to perform pRad experiments at LANSCE on well-characterized Eglin sand. Their goal was to take radiographic measurements of the particle flow field in the sand target as a function of time.

The scientists designed the pRad experiments for two kinds of shock drive and both wet and dry sand targets. The drives were either small buried charges or copper jets, known as “vipers,” which are generated by lined shaped charges. The individual sand particles were of such small size and so evenly distributed that the particles could not be tracked individually. Therefore, the researchers embedded a plane of scattered tungsten tracer particles that had very high radiographic contrast to the surrounding sand. These tracer particles allowed them to extract the velocity field as a function of position in the sand and time after the incident shock arrived. The figure at right (top) shows the time development of the particle field from a single dry sand experiment. The motion of the tungsten particles can be seen after the shock wave passes them. From this motion and the known time between the radiographic frames, the scientists could determine the velocity field of the particles and the surrounding sand.

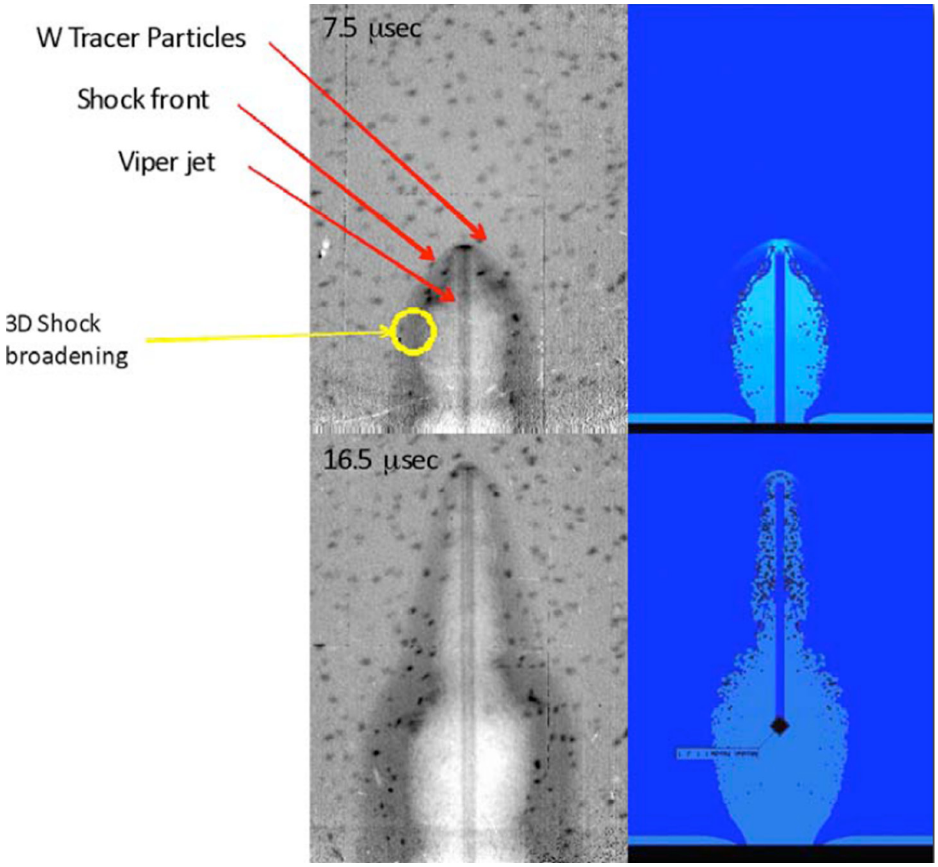
The researchers examined wet and dry flow fields under shock conditions. Even a small amount of liquid added to a dense granular material forms connections or bridges at the contact points between grains. The surface energy of those bridges forms an attractive force between the grains that is absent in dry granular materials. However, a coating of water on the grain contacts could reduce intergranular friction. Therefore, wet sand has both repulsive and attractive grain interactions, whereas dry sand has only the repulsive. Given that these microscopic interactions differ between wet and dry sand, it is not surprising that the macroscopic behavior also differs. The scientists observed that the penetration rate of the viper is greater in wet than dry sand, and the velocity field differs between wet and dry sand conditions. The grain level response with the heterogeneous target could result in asymmetric loading of the projectile, which could lead to variations in projectile performance. Continuum constitutive models fail to capture this complicated grain level response completely. The figure at right (bottom) shows a continuum model, calculated using the Autodyne software code with a simplified equation of state of sand, which simulates the dynamic response of a shaped charge projectile penetrating the sand. The researchers compared their simulation with two individual frames of proton radiography data selected from the figure at right (top). The scientists are using the data to develop a 2D mesoscale model to account for the asymmetric loading and the grain level effects, which could be crucial to predicting the penetration depth and rate and the overall effectiveness of the projectile.

Researchers include C. L. Schwartz (Neutron Science and Technology, P-23) and W. D. Neal (Institute of Shock Physics, Imperial College, London, UK) for the Granular Flow Collaboration. NNSA Science Campaign 3 (LANL program manager E. Mullen) funded the research in part.

The work supports the Lab's Nuclear Deterrence and Global Security mission areas and the Materials for the Future science pillar.



(Top): A copper "viper" jet penetrating a target of dry sand, radiographed 18 times, beginning at 1.5 microsecond after impact. Images are separated by one microsecond.



(Bottom): Comparison of experimental data frames 7 and 16 from top figure (left) to simulation (right).

Unstable Richtmyer-Meshkov Growth of Solid and Liquid Metals in Vacuum

LANL is actively engaged in the development and implementation of ejecta source and transport models. Past efforts supported theory and model development, with ejecta source and transport measurements taken from machine-roughened tin (Sn) surfaces. Currently, however, we are validating our models with experimental results from larger-scale perturbations that permit the study of the physics of ejecta production with dynamic penetrating proton radiography.

To support our modeling efforts, recent Richtmeyer -Meshkov (RM) experiments on Sn at LANL explore three aspects of ejecta physics: total mass ejected, ejecta mass velocity distributions, and driving conditions under which ejecta do or do not form. Our experiments span a sufficiently wide range of pressures to encompass ejecta formation resulting from the RM-unstable growth of both solid (low pressures) and liquid metals (high pressures),[1] but here we review the unstable liquid Sn growth.

We first consider the case for metals that liquefy on single shock compression or during isentropic shock release. The shockwave is driven through the metal into sinusoidal perturbations at the metal vacuum interface. When the shockwave arrives at the interface, it first releases to zero pressure (the metal is compressed, the vacuum is not) at the perturbation minima and then reflects back into the metal as a rarefaction wave. A brief time later the shockwave releases to zero pressure at the perturbation maxima, also reflecting back into the metal as a rarefaction wave. Under these conditions, the stresses produced by the shockwave interacting with the perturbations cause the perturbation minima to compress, invert, and then grow in tension as RM instabilities (spikes) into vacuum. Because the compressed RM spikes grow quickly relative to the initial perturbation maxima, the initial maxima invert and form bubbles that unstably grow into the metal, causing metal to flow into the spikes to support the spike growth. Bubbles and spikes (see bottom figure) refer to peak penetration depths on the opposite sides of the free surface, which is nominally defined as the plane through the inflections of the initial two-dimensional sinusoidal surface perturbations.

Our previous Sn ejecta work focused on shockwaves driven into millimeter-thick samples with machine-roughened surfaces. The roughened surfaces usually have periodic perturbations with wavelengths of the order of $\lambda = 100$ μm. The full peak-to-valley heights of the perturbations range from 2 to 25 μm, which nominally corresponds to amplitude wavenumber products on the of order $0.1 \leq \eta_0 k \leq 1$ ($k = 2\pi/\lambda$, where lambda is the period and η_0 is the perterbation amplitude). The standard diagnostics on these experiments has been laser doppler velocimetry (LDV, to measure high-speed velocities) and soft (low-energy) x-radiography (to measure ejecta masses).

Our small-scale ejecta experiments and standard diagnostics allow us to diagnose the ejecta velocities, the free-surface velocities, and the mass distributions, but we are not able to observe the bubble and spike dynamics directly with soft x-radiography. This inability to observe occurs because typical dynamic x-radiography techniques resolve only a few line-pairs per millimeter, i.e., a spatial resolution of $\approx$200 μm, which is to be compared with the small η_0 and $\lambda \approx$ 100-μm wavelength perturbations. Dynamic x-radiography also typically returns only a maximum of four radiographs in complex fielding geometries.

In contrast with the soft x-radiography work, pRad can provide a spatial resolution of the order of 80 μm when combined with the ×3 electromagnetic quadrupole lens. Given the structure of the linear accelerator, when combined with the magnifier and collimation system, it is possible to acquire up to 18 high-resolution images on a single dynamic event. The images have an exposure duration of $\approx$200 ns, which would include $\approx$20 proton pulses per exposure, with each proton pulse being $\approx$60 ps long. The transmitted protons are imaged onto a set of six gated, three-frame complementary metal–oxide–semiconductor (CMOS) cameras, the inter-frame times of which are set to be on the order of a microsecond for most dynamic experiments.

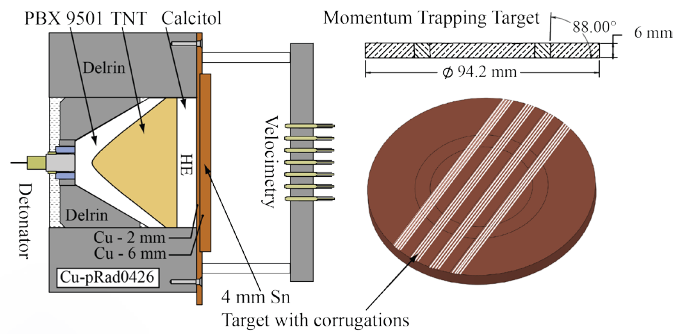
These x-radiography limitations and the RM physics requirements have driven us to do the experiments at the LANSCE 800-MeV pRad facility. Given that we wish to resolve the bubble and spike dynamics, we have moved our experiments to pRad. Thus, we can resolve the dynamics with adequate sampling perturbation wavelengths of $\lambda \gtrsim 450$ μm, and amplitudes of $2\eta \gtrsim 100$ μm.

In designing packages that addressed the full set of needs, we settled on using a P076 driver (76-mm-diameter HE lens), and we used Calcitol boosters for the Sn experiments. The final geometries are similar to the design seen in the top figure.

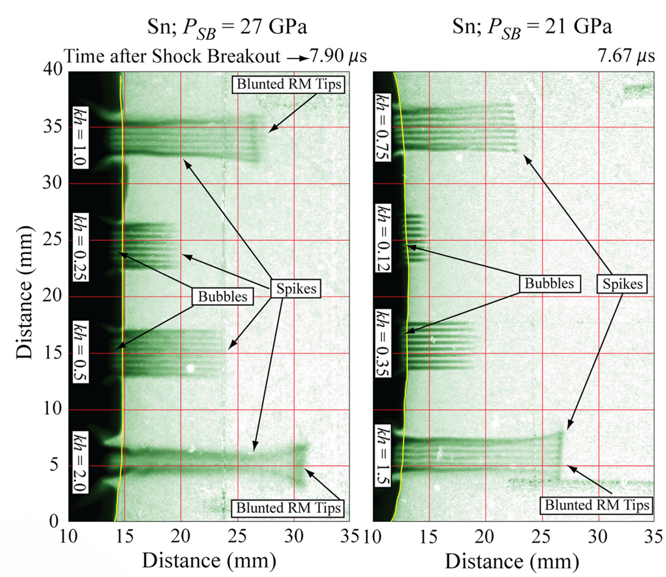
The bottom figure shows two late-time, ×3-magnified images from the pRad experimental geometry (see top figure): Sn at P_{SB} = 27 GPa is to the left, and Sn at P_{SB} = 21 GPa is to the right. The free-surface velocities were measured with LDV from the flat areas between each perturbation region, and the bubble and spike velocities were measured by LDV, as well.

Because the two Sn experiments released to a partial liquid phase, their spikes grew without bound. The Sn data present the opportunity to resolve bubble and spike dynamics that cannot be observed in smaller-scale experiments. For example, from our small-scale experiments, it is clear that the spikes quickly reach their asymptotic velocities much faster than we have been able to resolve. In addition, we have not been able to resolve any early-time bubble dynamics in the x-radiography.

Reference: [1] W.T. Buttler et al., "Unstable Richtmyer-Meshkov Growth of Solid and Liquid Metals in Vacuum," *J. Fluid Mech.* **703**, 60-84 (2012).



(Top). pRad RM experimental packages encase a 76-mm-diameter plane-wave Calcitol lens in acetal plastic. The lens detonates an HE booster that drives a buffer plate and three-piece target (on right). The targets included four λ = 550-μm bands of sinusoidal corrugations with varying amplitudes. Each corrugation band was separated by flat regions used to determine velocity histories.



(Bottom). Sn RMI instability pRad images. The time of shockwave breakout is given above each image. The perturbation wavelength was λ = 550 μm; $\eta_0 k$ is shown to the left of each perturbation region; u_{fs} was diagnosed with LDV (a).

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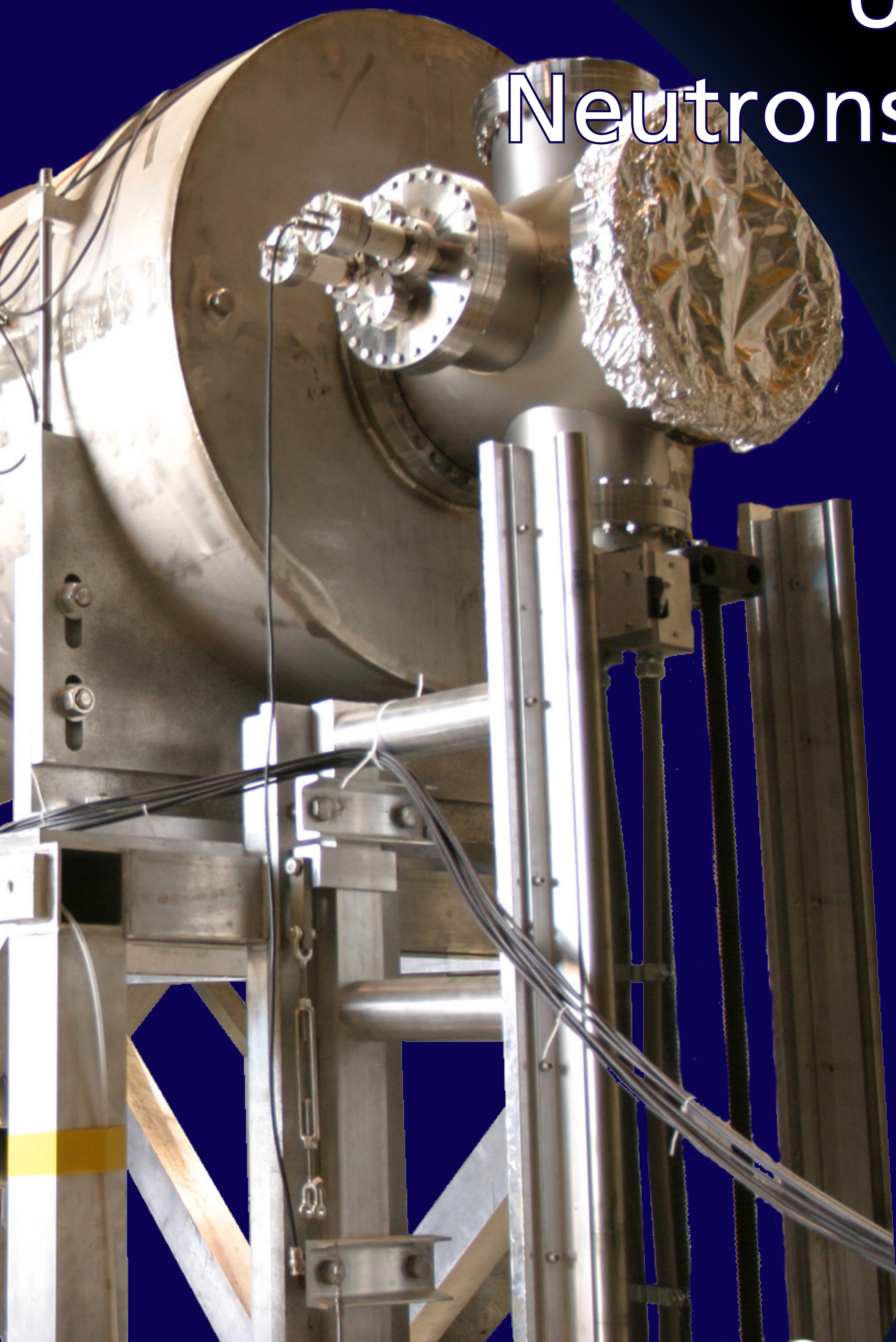
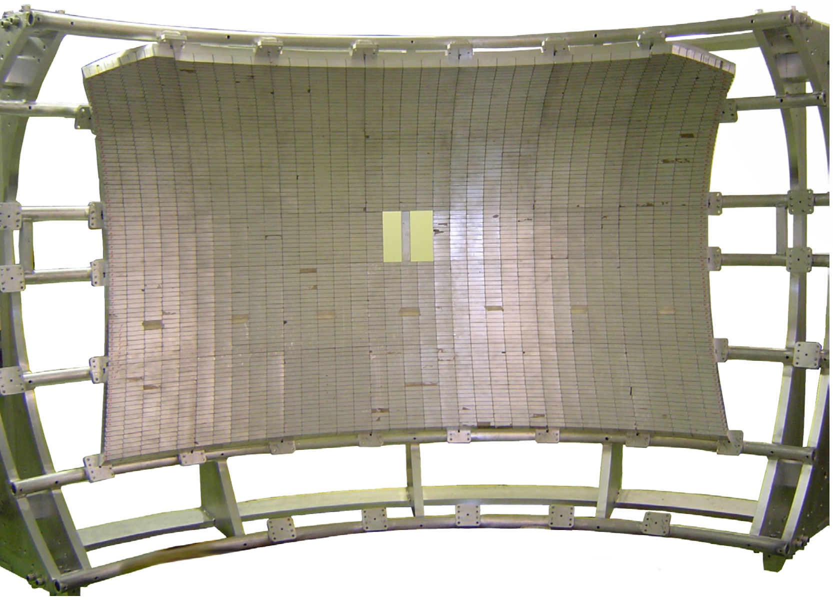
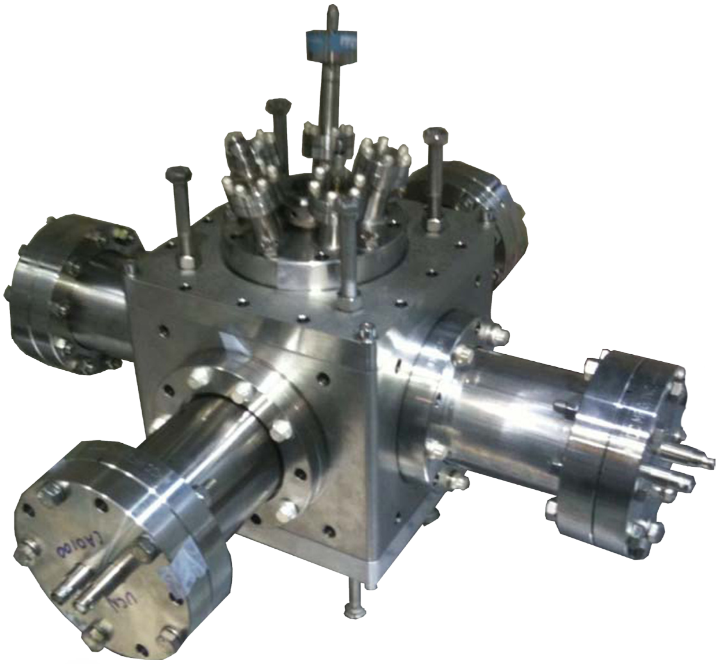


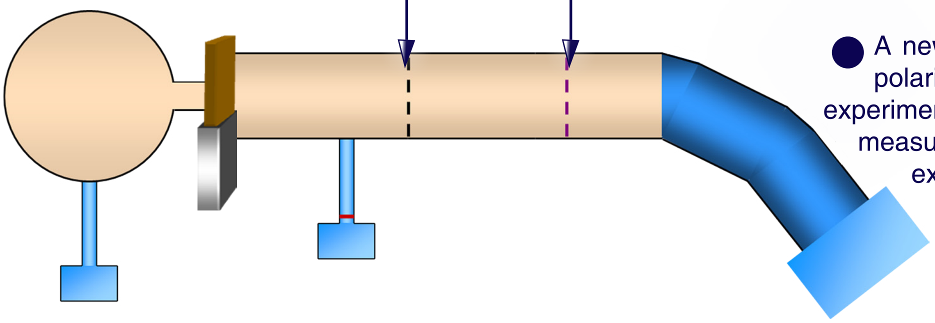
Instrumentation and Applications



● Neutron lifetime experiment magnetic trap: high field rare earth magnets are arranged in a Halbach array to form the walls and bottom of a trap that will hold ultracold neutrons. Because ultracold neutrons have very low energies, the top of the trap is formed by gravity (0.6 meters of gravitational potential is equal to the magnetic field potential at the bottom of the trap).



● UCNB spectrometer: Inside this vacuum chamber, a scintillator box holds UCN. When these UCN decay, the resulting beta particle creates light in the scintillator, which is detected by photo multiplier tubes on the sides of the box. This experiment is attempting to make the world's best beta spectrum from neutron decay to look for new physics.



● A new shutter system has been installed in the polarized beam line. This system has allowed experiments such as UCNA to get a more precise measure of the neutron polarization in the experiment.

Fundamental Physics with Ultracold Neutrons at LANL

The standard model (SM) of particle physics describes our current understanding of fundamental particles and interactions that govern the universe. To test these particles and interactions predicted by the SM, physicists measure observables, such as particle lifetimes, decay products, and decay correlations. The typical place to test these observables is at one of the world's high-energy particle accelerators, such as the Large Hadron Collider (LHC) near Geneva. At LANL, the UCN team is testing the theory using neutrons from the opposite end of the spectrum (neV) because of their unique properties.

Ultracold neutrons are defined as neutrons that can be trapped in material bottles and guides because their kinetic energies are less than the effective potential V_F (the volume average of the Fermi potential) potential,

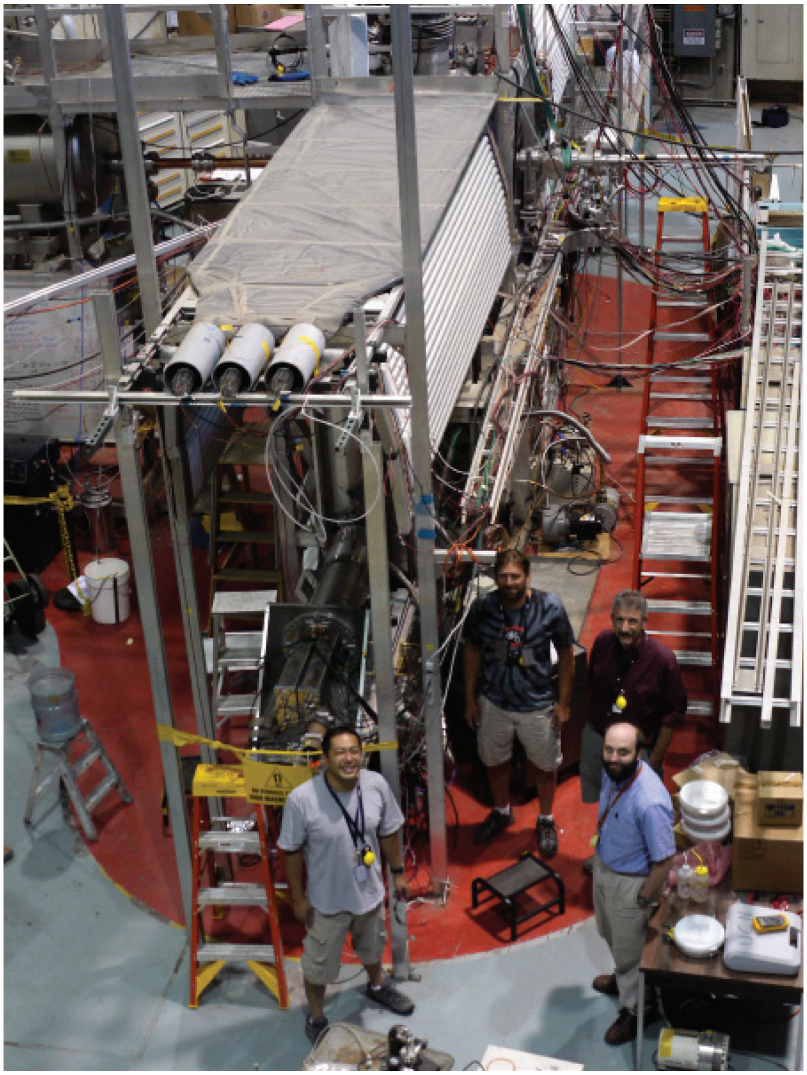
$$V_F = \frac{2\pi\hbar^2}{m} N_A \,,$$

where *N* is Avagadro's number, *A* is the material's nuclear scattering length, and *m* is the neutron mass. Nickel-58 (^{58}Ni) exhibits one of the largest potentials of available materials, 342 nV. Neutrons with kinetic energies below this (i.e., velocities below 8.09 m/s) can be trapped in a ^{58}Ni bottle. In addition to being trappable in material bottles, UCN can be trapped by strong magnetic fields (u.B~60 neV/Tesla) and gravity (1 meter of height gives 102 neV of potential). Two books and a recent review highlight the wide variety of physics that can be performed using trapped UCN.

In the past decade, experiments have demonstrated several advantages of using ultra-beta decay experiments. Measuring the decay of neutrons contained in material bottles eliminates systematic errors associated with defining the volume that plagued neutron lifetime experiments with cold neutron beams and therefore allows more precise measurements. More recently, results obtained with the LANSCE UCN source have demonstrated that the high polarizations and low backgrounds that can be obtained with spallation-driven, pulsed UCN sources can reduce the systematic errors in measuring the spin dependence of neutron beta decay relative to cold neutron beam-based experiments.

UCNA is the flagship experiment for the LANSCE UCN source, and it looks at the decay of polarized UCN by measuring the correlation between the momentum of the decay electron and the parent neutrons polarization. The UCNA experiment is currently taking data, and preliminary results have been published (see the highlight for a full description). The ratio of the vector and axial vector coupling constants.

An experiment (UCNt) using a permanent magnet walled bottle is under development to measure the lifetime of the neutron. The trap uses a uniquely arranged Halbach array to form a trap where UCN interact only with magnetic and gravitational fields. (A Halbach array is an array of permanent magnets with sequentially rotated orientations. It has the property that the field strength drops off exponentially as a function of distance from the magnet surface and is effectively a very high-order multipole magnet arrangement.)



UCNA East Detector: The UCNA experiment is run by a collaboration of universities and LANL. Pictured here is the east detector, consisting of the Caltech-built electron detector and LANL-built muon shield.

UCNA

UCNA continued to take data in 2011, with a renewed emphasis on measuring and eliminating sources of systematic error.

Achieving a result with the desired total error requires a strong understanding of the polarization of the neutrons in the decay trap, with depolarization being of paramount concern.

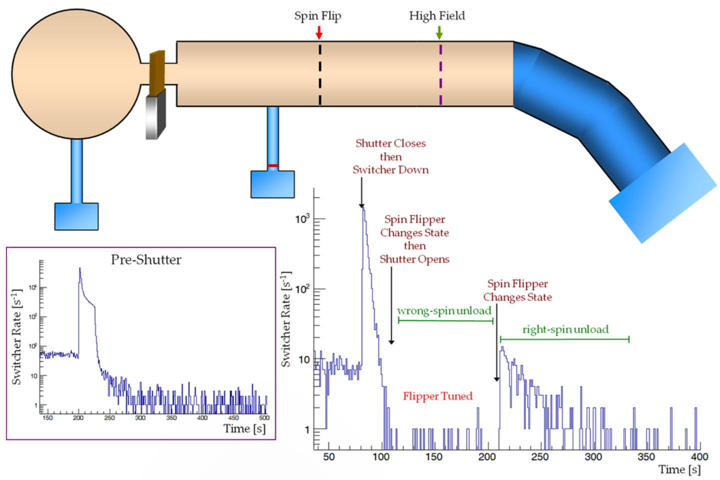
To address this issue, a shutter system was implemented that allows a much more precise measurement of the fraction of depolarized neutrons present in the system.

Initial results indicate that the uncertainty due to depolarization should be reduced by a factor of five.

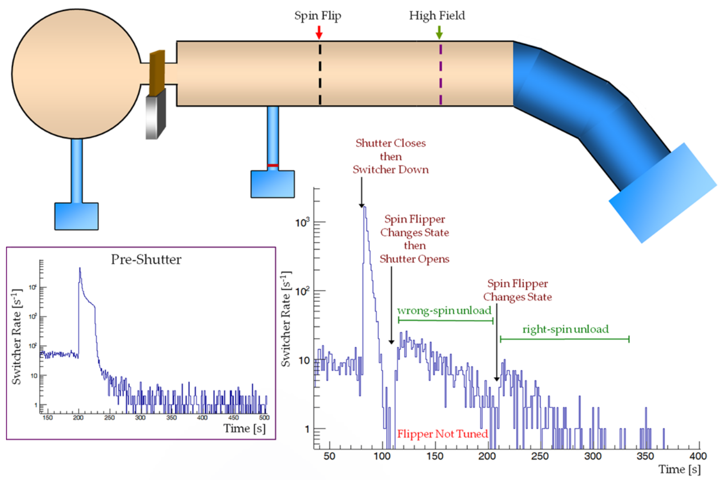
Additionally, new work in detector calibration has improved our understanding of the detector response, and a new set of thinner decay trap end foils has been developed that will decrease backscattering and energy loss effects.

While running during the 2011 beam cycle, UCNA counted approximately 34 million beta decay events, which is a strong push toward the final goal of 100 million beta decay events that is the ultimate goal of the UCNA project.

After the cycle completed, a concerted effort to improve the delivery of beam to the target was pursued. Although the effects of this effort have not yet been established, the expected improvement may result in the most intense ultracold neutron source in the world.



Flipper tuned.



Flipper not tuned.

(Top and Bottom). Changes in the switcher rate presented in the graphs highlight the improvement in sensitivity to the incorrectly polarized neutrons.

UCNB

The UCNB experiment will measure the correlation between the antineutrino's momentum and the neutron's spin as a function of the electron energy.

It is necessary to measure both the electron and the proton from the decay to deduce the momentum of the antineutrino.

Large-active-diameter (12.5-cm), highly segmented (128-pixel) silicon detectors will be used to measure the electrons and protons.

The whole detector apparatus will be biased to -30 kV to facilitate proton detection because the maximum kinetic energy of the beta decay protons is approximately 800 eV.

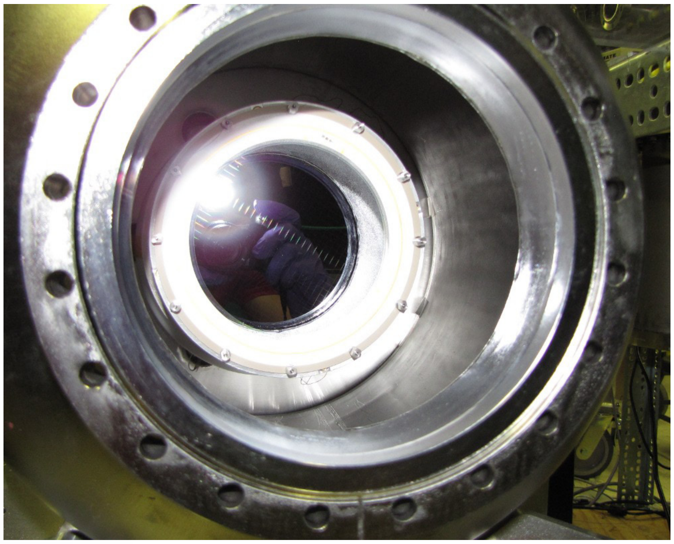
Coincident measurement of both the electron and proton will eliminate backgrounds and enable identification and control of systematic errors.

The segmentation of the detectors provides spatial resolution, which strengthens coincidence conditions because the electron and proton must arrive within roughly two Larmor radii of each other in the magnetic field of the superconducting solenoid (SCS).

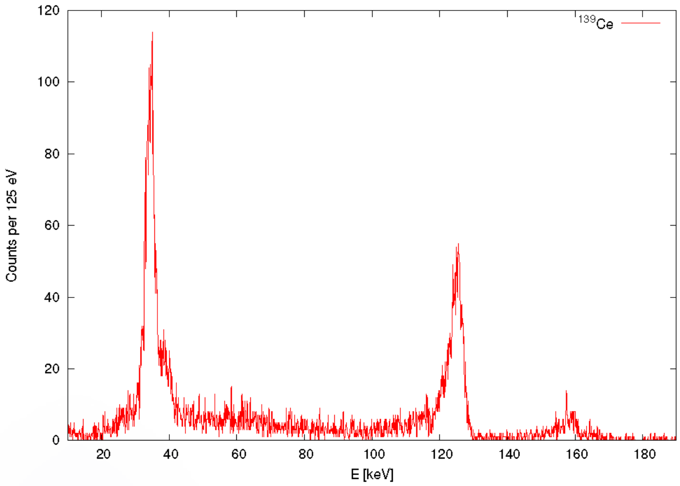
The electronics and data acquisition system must be capable of fast timing (approximately a few nanoseconds) to identify electrons that scatter from the silicon detectors before depositing their energy.

Custom amplifiers have been developed to instrument our detectors, and development of the firmware on a 12-bit, 250-MHz flash analog-to-digital converter (ADC) is ongoing to simultaneously achieve the necessary timing and energy resolution.

We are in the process of refining the detector apparatus to accommodate full bias voltage with sufficiently small leakage currents.



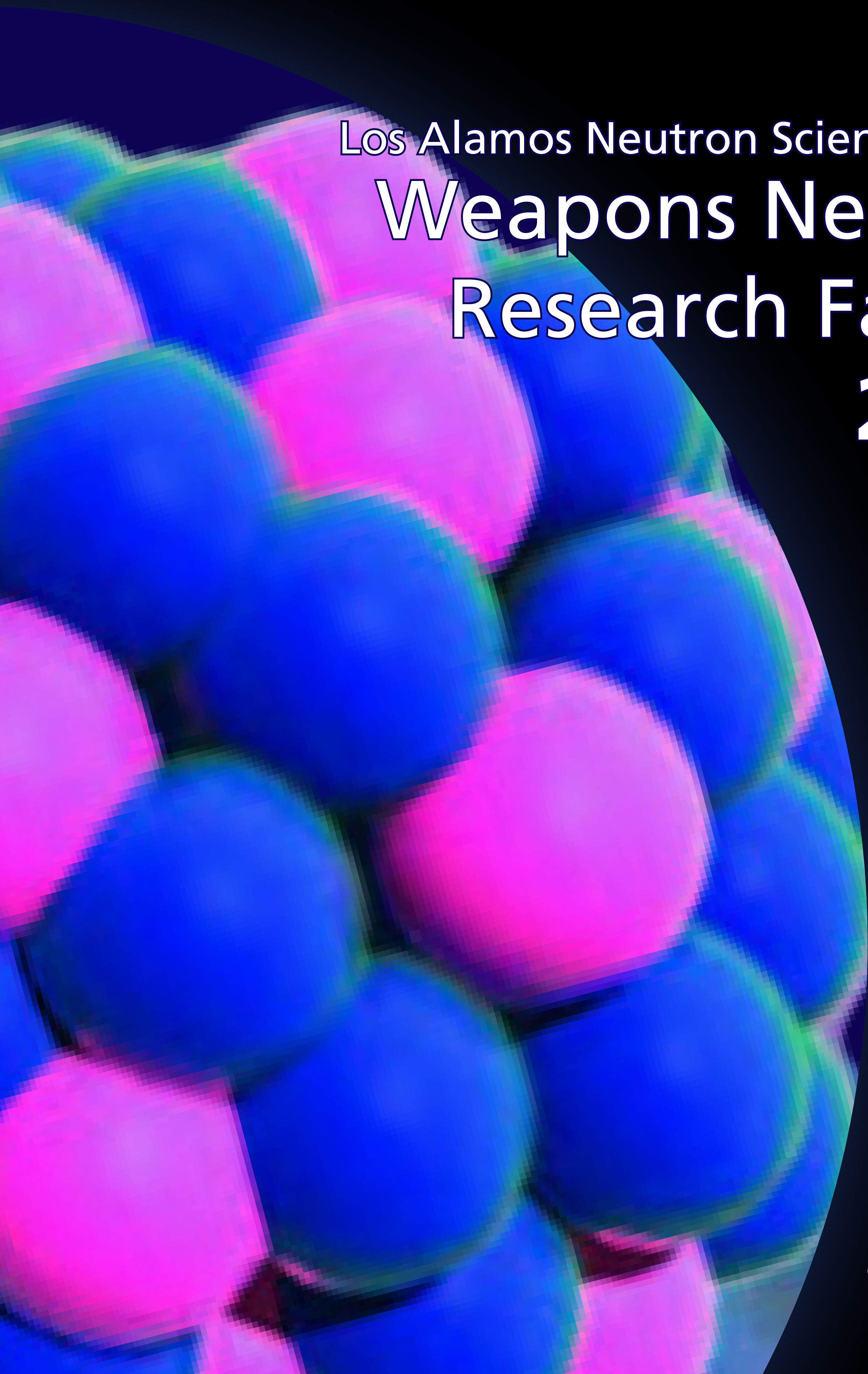
A 12.5-cm-diameter, 128-pixel silicon detector in a vacuum chamber for testing.



A spectrum of x-rays and conversion electrons from ^{139}Ce free of noise down to energies of 10 keV.

Los Alamos Neutron Science Center

Weapons Neutron Research Facility 2011



LANSCE
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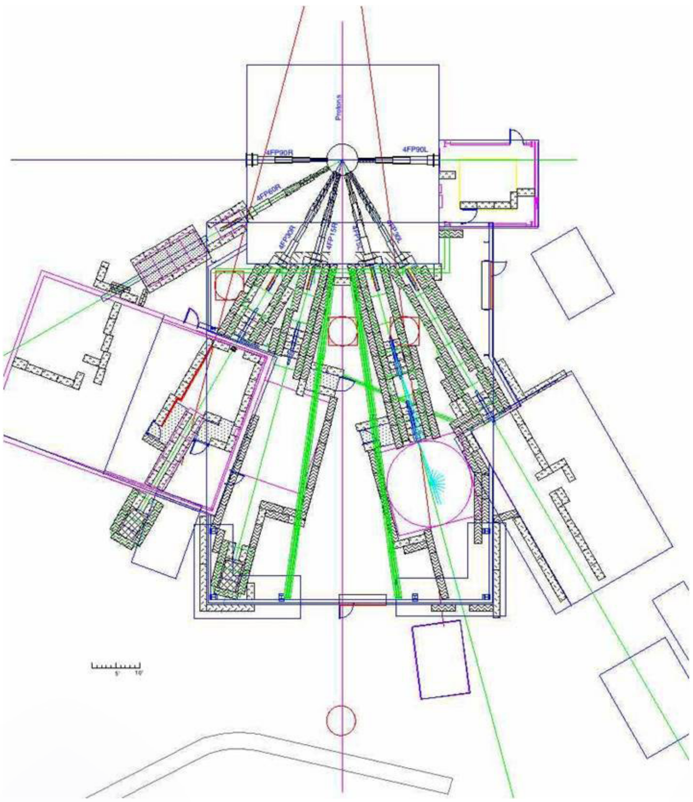
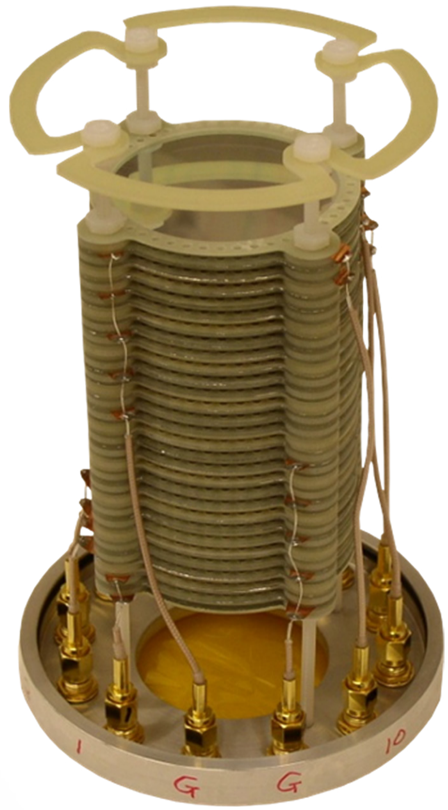
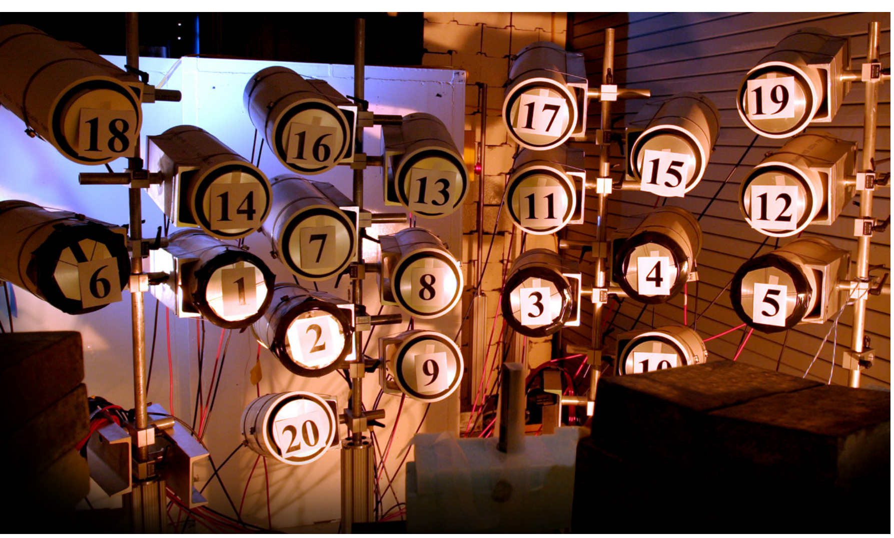
Instrumentation and Applications



WNR flight paths, including the new 15R and 15L.



ChiNu fission sample/detector: A parallel plate avalanche counter from Lawrence Livermore National Laboratory (LLNL) is much faster (1 ns) and has a much lower scattering mass than conventional ionization chambers.



Fast Neutron-Induced Gamma-Ray Observer (FIGARO) is an array of neutron detectors that are used to measure neutron emission from neutron-induced reactions at LANSCE.

New WNR Building

Construction of a new building to expand our capabilities at the LANSCE/WNR Target-4 experimental area has started. The building doubles our capacity for neutron testing of semiconductor devices with the same neutron spectrum that presently exists at the Irradiation of Chips and Electronics (ICE) House.

The new building also provides a special flight path essential for the success of neutron output measurements following fission (Chi-Nu). On this flight path, a pit in the floor under the detectors reduces the background from neutrons scattered from the concrete.

The new building will cover the 15-degree right and left flight paths, as well as parts of the 30-degree right and left flight paths, and will have a crane to move heavy shielding and equipment.

Contractors are presently excavating in preparation for framing and pouring the foundation for the building.

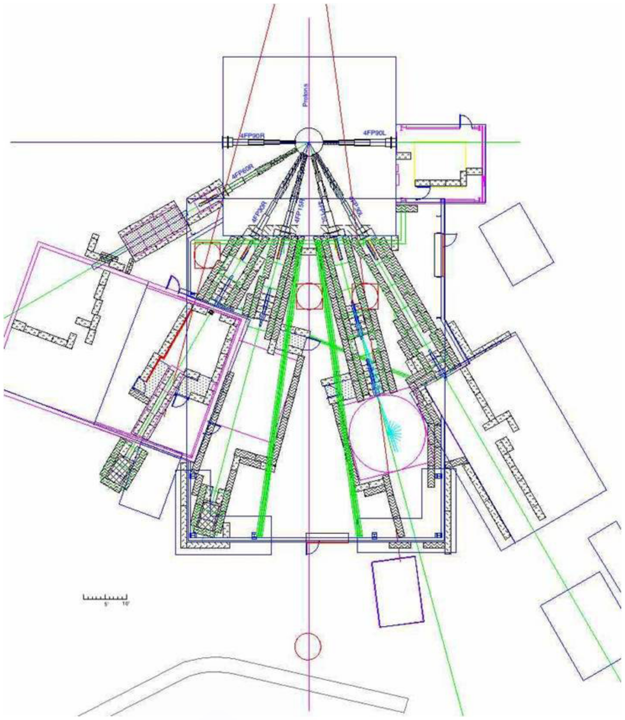
A detailed schedule is being developed that will couple the construction schedule with the installation of the flight paths. We will bring up the Target-4 flight paths in a staged sequential manner: the 90-degree left Time Projection Chamber (TPC) and the 60-degree right GErmanium Array for Neutron Induced Excitations (GEANIE) flight paths will be the first to receive beam because they are outside of the building construction area.

The next flight paths to be brought on line will be the 30-degree flight paths (ICE House and ICE-II). The last flight paths will be the 15-degree right and 15-degree left flight paths because they require the most installation effort. We will keep users informed as the work progresses, and we look forward to operations in our new facility.

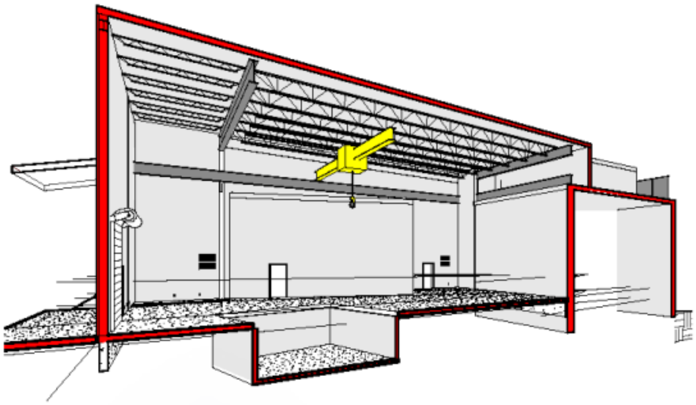
Excavation and preparation.

Installing the foundation.

Pouring the slab.



WNR flight path.



Schematic of finished building.

New Technique Developed to Measure Uranium-237

In December 2010, scientists from Nuclear and Radiochemistry (C-NR) and WNR collaborated with Oak Ridge National Laboratory (ORNL) to field a uranium-237 (^{237}U) sample at LANSCE's Lead Slowing-Down Spectrometer (LSDS). The LANSCE Accelerator Operations group and the Radiation Protection (RP-1) group provided technical support. The goal was to measure the neutron-induced fission cross section for the short-lived isotope ^{237}U (a beta emitter with a half-life of 6.75 days) for incident neutron energies between 1 eV and 100 keV. The measurement required sole use operation of the LANSCE accelerator facility.

ORNL's High Flux Isotope Reactor irradiated 1.5 mg of highly enriched uranium-236 (^{236}U) to prepare the ^{237}U sample. Then ORNL chemists used anion exchange and extraction chromatography to remove fission products and neptunium-237 (^{237}Np), the decay daughter of ^{237}U, and prepared an electroplated target. RP-1 prepared dose rate estimates as part of the planning for the measurement. The calculations indicated that there would be a substantial radiation field around the ionization chamber once the ^{237}U target had been loaded. To reduce radiation exposure to personnel, LANL scientists designed the detector with 1-cm-thick lead on all exterior surfaces. ORNL used remote handling methods to load the target and close the detector.

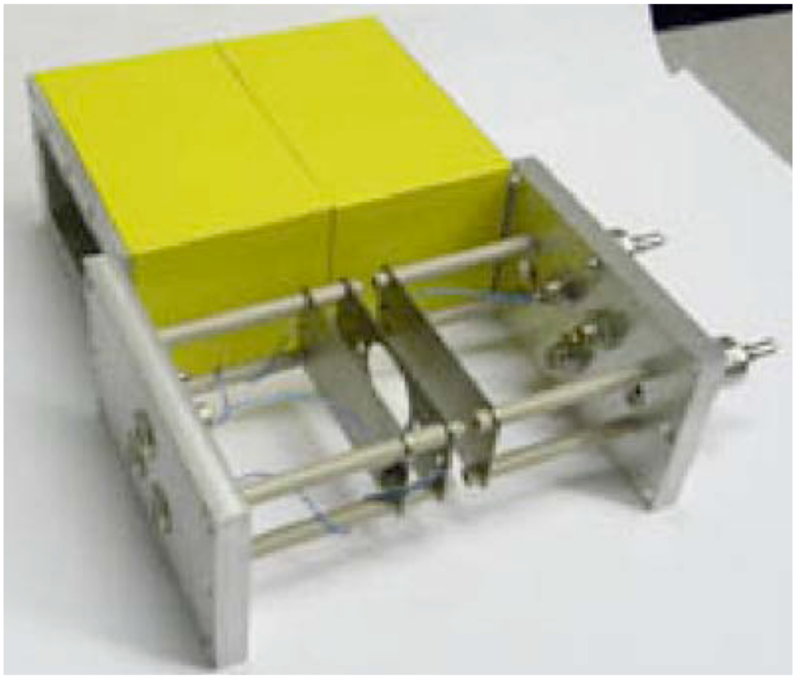
After the assembly arrived at LANSCE, researchers and RP-1 unpacked the assembly and loaded it into the LSDS. Scientists collected data for the remaining 5 days of the scheduled LSDS run. The top figure shows preliminary data for neutron energies between 2 eV and 2 keV. The data are a combination of F^{236}U(n,f) and ^{237}U(n,f), which were present in the target, with a mass ratio of approximately 500 and 2 micrograms, respectively.

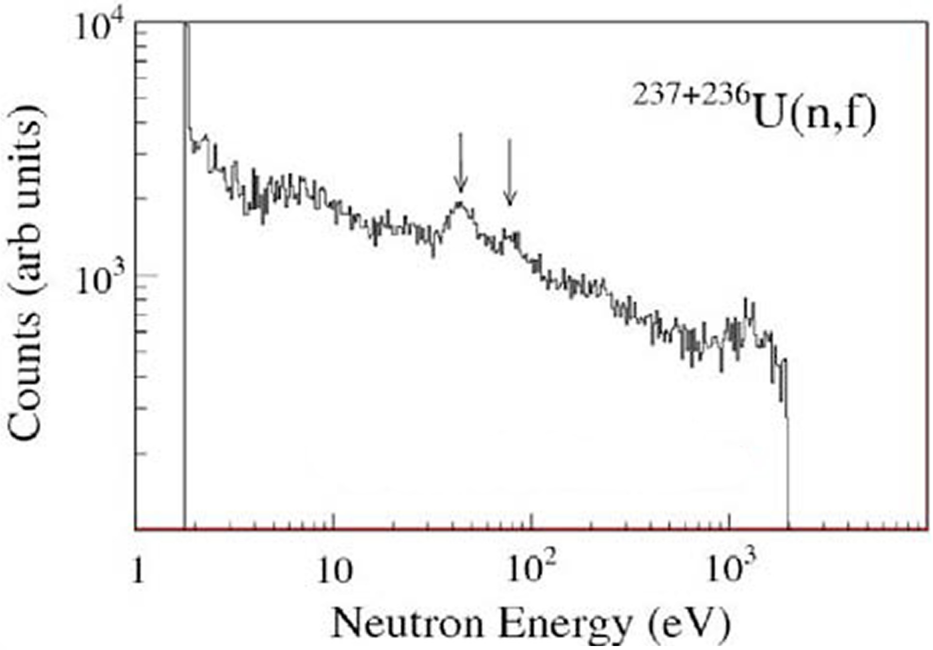
Although ^{236}U is a threshold fissioning isotope (low-fission cross section below a threshold neutron energy), the greater mass present in the target resulted in a fission rate comparable to the expected rate for ^{237}U fission. The two arrows in the bottom figure indicate fission resonances that are most likely derived from ^{237}U.

The scientists plan to repeat the measurement with the same target after the ^{237}U has decayed away, which will provide a "blank" data set to enable subtraction of the ^{236}U contribution to the data. Kim Scott is the LANL program manager for this work, which is funded by Science Campaign 4 and has national security applications.

LANL staff involved are Evelyn Bond, Todd Bredeweg, Marian Jandel, David Vieira, and Jerry Wilhelmy (C-NR); Leo Bitteker, Matt Devlin, Robert Haight, Ronald Nelson, and Stephen Wender (WNR); Michael Duran, Daniel Gallegos, William Knight, David Lee, and Markilee Martinez (RP-1).

Collaborations included the CEA (French Alternative Energies and Atomic Energy Commission) and ORNL.





(Top). Photo of LANL-designed ionization chamber used to measure the ^{237}U(n,f) cross section at the LSDS. The internal components (foreground) slide into either end of the lead-lined detector body.
(Bottom). Preliminary data from the December 2010 experiment at the LSDS.

Measuring the Fission Neutron Spectrum at LANSCE

Scientists from LANL, Japan (Kyushu University), and France (CEA Bruyères-le-Châtel) have measured the energy distribution of neutrons from neutron-induced fission. The data are used as constraints in the LANL model of nuclear fission to obtain information on the total kinetic energy of the fission fragments. Moreover, the data will improve the evaluated data libraries, which are used in applications to nuclear energy, criticality safety, and nuclear weapons development.

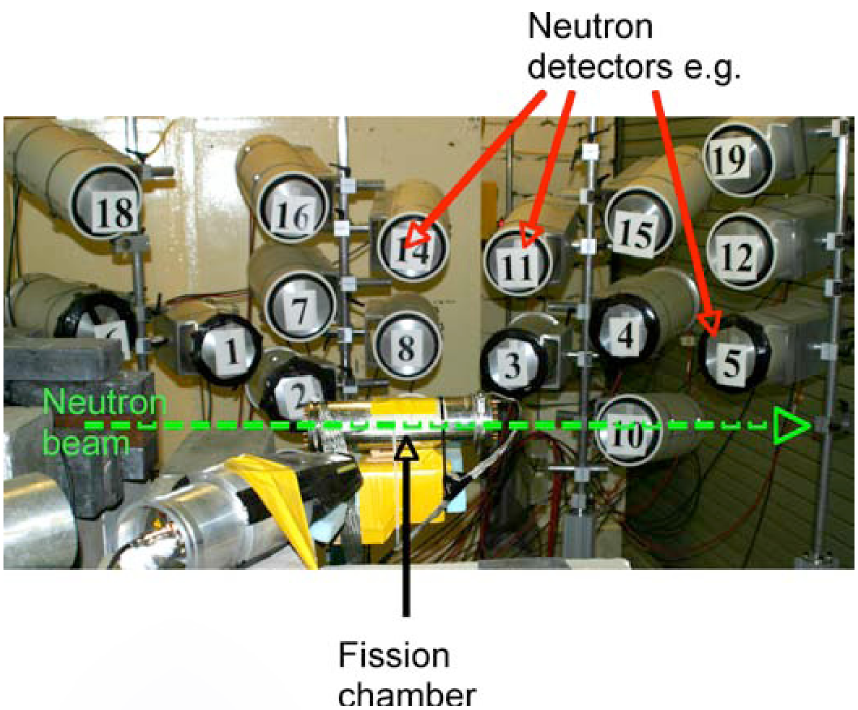
A nucleus of uranium, plutonium, or certain other elements can be induced to fission, or split into two lighter nuclei, by the addition of a neutron. When fission occurs, the two fission fragments can emit energetic neutrons, which then can induce further fissions: the principle of the chain reaction. For reactors, the chain reaches a steady state, whereas for weapons and other super-critical systems, the number of fissions increases exponentially with time. Because the probability of fission depends on the neutron energy, the energy spectra of the neutrons from fission must be known to calculate the neutron multiplication of a fissionable system. Although several measurements have been made of the neutron emission spectrum from fission induced by thermal neutrons (a neutron energy distribution characteristic of room temperature), very few measurements have been performed for fission induced by fast neutrons (neutrons with a kinetic energy in excess of 0.1 MeV). The two measurements for the important isotope plutonium-239 (^{239}Pu) are inconsistent. Therefore, the researchers' goal in the measurements at WNR is to make significant improvements in these basic data.

The approach uses a double time-of-flight technique. The WNR neutron source is pulsed to give the "start" signal, and the time of flight of neutrons to the fission detector located 22.7 meters away gives the energy of the neutron inducing the fission. An electronic pulse created when fission takes place is the "stop" signal for the timing. The fission pulse is also used as the "start" signal to time neutrons from fission in the fission chamber to neutron detectors placed 1 meter away. These detectors are called the Fast Neutron-Induced Gamma-Ray Observer (FIGARO) array. By collecting data from many fission events, a distribution of the energies of the fission neutrons is obtained and can be compared with predictions of the LANL Model. The fission chamber, which was supplied by the French colleagues, and the neutron detector are pictured in the photo. Samples of the results, are compared with data in the evaluated neutron data file, ENDF/B-VII.0, which is used around the world for applied calculations, and with predictions of the revised Los Alamos Model. Their results are in agreement with the data found in ENDF/B-VII.0. Scientists are continuing the work to reduce the size of the error bars and to extend the measurements to neutrons with energies below 1 MeV. The work supports the LANL's Nuclear Deterrence and Energy Security mission areas and the Science of Signatures and Materials for the Future science capabilities.

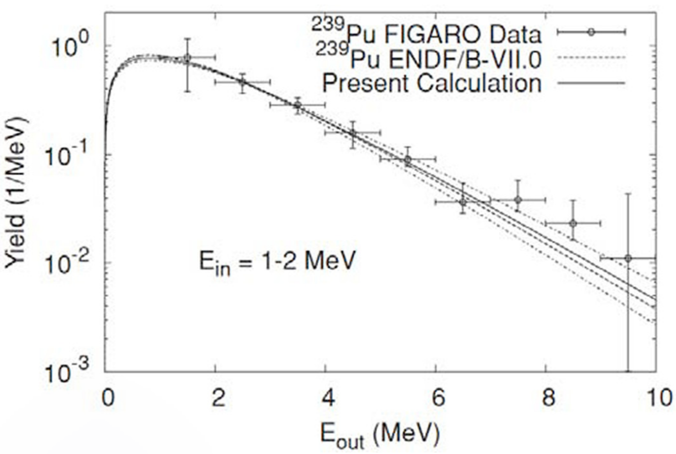
Scientists participating in the research include Shusaku Noda [Kyushu University, Neutron Science (WNR), and Nuclear and Particle Physics, Astrophysics and Cosmology (T-2)], Robert Haight, Ronald Nelson, Matthew Devlin, and John O'Donnell (WNR); Audrey Chatillon, Thierry Granier, Gilbert Belier, and Julien Taieb (CEA); Toshihiko Kawano and Patrick Talou (T-2).

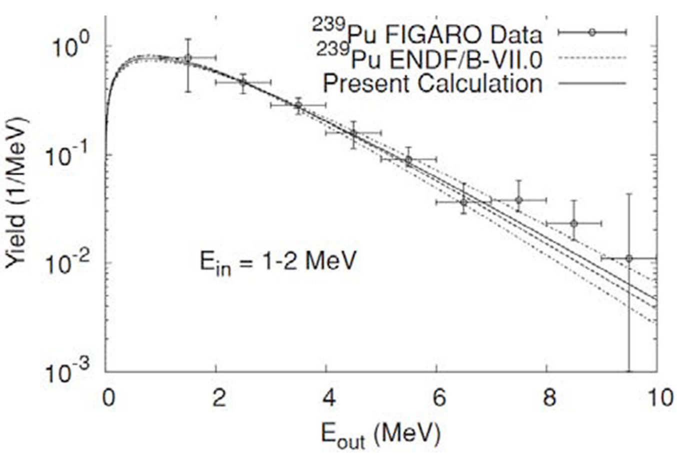
Reference: "Measurement and Analysis of Prompt Fission Neutron Spectra from 1 to 8 MeV in Neutron-Induced Fission of ^{235}U and ^{239}Pu Using the Double Time-of-Flight Technique," *Physical Review C* **83,** 034604 (2011); doi:10.1103/PhysRevC.83.034604.

AOT and LANSCE - The Pulse, October 2011.
LALP-11-017



Fission chamber and neutron detectors (numbered).





Sample results of the prompt fission neutron spectra for two incident neutron energies, 1-2 MeV and 5-6 MeV. The data (FIGARO) are compared with those in the Evaluated Nuclear Data Library (ENDF) and with predictions of the modified the Los Alamos Model (present calculation). Scientists adjusted input parameters of the latter to fit the present data.

Los Alamos Neutron Science Center

User Program 2011

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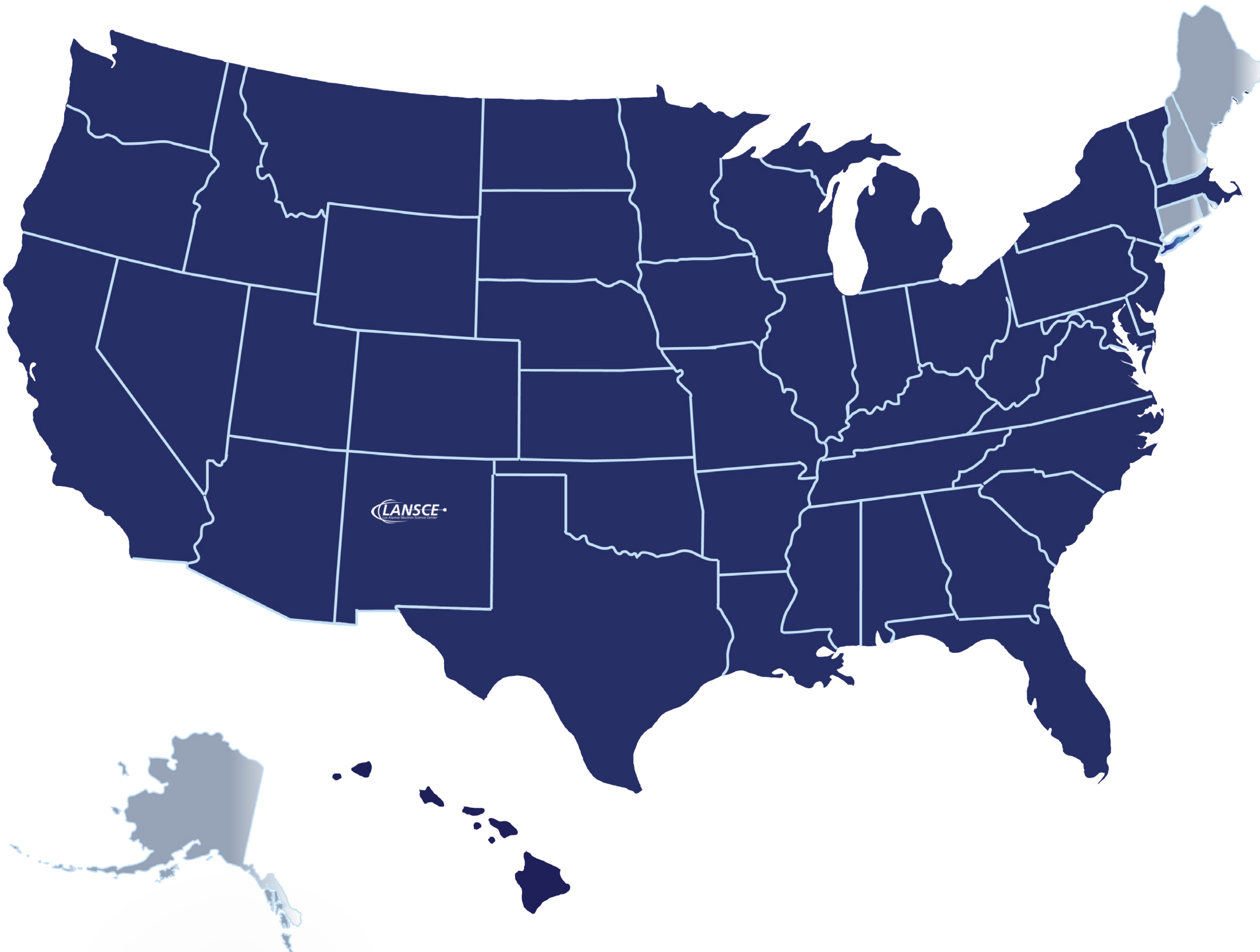
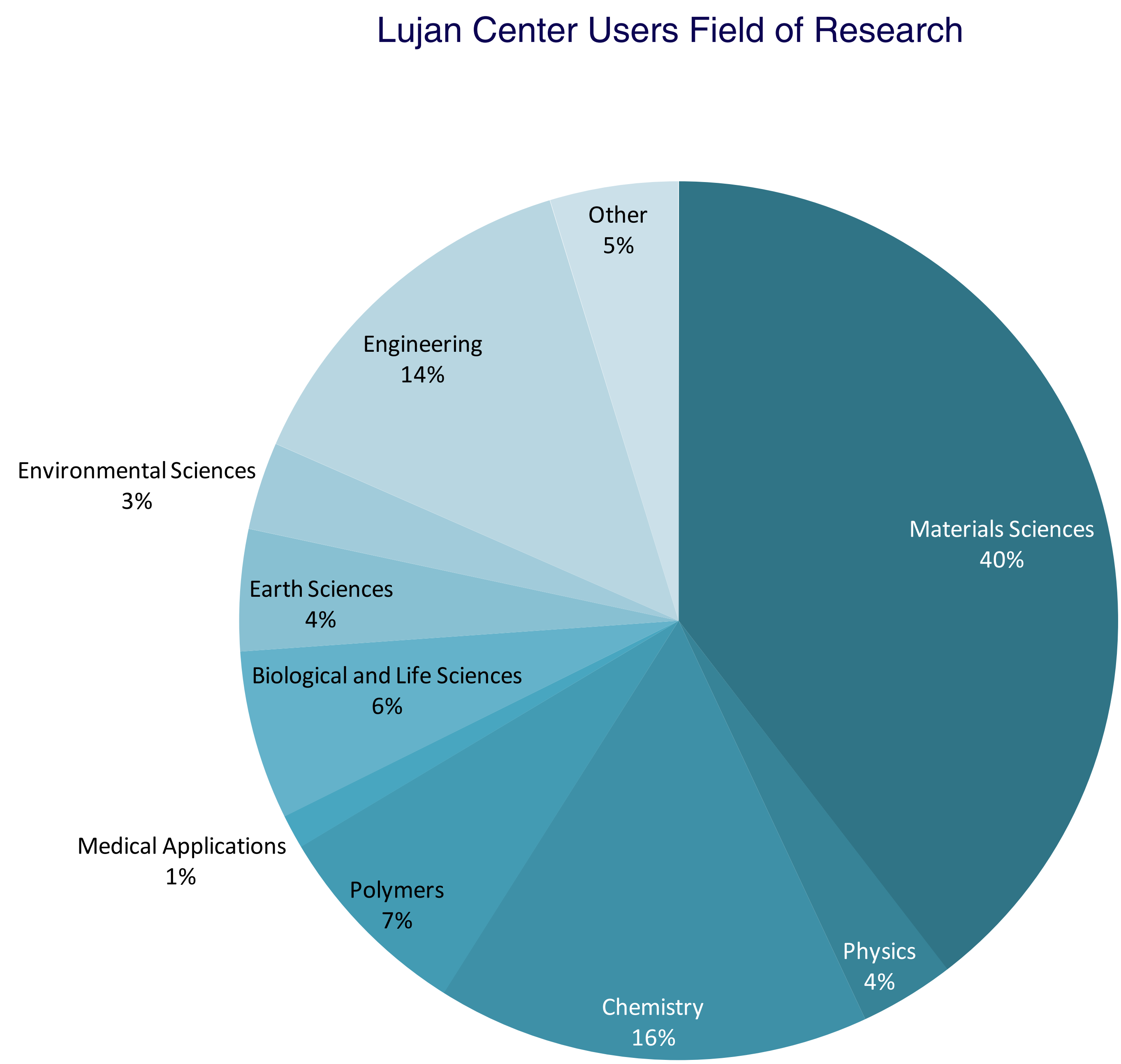


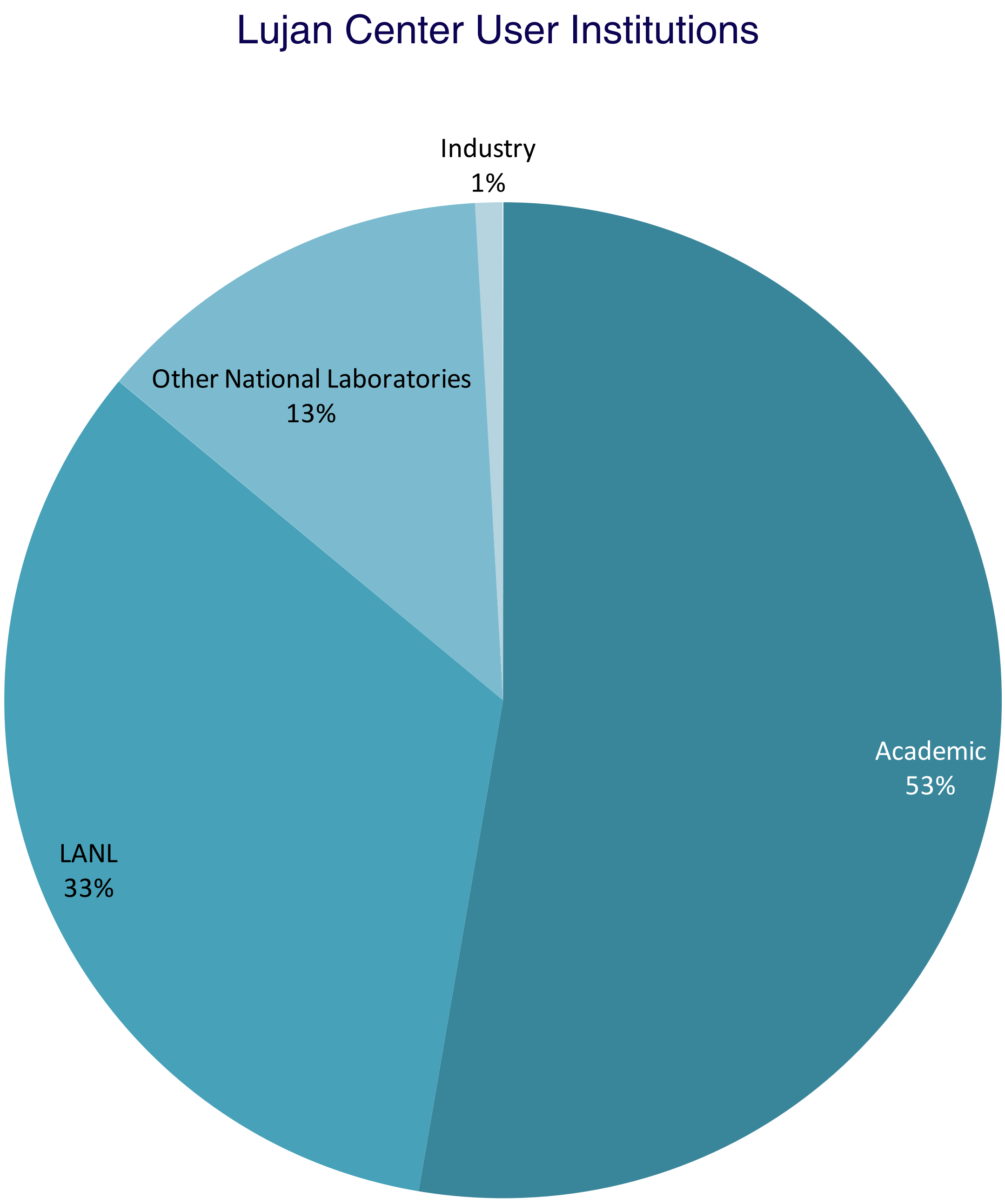
US States Represented by LANSCE Users

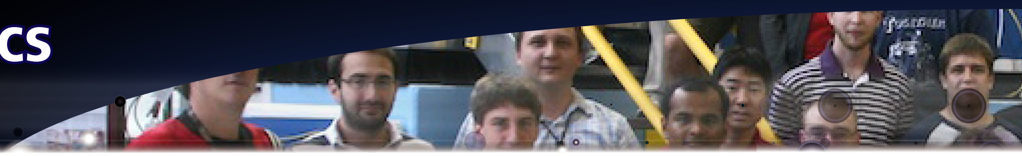
LANSCE's designated National User Facility Program hosts users from nearly all 50 states in the US.

Lujan Center Users

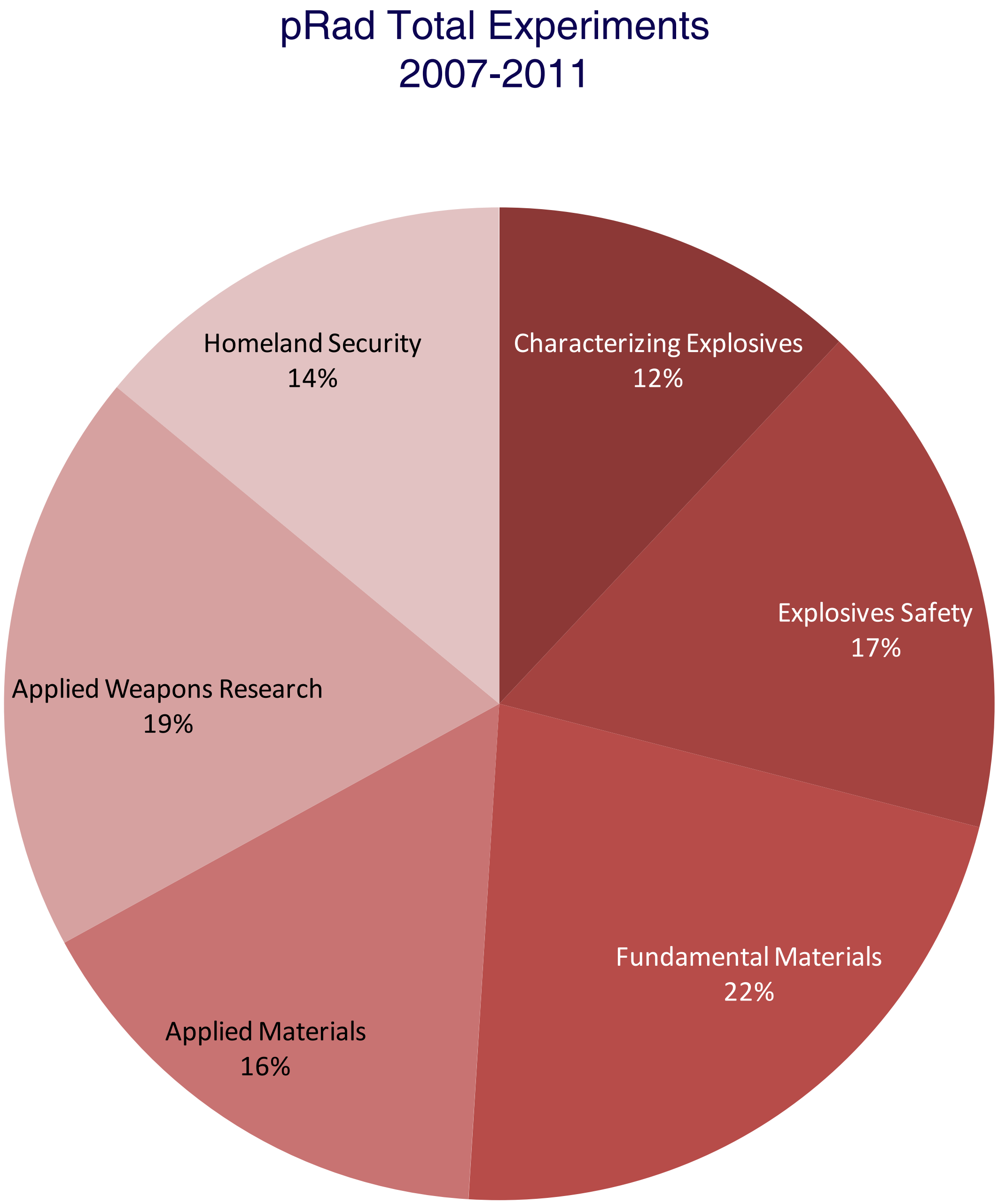


Lujan Center Users





pRad Users


pRad Total Experiments
2007-2011
Characterizing Explosives
12%
Explosives Safety
17%
Fundamental Materials
22%
Applied Materials
16%
Applied Weapons Research
19%
Homeland Security
14%

pRad User Program

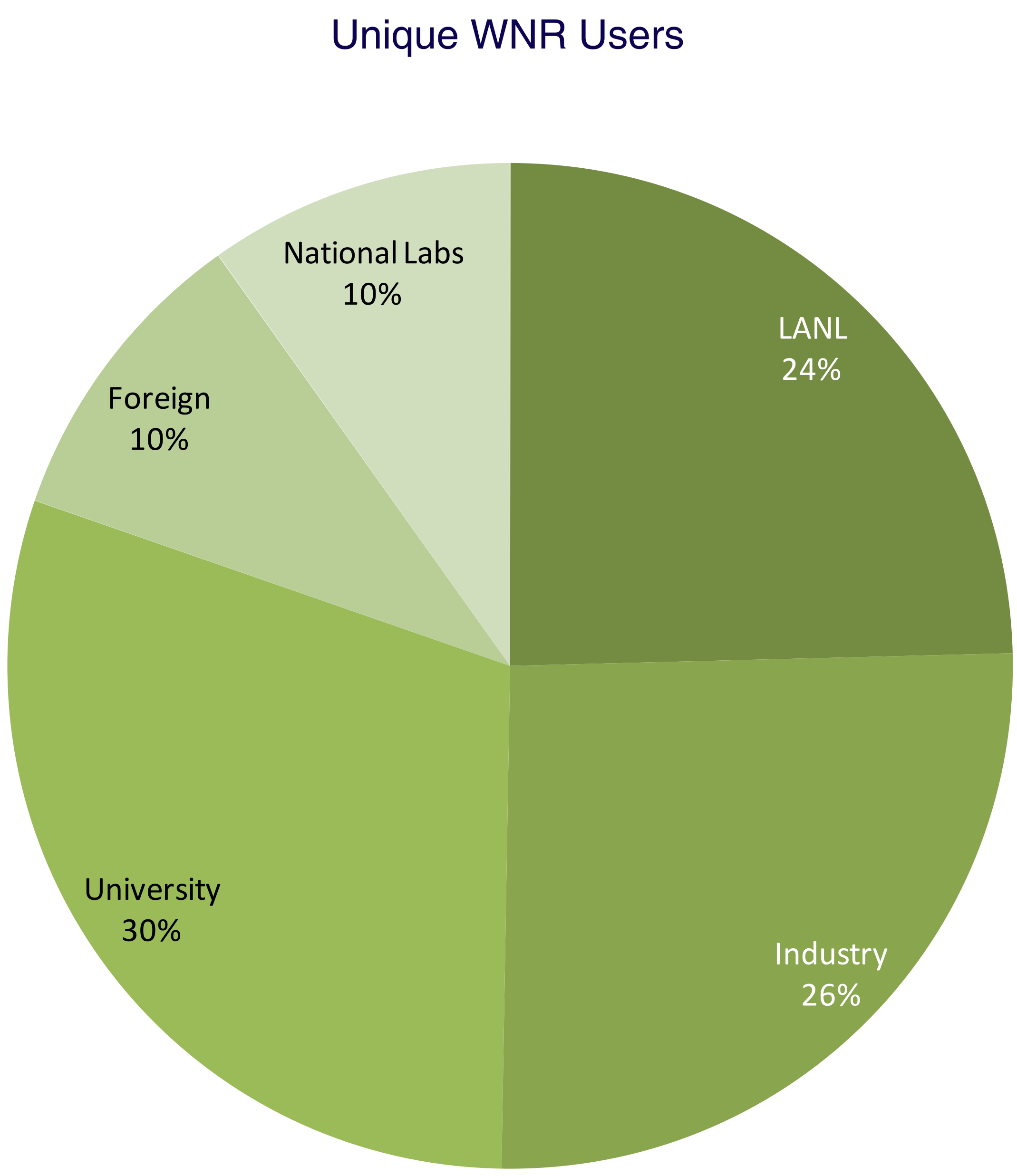
The pRad effort at LANSCE has operated as a user facility since 2003 and has recently been designated as one of the three DOE user facilities at LANSCE. Currently, the user community extends from the DOE-NNSA national laboratories (LANL, LLNL, SNL, and ORNL) to international users (AWE, CEA, and VNIIEF) and has recently grown to include DoD laboratories (ARL, and Eglin AFB), as well as university interest (Harvard, Imperial College, and the Technical University of Darmstadt).

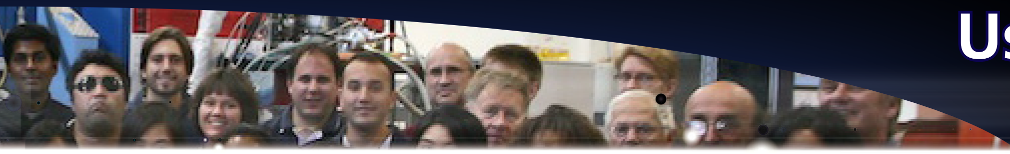
Currently, pRad at LANSCE is a dual-use facility, which allows access for users interested in classified research, as well as for external users interested in unclassified research. This user program will continue to provide a pool of scientific talent for recruitment into the national weapons program.

The LANL pRad team also offers mentoring, research, and employment opportunities for students and postdoctoral researchers.

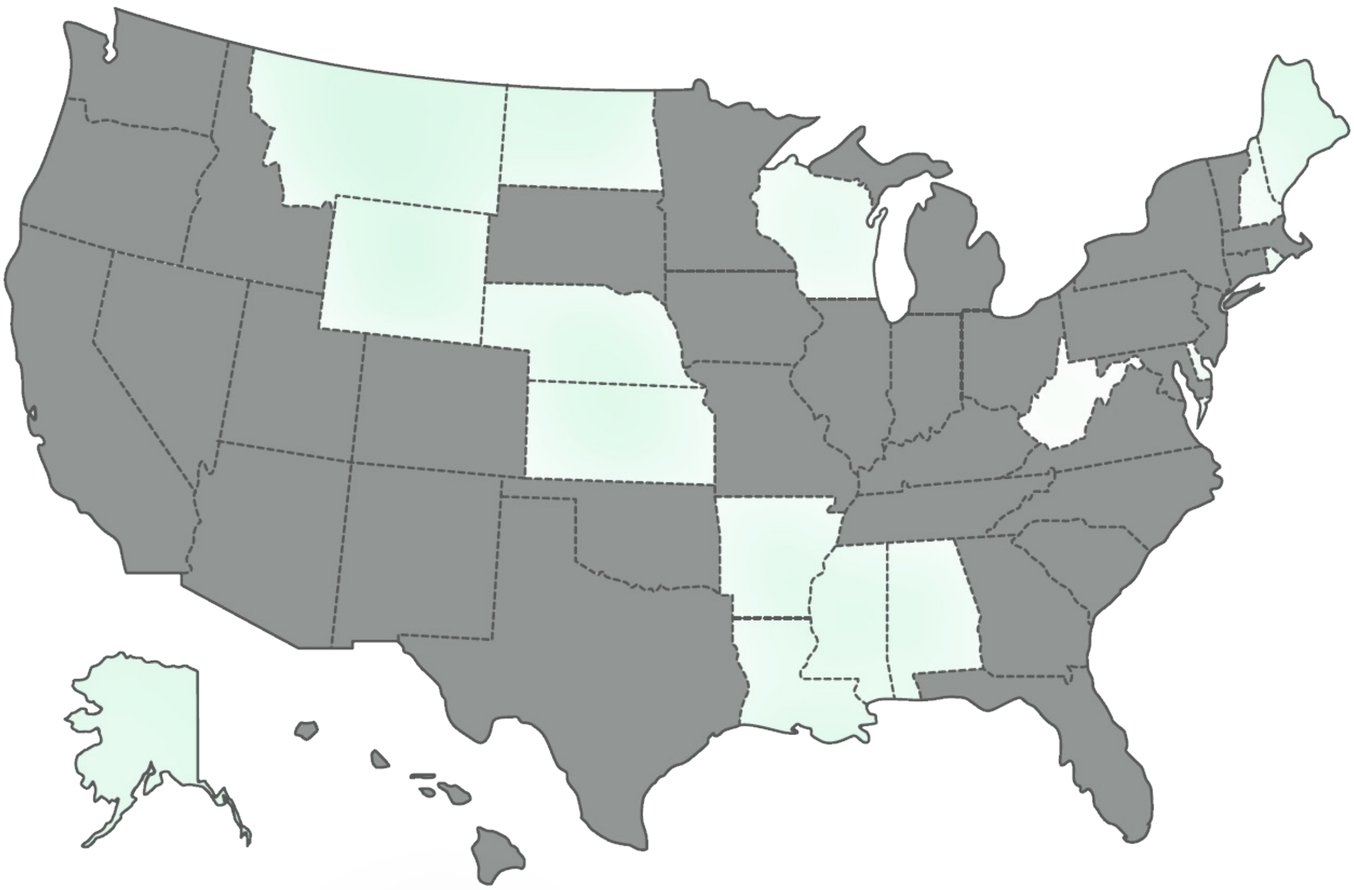
Summer students working with pRad

WNR Users


Unique WNR Users
National Labs
10%
LANL
24%
Foreign
10%
University
30%
Industry
26%



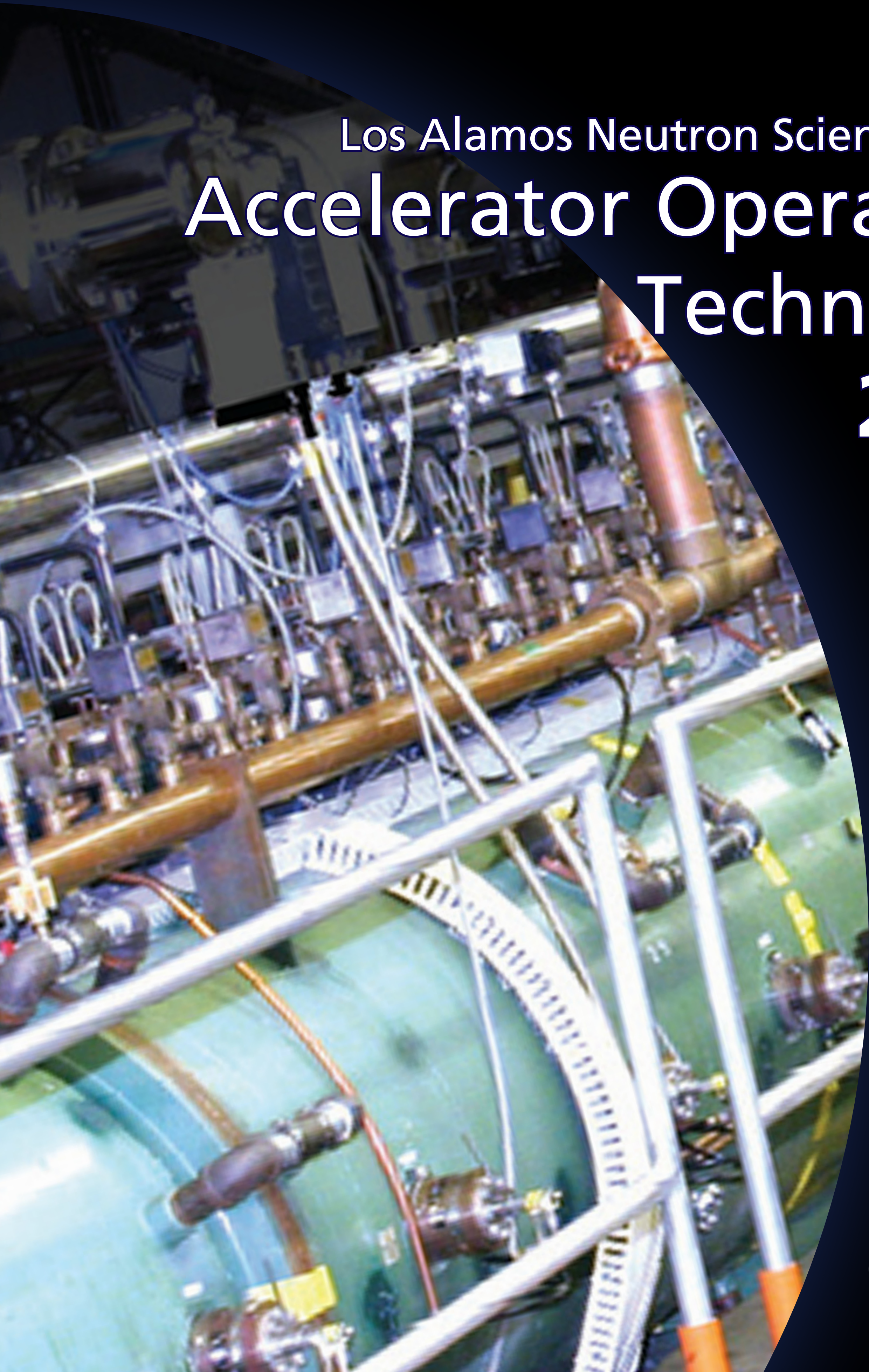
WNR Users



States represented by WNR users.

Los Alamos Neutron Science Center

Accelerator Operations Technology 2011



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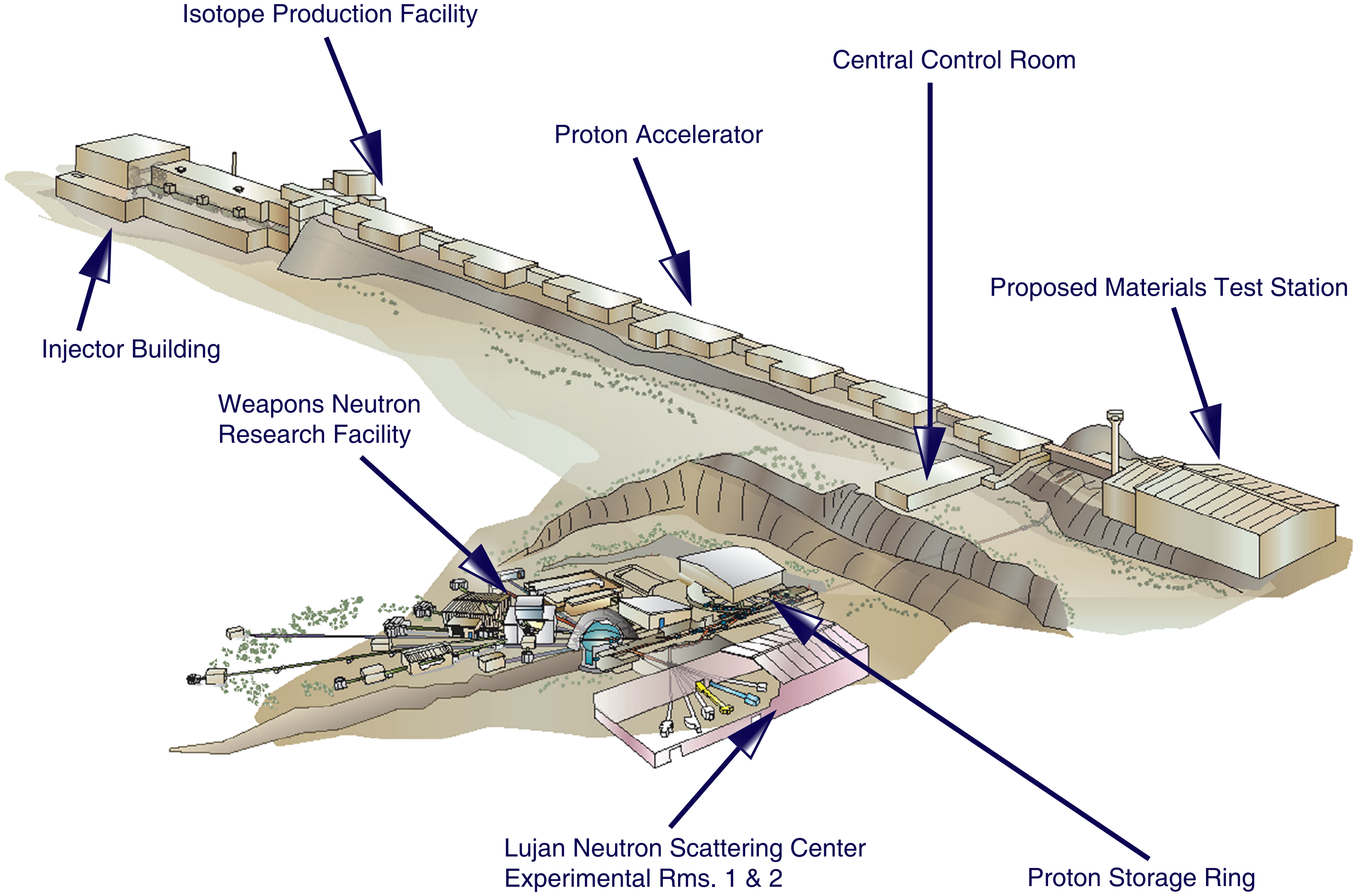


Schematic of LANSCE's beam delivery.

LANSCE Beam Facts

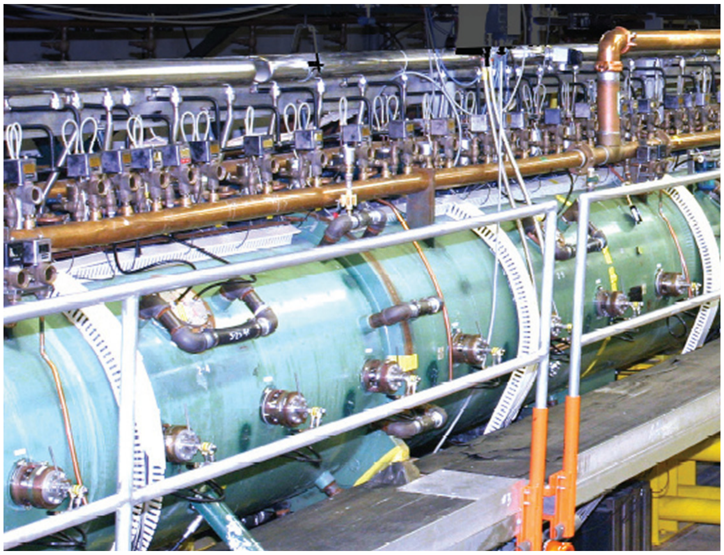
One-hundred-million-electronvolt (MeV) protons are used at IPF to produce radioisotopes for both research and nuclear medicine.

Pulses of 800-MeV negative hydrogen ions are used at the pRad to image dynamic events related to nuclear weapons performance and are also sent to heavy-metal targets at WNR, where proton-nucleus collisions in the targets generate large numbers of neutrons through a process called nuclear spallation. The neutron pulses are used for materials irradiation and fundamental and applied nuclear physics research.

The negative hydrogen ions are injected into a 90-m-diameter proton storage ring (PSR) that compresses the 625-ms pulses into a 250-ns intense burst of protons, which, through nuclear spallation, produces bursts of neutrons for neutron scattering studies of material properties at WNR and the Lujan Center. The Lujan Center is a major national research center annually hosting more than 300 scientists from around the world who perform materials science research and low-energy neutron nuclear physics studies using a variety of uniquely designed instruments.

At UCN, 800-MeV protons hit a tungsten target and produce approximately 14 neutrons at energies of a few million electronvolts, which are reduced to cold neutron temperatures of 40 K by scattering in polyethylene moderators. As they interact with the solid deuterium inside a guide tube coated with ^{58}Ni, the cold neutrons become ultra cold.

The ultracold neutrons then travel through a guide tube and are detected by a helium-3 detector, allowing for the research of fundamental nuclear physics and allowing researchers to test the standard model of elementary particles.



At the core of the LANSCE international user facility is a highly flexible linear accelerator (LINAC) system, which is overseen by the Beam Delivery team.

2011 Production Delivery Statistics

Area	Scheduled Hours	Delivered Hours	Reliability
IPF	3845.2	3468.1	90.2%
Lujan	3358.0	2872.5	85.5%
pRad	922.5	782.3	84.8%
UCN	1323.3	1199.4	90.6%
WNR	1188.2	1061.7	88.2%
Total	**10637.2**	**9384**	**87.9%**

LANSCE Linear Accelerator (LINAC) Risk Mitigation Status

The LANSCE-LINAC Risk Mitigation (LRM) project will replace obsolete and end-of-life equipment at LANSCE and will provide new capabilities. To date, it has received funding of $59.3M, and the agreement with the National Nuclear Security Administration (NNSA), which began in FY10, represents a total investment of $250M over 10 years.

The core elements of the first phase of the LRM project are the radio frequency (RF) system upgrade; improvements to the instrumentation, control, and diagnostic systems; and accelerator system upgrades. These upgrades emphasize early restoration of 120-Hz operation for the LANSCE facility, which will be of significant impact and benefit to WNR, where the available beam current will increase by a factor of 2.5.

RF System Upgrades

The near-term focus for the RF system upgrades is two-fold: establish a new vendor pipeline for the 1.25-MW peak power 805-MHz klystrons, and develop and install new 201.25-MHz amplifier systems to replace the present systems that limit the LANSCE facility operation to 60 Hz. The goal is to restore 120-Hz operation coming out of the FY14 maintenance outage in 2014.

Klystron Replacement

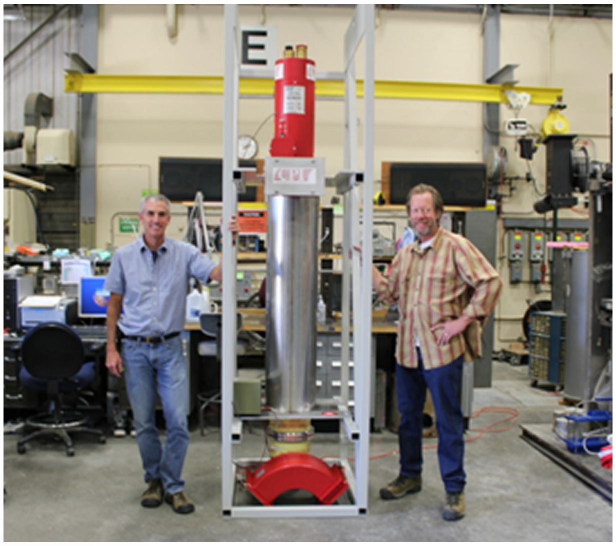
The 805-MHz Coupled Cavity LINAC (CCL) receives power from 44 klystrons rated at a maximum peak RF power of 1.25 MW at a 13.2% electron beam duty factor and a 12% RF duty factor. The klystrons have a maximum voltage of 86 kV and operate at a nominal beam current of 29 A to produce the rated peak power. Typical operation at LANSCE is nominally a 1-MW peak at a 120-Hz pulse repetition frequency and a 10% RF duty factor. The average klystron installed had in excess of 125,000 filament hours at the start of 2010.

In 2010, the prototype for the replacement klystron was ordered from Communications and Power Industries (CPI).

This klystron was successfully tested and delivered in 2011. The production order for an additional 45 replacement klystrons was placed in 2011. These new klystrons are almost identical in design to the original LANSCE klystrons manufactured by CPI in the 1970s. Eight new klystrons have been delivered to date, and the production schedule calls for 2 klystrons to be delivered per month until the order for 45 klystrons is filled.

201-MHz RF System Replacement

A prototype 201-MHz RF final power amplifier (FPA) has been designed and fabricated. This prototype demonstrated the design requirements to generate



First article replacement: LANSCE klystron being prepared for testing at LANSCE.

2.0 MW of peak and 200 kW of average power in 2011 and is currently undergoing extended life testing. The amplifier features a tuneable input-and-output transmission-line cavity circuit; a grid decoupling circuit; an adjustable output coupler; transverse electric (TE) mode suppressors; blocking, bypassing, and decoupling capacitors; and a cooling system. The tube is connected in a full wavelength output circuit, with the lower main tuner situated ¾λ from the central electron beam region in the tube and the upper-slave tuner ¼λ from the same point.

A pair of FPAs of this design will be power-combined for each of the three high-power Drift Tube LINAC (DTL) tanks, resulting in significant headroom for both peak and average power over existing 201.25-MHz systems. All major procurements have been placed for the new 201-MHz amplifier assemblies. In Module 2, the 201-MHz RF system will be replaced. This module has the highest power module of the four that power the drift tube LINAC. The other modules will be replaced in FY15 and FY16. A hybrid approach is being pursued to restore the facility to 120-Hz operation after the FY14 maintenance outage.

Prototype 201-MHz FPA under test.

Upon completion of the FY14 maintenance outage, we will have replaced the highest-power 201-MHz RF station with the new system. The remaining modules will still have the existing Burle triodes. These triodes have been incapable of supporting 120-Hz operation in our highest-power modules in recent years. An aggressive purchasing and testing effort is being pursued to acquire Burle triodes that will operate at 120 Hz on the lower-power modules (1, 3, and 4), which would allow us to exit the 2014 outage with 120-Hz operation. The success with this hybrid plan will be determined by the ability to identify 120-Hz-capable Burle triodes for the next two highest power modules (3 and 4).

Low-Level RF (LLRF) Feedback Controls, High-Voltage Systems, and Modulators

As part of the 201-MHz RF system replacement, it was necessary to change the approach for cavity feedback control. The Burle triodes use modulation of the anode voltage for field control because of tube stability issues. The new 201-MHz RF system will use drive modulation to affect cavity field control. The LLRF design is being executed so that it will support both the 201-MHz DTLs and the 805-MHz CCLs. The prototype units for the LLRF modules are being completed in FY12 in preparation for FY13 production and FY14 installation.

The LANSCE klystron modulators are based around a modulator tube that is no longer available. LANSCE LRM is funding the design of a new modulator topology around a modern modulator tube. The prototype of this modulator was completed in FY11 and is undergoing long-term testing in FY12, with production scheduled to start in FY13.

Instrumentation, Control, and Diagnostics

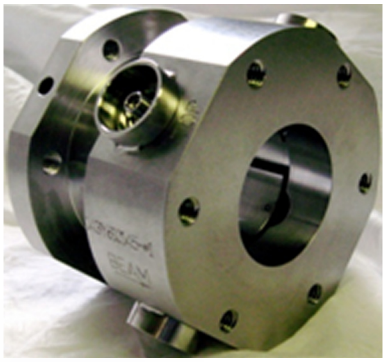
To date, the progress of the instrumentation, controls, and diagnostic system replacements includes the completion of the installation of the new control system network, using a fiber-optic backbone as the communication path. Beginning with the 2012 run cycle, over 200 accelerator front-end devices will use a direct network connection for monitoring and control functions. Important progress was made on Field Programmable Gate Array (FPGA) firmware that will allow the LLRF System also to be directly connected to the network. This firmware makes use of the Nios II processor core in an Altera FPGA. The advancement implemented RTEMS, a real time operating system, on the processor core and improved the Nios II Ethernet driver for more stable operation at higher throughput.

The significance of this advancement is that the Experimental Physics and Industrial Control System (EPICS) Input-Output Controller (IOC) suite of software can now run directly on the Nios II core, eliminating the need for additional hardware and software to interface the LLRF System to the LANSCE Control System.

BiRIO industrial controls hardware.

This FPGA EPICS implementation may also find application in the Timed Data System, which will replace some of the Remote Indication and Control Equipment (RICE) functionality and the Beam Position and Phase Measurement (BPPM) System. Additional enhancements to EPICS required for implementation of the Timed Data System were made.

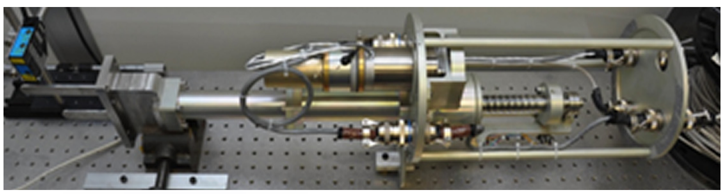
The EPICS data server, event queue, and data access library have all been updated. A great deal of effort has been and will continue to be directed at interfacing issues that must be addressed to allow operation of the new and old systems during the staged installation phase of the project. Construction and hardware purchasing for the Industrial Control System, which will replace the remaining RICE functionality, is underway. To replace old control system computers, replacement of the RICE must go hand-in-hand with replacement of the LANSCE Timing System.



CCL BPPM sensor.

The new event-based timing system design has been refined to the point that construction can begin. Equipment has been ordered, and plans are in place to attempt to install the new event-based timing master during the FY13 maintenance outage. There are also plans to install a “Legacy Gate Replicator,” which will service those accelerator areas and systems not yet converted to the new event system. The event-based timing system and the legacy gate replicator will be capable of operating new and old accelerator systems, along with the new beam diagnostic systems.

Installation of the BPPM sensors continues, as does the development of a measurement system for sensor and BPPM data acquisition system testing. Development of the wire scanner beam-profile measurements system with several prototyping exercises continued. The data acquisition system for the wire scanners was finalized, and purchasing of the hardware has begun. Designs for several wire scanner actuators are nearing finalization, and end-to-end software and system testing is scheduled for early in the run cycle.



Wire scanner actuator prototype.

Accelerator Systems Upgrades

Drift Tube LINAC (DTL) Water Cooling System (WCS)

Over the past year, the DTL WCS team completed the final design for the refurbishment of the DTL Tank 2 WCS. In addition, the team completed the designs for the majority of the DTL Tanks 1, 3, and 4 WCSs. Each DTL Tank WCS includes three pumping skids, a water manifold distribution system, a control system and instrumentation electronics rack, and a distributed cabling and junction box network.

In addition to completing the engineering designs, the DTL WCS team started the detailed development of the control system software and operator interfaces and continued the development of a simulator/tester unit for certifying the functionality of the mechanical hardware, instrumentation, and control system.

Vacuum Systems

Over the past year, modern switching vacuum ion pump supplies have been purchased and installation of these units has begun. Additional supplies will be installed over the coming year as beam delivery schedules and resources allow. Each unit is integrated with the control system and provides real-time data to operators and service personnel.

Additional improvements will include the installation of air-cooled chillers to minimize downtime events for the 201-MHz DTL cryogenic pumping system. Designs are in process to install new fast valves in several partitions of the accelerator, which will protect the 805-MHz section of the accelerator from catastrophic loss-of-vacuum events.

Diagnostics

One of the main goals is to construct the new wire scanners (WSs) with as many commercially available off-the-shelf components as possible. In addition, faster beam scans (both mechanically and data acquisition) are desired for better operation of the accelerator. Two prototype actuators have been fabricated and have undergone extensive testing over the past year. One device will serve the low-energy beam transport region, the DTL, and the coupled cavity 805-MHz portion of the accelerator. The other actuator was designed with a 12-in.-long stroke and will service the high-energy-beam transport lines. LANSCE-RM funding profiles will require that the WSs be purchased and installed over several years.

Radio Frequency Quadrupole (RFQ) and Pulse Stacking

Several new scope elements were added to the LANSCE Risk Mitigation project in 2011, including the eventually replacing the two aging Cockcroft-Walton (CW) high-voltage injectors with more reliable and maintainable 750-keV RFQ injectors. However, to maintain all of the present LANSCE beam-delivery capability, up to three new RFQ injectors may be needed. Conceptual studies indicate that replacement of the H+ injector that provides beam for the IPF and the future Material Test Station is straightforward but that replacement of the H-injector that serves all other experimental facilities may require two new RFQs.

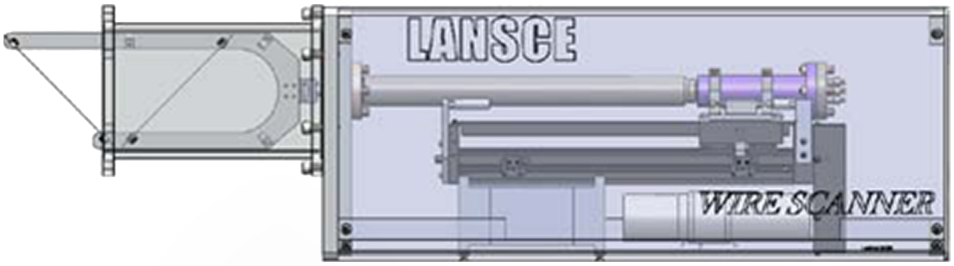
This requirement may be needed because the unique micropulse beam structure required by the WNR and pRad facilities is not compatible with the more standard RF structure of the beams for the Lujan Center and the UCN source. Replacing the present CW injectors with RFQs will enable us to increase the peak beam current to the Lujan Center and pRad. A new low-frequency RFQ is needed for long-pulse operations to WNR. Initial efforts will focus on replacing the H+ injector to ensure long-term reliability and to minimize programmatic risk to the National Isotope Program.

A successful internal technical review of the design, procurement, and implementation plan for the H+ RFQ injector was held in February 2012.

This review also included discussions of technical issues that require attention to minimize the risk of implementation. Additional parametric physics studies are being performed, and electromagnetic and thermal models are being developed in preparation for entering into the design phase. The design and fabrication of the RFQ will be a collaborative effort between LANL/AOT and industry. Design of the RFQ is expected to start this year. Final design and start of RFQ fabrication is expected in FY13.

An additional new capability enhancement is a set of modifications to the Proton Storage Ring (PSR) to enable "pulse-stacking" of WNR-like micropulses on selectable machine cycles; this capability would significantly enhance the low-energy neutron spectra in the 100-keV range at WNR. Required modifications include ring RF bunching, extraction, and kicker systems necessary to direct such pulses "on demand" to WNR rather than the Lujan Center. A preliminary-design study and cost estimate have recently been completed. Other supporting beam physics calculations are ongoing, as is the development of a plan to define required enabling pulsed-power or magnet R&D necessary to realize this capability. More detailed design efforts will be started in the future as funding is made available.

Line D ion pump power supply rack.



Switchyard 12-in.-long stroke WS.

Los Alamos Neutron Science Center

News

2011

LANSCE
Los Alamos Neutron Science Center

News Briefs

2011, Record Proposals for First Call

LANSCE facilities received a record number of proposals for this first FY11 call.

LANSCE Welcomes Japan Proton Accelerator Research Complex (JPARC) Users

LANSCE welcomes proposals from JPARC users displaced by the earthquake. Proposals will be accommodated on a Fast Access basis.

Record Isotope Production Supports US Cardiac Care

Demand for this particular isotope is increasing because of the current shortage of molybdenum-99 (^{99}Mo) used in single photon emission tomography (SPET) cardiac scans.

Basic Energy Sciences (BES) Neutron User Facilities Present Collaborative Exhibit at 2011 ACA Meeting

The 2011 American Crystallographic Association (ACA) marked the first collaborative exhibit of all US DOE BES neutron facilities: the Spallation Neutron Source (SNS), the High Flux Isotope Reactor (HFIR) at Oak Ridge National Laboratory (ORNL), and the LANSCE Lujan Center at LANL. The large-format exhibits presented the unique capabilities and research opportunities of the BES neutron facilities to the crystallographic community.

NUFO Poster Session on Capitol Hill

Representatives from LANSCE attended the National User Facility Organization (NUFO) poster session on Capitol Hill in April. The NUFO-sponsored session was an opportunity for LANSCE to showcase our science and user outreach to attending members of the House and Senate.

New Rosen Scholar Fellowship Created

The Rosen Scholar Fellowship is intended to attract visiting scholars to LANSCE in the fields of nuclear science, materials science, defense science, or accelerator technology. This fellowship is reserved for individuals whose career accomplishments in the fields of research covered by LANSCE facilities are recognized as outstanding by the scientific community and exemplify the innovative and visionary qualities of Louis Rosen. The Rosen Scholar is expected to be resident at LANSCE and bring his/her scientific expertise to LANSCE, as well as the broader LANL scientific community.

Lujan Center Research Featured on Cover of *Langmuir*

Work performed on the surface profile analysis reflectometer (SPEAR), the neutron time-of-flight reflectometer at the Lujan Center, is featured on the cover of a top-ranking scientific journal. The image, which appears in the November 15, 2011, issue of *Langmuir*, shows a structural phase.

Langmuir, an interdisciplinary journal published by the American Chemical Society, ranks number 2 in citations out of 121 journals in the field of physical chemistry.

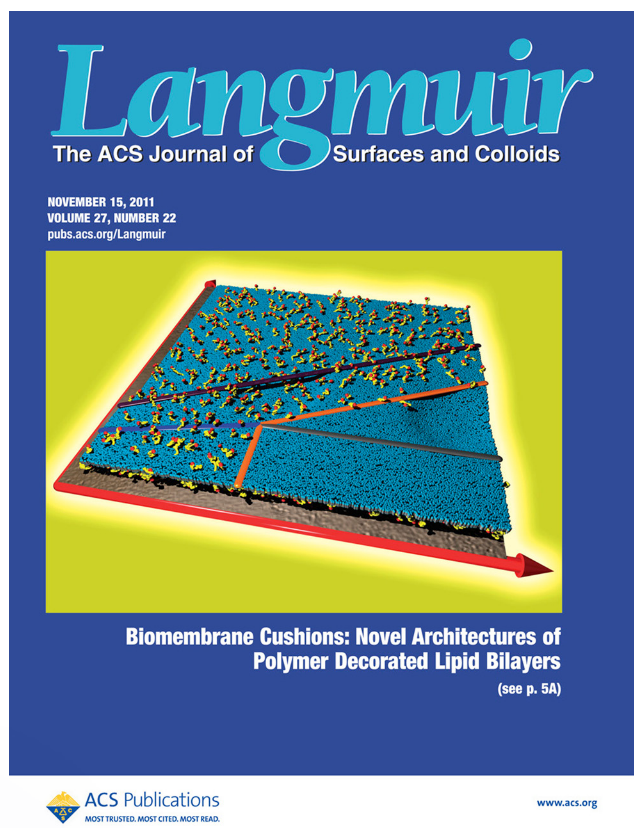
The image accompanies research on the structure and thermodynamics of lipid bilayers on polyethylene glycol cushions. Important for novel biosensors applications, embedded functional lipids provide a simple means of controlling the biomembrane architecture and its properties. By controlling the interaction energy of the polymer with the underlying surface, the membrane can be made to float on top of a well-anchored polymer cushion. It also can be rearranged to expose a polymer chain forest to the environment or to create a hybrid system where the membrane is decorated on both sides with the polymer chains.

In developing well-hydrated polymer cushioned membranes, scientists often neglect structural studies. In this project, neutron and x-ray reflectivity studies reveal that hybrid bilayer/polyethylene glycol (PEG) systems created from mixtures of phospholipids and PEG-conjugated lipopolymers do not yield a hydrated cushion beneath the bilayer unless the terminal ends of the lipopolymers are functionalized with reactive end groups and can covalently bind (tether) to the underlying support surface.

Reference: "Structure and Thermodynamics of Lipid Bilayers on Polyethylene Glycol Cushions: Fact and Fiction of PEG Cushioned Membranes," by Jaroslaw Majewski (Lujan Center); Chad Miller (Stanford Synchrotron Radiation Lightsource); Erik Watkins, Rita El-khouri, Brian Seaby, and Tonya Kuhl (University of California, Davis); and Carlos Marques (Université de Strasbourg, France).

The National Science Foundation's Division of Chemistry supported the work. Neutron measurements were performed at the SPEAR reflectometer at LANSCE and the Advanced Photon Source, which are funded by the DOE.

AOT and LANSCE - The Pulse, November 2011.
LALP-11-017



Biomembrane as featured on the cover of the November 15, 2011, issue of *Langmuir*.

Gearing Up for a Promising New Weapon against Cancer

In the emerging field of treating cancer with radioactive drugs, the National Research Council has made actinium-225 (^{225}Ac) one of its research priorities. Meanwhile, the National Institutes of Health and the Nuclear Science Advisory Committee have identified ^{225}Ac as a critical isotope that must be manufactured if it is to be studied.

Until now isotopes of the silvery metal were mined from decaying uranium, but the demand for ^{225}Ac has outstripped the supply available from the nation's uranium stockpile.

LANL scientists are close to determining whether the nation's two accelerators are capable of providing a stable supply of ^{225}Ac for research efforts and clinical trials. "Preliminary results show great promise for large-scale production at LANL and Brookhaven National Laboratory," physicist Meiring Nortier said. At LANL, both the IPF and the planned Materials Test Station (MTS) have that potential.

Using proton beams available at LANSCE and the Blue Room of WNR, scientists successfully produced ^{225}Ac from thorium-232 (^{232}Th). In the process, they documented the world's first set of cross-section measurements at these high energies for this specific set of nuclear reactions. When published, the data will help isotope production scientists worldwide to fine tune production parameters for the highest product yield and highest product quality.

Graduate student John Weidner took the lead in executing the experiments and analyzing the data. He helped irradiate ^{232}Th foils with 800-MeV protons in the Blue Room and then transported the foils to the hot cell facility for gamma counting and alpha assay. In other test runs, he used the 100-MeV beam at the IPF and a specially developed 200-MeV beam at WNR.

The researchers from the Laboratory's theoretical and computational physics, chemistry, and neutron and nuclear science fields will now shift their focus to production scale-up investigations, including the development of high-power targets and chemical recovery methods.

Targeted alpha therapy, also known as alpha radioimmunotherapy, is a medical treatment that could kill malignant cells without damaging the body's healthy cells. If clinical trials lead to product development, the annual demand for ^{225}Ac could reach 50,000 millicuries by 2014, according to the Nuclear Science Advisory Committee Isotopes Subcommittee.

Actinium-225 holds the most promise for treating leukemia and other cancers that embody small clusters of cells or individual cells. For the first clinical study testing ^{225}Ac in people, New York's Memorial Sloan-Kettering Cancer Center and the National Cancer Institute were recruiting participants in 2011. "The antibody HuM195 will be used to deliver ^{225}Ac directly to leukemia cells throughout the body," according to the study. "Once ^{225}Ac reaches these cells, it gives off four alpha particles, killing the leukemia cells. Experiments show that actinium-225-HuM195 should be approximately 1,000 times more potent than bismuth-213-HuM195."

AOT and LANSCE - The Pulse, August 2011.
LALP-11-017

Using proton beams available at LANSCE and the Blue Room of WNR, scientists successfully produced ^{225}Ac from ^{232}Th.

UCN Probes Existence of Interactions beyond the Standard Model

In 2011 UCN was awarded a Laboratory Directed Research and Development (LDRD) Directed Research (DR) to probe the existence of new interactions Beyond the Standard Model (BSM) at the TeV scale by (1) performing precision measurements of neutron decay parameters at the LANL UCN source and (2) performing the theoretical studies necessary to assess the discovery potential of these measurements.

UCN will focus on two quantities that provide maximal sensitivity to new physics because their theoretical standard model (SM) backgrounds are known at the level of 10^{-5}: the Fierz interference term b, which characterizes the energy spectrum of the electrons emitted in neutron decay, and parameter B, which measures the antineutrino asymmetry relative to the neutron spin.

Measurements of b and B at the 10^{-3} level probe the existence of BSM scalar and tensor interactions generated by the exchange of particles with masses up to 10 TeV.

Motivated by these considerations, we will perform the first-ever measurement of b, with a sensitivity of 10^{-3}, and a measurement of B, with a factor of five improvement over the most precise existing result.

These two measurements will inaugurate a new class of precision neutron decay experiments, enabled by the unique features of the LANL UCN source: a high density of UCN with the world's highest degree of polarization, low background from the spallation source, and our previously developed large-area silicon detectors.

Simultaneously with the experimental effort, we will carry out a theoretical program to elucidate the implications of b and B measurements at 10^{-4} for extensions to the SM.

To reach this goal, we will on the one hand use lattice QCD to calculate from first principles the nonperturbative neutron-to-proton matrix elements of the operators generated by exchange of new BSM particles. On the other hand, we will identify the contributions to B and b within well-motivated extensions of the SM, such as models of warped extra dimensions and supersymmetry.

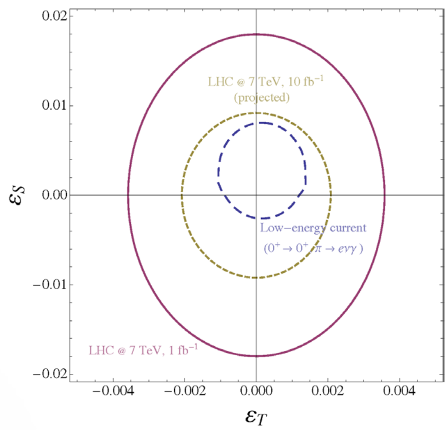
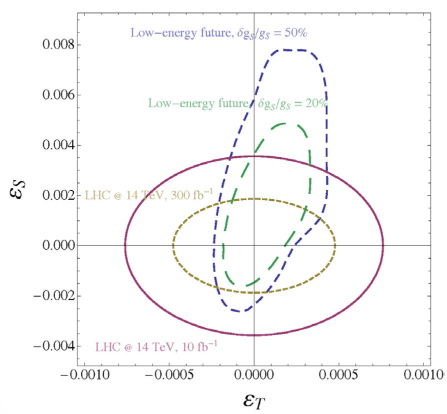


Illustration of the 90% Confidence Level allowed regions for the scalar and tensor effective couplings (the allowed region is the one inside the various curves). The three curves correspond to constraints from: (i) current low-energy experiments including our own (blue, dashed) (ii) current results from the Large Hadron Collider (LHC) searches at center-of-mass energy of 7 TeV; (iii) projected LHC searches with statistics increased by one order of magnitude (gold, dotted).



The various curves correspond to: (i) LHC searches at center-of-mass energy of 14 TeV for two different values of the accumulated statistics (solid, red and gold, dotted ellipses). (ii) Anticipated bounds from future low-energy experiments such as ours (dashed green and blue curves). The latter two curves correspond to two different scenarios for the theoretical uncertainties on scalar and tensor matrix elements. dotted).

Las Conchas Fire and LANSCE

The Las Conchas Fire started on June 26, 2011. The fire burned 156,593 acres and resulted in 15 reported injuries; the fire was 100% contained as of August 2, 2011 (http://www.inciweb.org/incident/2385/). At the time, it was considered to be the largest fire in New Mexico history. LANSCE was essentially unharmed by the Las Conchas Fire, which burned near Los Alamos and on an outlying portion of LANL property.

While the townsite was evacuated and the majority of LANL was shut down, a crew of essential workers remained at LANSCE to look over the facility and ensure its safety. After LANL's site evacuation was lifted, some adjustments in maintenance and production schedules were made in response to both restart activities and lost beam.

The evacuation of the Los Alamos townsite was lifted on Sunday, July 3. Both LANL and LANSCE re-opened on Wednesday, July 6. Thanks to the hard work of our staff, LANSCE went back into scheduled production after the emergency shutdown.

Smoke from the Las Conchas Fire billowing over the National Security Sciences Building at LANL.

Los Conchas Fire looms near Los Alamos.

A member of the Zig Zag Hotshots monitors for spots during a burnout operation on the west side of the fire.

Los Alamos Neutron Science Center

Conferences, Workshops & Tours 2011

LANSCE

Los Alamos Neutron Science Center

2011 LANSCE School on Neutron Scattering: Energy & Environment

LANSCE will hold its 2011 Neutron School on July 12-22 in Los Alamos. The DOE, National Science Foundation (NSF), LANSCE, and New Mexico State University (NMSU) jointly sponsor the school. The annual school focuses on specific science topics to which neutron scattering makes a critical impact. This focus makes it distinct from other national neutron schools.

This year's theme focuses on the study of materials for energy and environment research. Novel approaches to energy production, storage, and distribution; pollution prevention; environmental cleanup and protection; carbon sequestration; and raw materials sources are urgently needed. The development of new functional materials and a better understanding of natural materials and processes will play a central role in this endeavor. Neutron scattering, in all its diversity, will contribute significantly to the arsenal of sophisticated materials characterization techniques needed for energy and environmental research.

The goal of the neutron school is to introduce a variety of neutron scattering techniques to the students and to demonstrate how they complement other analytical methods to elucidate material structure and properties. In addition to introductory lectures on neutron scattering, experts will present contemporary research on materials science aspects of energy and environmental research. Afternoons will be devoted to hands-on neutron scattering experiments (small-angle scattering, reflectometry, powder diffraction, pair distribution function analysis, neutron vibrational spectroscopy, and radiography) and data analysis. A variety of materials related to energy and environmental issues will be selected for these exercises.

James Rhyne (Lujan Center) is the School's Director, Heinz Nakotte (NMSU) is the School's Co-Director, and local organizing committee members include Luke Daemen and Monika Hartl (Lujan Center), John Gordon (Inorganic, Isotope and Actinide Chemistry, CIIAC), and Donald Hickmott (Earth and Environmental Sciences, EES-DO).

Laboratory presenters include Kevin Ott (Applied Energy, SPO-AE) – keynote speaker, Greg Kubas (CIIAC) – banquet speaker, and lecturers David L. Clark (Institutes, INST-OFF), S. Zoe Fisher (Bioenergy and Environmental Science, B-8), Victor Klimov (Physical Chemistry and Applied Spectroscopy, C-PCS), and Andrew Sutton (C-IIAC). Leads for the hands-on experiments include Katharine Page, Sven Vogel, Michal Mocko, Jarek Majewski, Rex Hjelm, and Luke Daemen (Lujan Center).

AOT and LANSCE - The Pulse, April 2011.
LALP-11-017

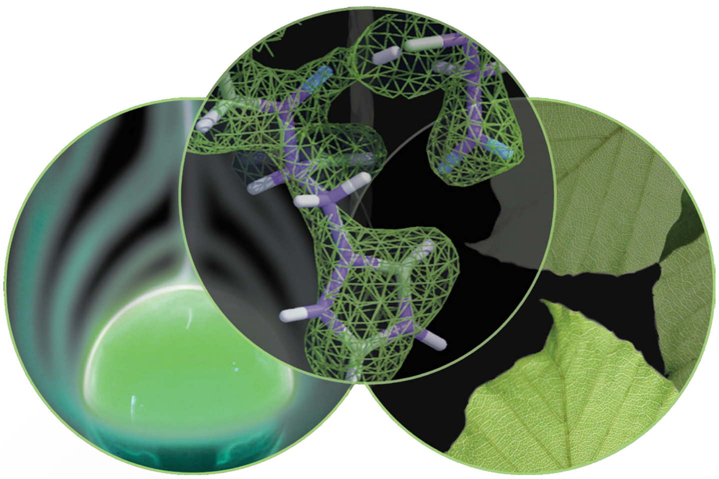


Image: Neutron scattering: energy & environment.

Workshop Spotlights Lujan Center Neutron Scattering Expertise

Hongwu Xu (Earth System Observations, EES-14), Sven Vogel (Lujan Center), and Rudy Wenk [University of California-Berkeley (UCB)] organized the workshop “Applications of Neutron Scattering to Materials and Earth Sciences.” UCB sponsored the workshop, which included lectures and tutorials. More than a dozen talks at the event featured the use of research techniques and instruments at LANL’s Lujan Center. LANL presenters included Alex Lacerda (LANSCE-DO); Luke Daemen, Katharine Page, and Claire White (Lujan Center); and Levente Balogh (Structure/Property Relations, MST-8).

The workshop was intended for University of California (UC) graduate students, postdoctoral researchers, and other scientists in earth sciences, physics, chemistry, materials science, and engineering interested in applying neutron scattering to studies of synthetic and natural materials. Talks covered the basics of the instruments, as well as examples of research by external users of specific applications. The workshop also included data analysis tutorials for information collected from the Lujan Center instruments High-Pressure-Preferred Orientation (HIPPO), Spectrometer for Materials Research at Temperature and Stress), NPDF (Neutron Powder Diffractometer (SMARTS), and Filter Difference Spectrometer (FDS). These instruments, among others at LANSCE not covered during this workshop, are used to characterize the atomic structures of materials and the response of the structure to changes in pressure, temperature, and stress.

Approximately 90 interested students and faculty members applied to attend the workshop, but space concerns limited participation to 60. The event was the fourth UC-sponsored neutron Lujan Center workshop and the first held since 2006.

Several attendees from non-UC institutions received travel funding. Several attendees from non-UC institutions received travel funding from the Consortium for Materials Properties Research in Earth Sciences (COMPRES) network which fosters research on high-pressure science. The UC Office of the President also supported travel for UC students and faculty for experiments at LANSCE through a grant awarded to Vogel and Wenk.

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LALP-11-017

Workshop attendees performing data analysis.

2011 High-Energy Proton Microscopy (HEPM)

LANL and the LANSCE National User Facility held the 2011 3rd International Workshop on High-Energy Proton Microscopy on October 27–28.

An international panel of collaborators discussed high-energy proton microscopy, its current status, technical specifications, the enablement of scientific experiments, and future advances for the optimization of proton microscopy systems. This workshop focused on defining a class of material science experiments that can effectively use high-resolution proton microscopy to achieve new scientific discoveries. Some of these experiments could be fielded at the GSI Helmhotlz Centre for Heavy Ion Research, Germany, using the **Pr**oton M**i**crosc**o**pe for FAI**R** (PRIOR) microscope.

Workshop Goals:

(1) Advance the science case for using high-energy (~1-GeV and higher) proton microscopy for the basic science of matter in extremes, and (2) determine one or a few "first experiments" so that the PRIOR collaboration can begin using the present and imminent capabilities at LANL's pRad and GSI's **H**igh-Energy **H**igh **T**emperature (HHT).

This workshop focused on defining a class of material science experiments that can effectively use high-resolution proton microscopy to achieve new scientific discoveries. Some of these experiments could be fielded at GSI using the PRIOR microscope.

Presenters and attendees of the 2011 HEPM Workshop.

Collaboration Meeting on Fission Measurements

LANL, Lawrence Livermore National Laboratory (LLNL), and other national laboratories and universities are collaborating on a major experimental effort to measure the fundamental fission properties that govern nuclear weapons and nuclear reactors. The goals of these projects are to (1) reduce the uncertainties in the fission cross section for plutonium-239 (^{239}Pu) and uranium-235 (^{235}U) to less than 1% and (2) measure the neutron output spectra in energy regions that have not been previously measured. LLNL leads the development of a Time-Projection Chamber (TPC) to obtain the required precision in the cross-section measurement. To measure the neutron output spectra, LANL leads the effort to develop a new neutron detector array (ChiNu) for both low and high-energy neutrons. The experiments are performed at WNR.

Approximately 50 collaborators gathered for a 2-day meeting at LLNL to review the status of these efforts, discuss emerging issues and concerns, and develop plans to achieve important milestones and complete these projects. This meeting was the second of this group; the first meeting took place a year ago at LANL. The LANL and LLNL Campaign-1 program managers and the DOE Nuclear Energy program manager described the importance of these measurements to their respective programs. Bob Haight (Neutron Science, WNR) presented the status of the ChiNu experiment. Experimenters described the status of their particular responsibilities and the theoretical basis for these measurements. Mark Chadwick (X-Computational Physics, XCP-DO) discussed how the data will be incorporated into the nuclear weapons design codes.

The work supports the Laboratory's Nuclear Deterrence and Energy Security mission areas and the Science of Signatures and Information and Knowledge Science capabilities.

AOT and LANSCE - The Pulse, June 2011.
LALP-11-017

Hye-Young Lee (WNR) presents the results of testing lithium-6 glass detectors.

Tours at LANSCE

Throughout the year, LANSCE hosts a variety of visitors, many of whom request tours of the accelerator, instruments, and laboratories. These visitors are either US or foreign citizens and can represent, for example, academia, industry, national laboratories, and local, tribal, state, or federal government.

As a National User Facility, LANSCE encourages visitors to schedule tours.

Institutions (A - H)	Number of Visits	Number of Attendees
Albuquerque Journal	1	2
Argonne National Laboratory (ANL)	1	1
Arizona Department of Education	1	1
Arizona State University	1	10
Army Research Laboratory (ARL)	1	2
Bechtel Corporation	2	2
Boeing Company	1	5
Boy Scouts of America	1	97
California Institute of Technology	2	2
Campinas State University, Brazil	1	1
Carson City Public Library	1	1
Columbia University	2	2
COSMOS | California State Summer School for Mathematics & Science	1	25
Department of Defense (DoD)	1	1
Department of Energy (DOE)	4	9
Duke University	1	1
Federal Bureau of Investigations (FBI)	1	2
Fermi National Accelerator Laboratory (Fermilab | FANL)	2	3
Florida State University - Sarasota Regional Medical Campus	1	2
Forsytr	1	3
Fuel Co	1	17
George Washington University	1	1
Harvard University	1	14

Institutions (I - P)	Number of Visits	Number of Attendees
IBM	1	1
Idaho National Laboratory (INL)	1	1
Imperial College	1	1
INTEL	1	1
Indiana University Cyclotron Facility (IUCF)	1	1
Kansas City Plant	1	1
KEK - High Energy Accelerator Research Organization, Japan	1	1
KNME TV (New Mexico PBS)	1	1
Lawrence Livermore National Laboratory (LLNL)	8	9
Los Alamos Chamber of Commerce	2	2
Los Alamos City Council	1	1
Los Alamos Public Schools	1	1
Los Alamos School Board	1	2
Los Alamos Site Office (LASO)	9	17
Massachusetts Institute of Technology (MIT)	2	2
National Nuclear Security Administration (NNSA)	9	20
National Security Technologies (NSTEC)	7	9
National Superconducting Cyclotron Laboratory	1	1
Native Hispanic Institute	1	1
New Jersey Institute of Technology	1	1
New Mexico Community Foundation	1	1
New Mexico Environment Department	1	2
New Mexico Higher Education Department	1	2
New Mexico State University (NMSU)	2	22
New York University	1	1
Nuclear Regulatory Commission	1	1
Oak Ridge National Laboratory (ORNL)	2	2
Pacific Northwest National Laboratory (PNNL)	1	1
Pojoaque Valley School District	1	3
Qyenergy Corporation	1	2
Rio Arriba County	1	1
Rockefeller University	1	2
Rosatom State Nuclear Energy Corporation	1	3
Russian Federal Nuclear Center	1	5
San Ildefonso Pueblo	1	5
Pantex Plant	3	3

Institutions (S - Y)	Number of Visits	Number of Attendees
Sandia National Laboratories	4	11
Savanna River National Laboratory	1	1
Savanna River Nuclear Solutions (LLC)	1	1
Stanford University	1	6
State Department	1	2
Triangle Universities Nuclear Lab (TUNL)	1	1
TUFTS University	1	1
University of Arizona	1	2
University of British Columbia	1	1
University of California	3	3
University of California - Los Angeles	1	1
University of California-San Diego	1	1
University of Illinois	2	4
University of Michigan	2	2
University of Missouri	1	2
University of Nevada, Las Vegas	1	4
University of New Mexico	4	12
University of Notre Dame	1	1
University of Tennessee	2	2
University of Texas	1	1
University of Texas El Paso	1	1
University of Utah	1	1
University of Delaware	1	1
University of Illinois at Urbana Champagne	1	1
US Government Accountability Office	1	4
Western Electricity Coordinating Council (WECC)	1	10
Yale University	3	3

Los Alamos Neutron Science Center

Celebrations

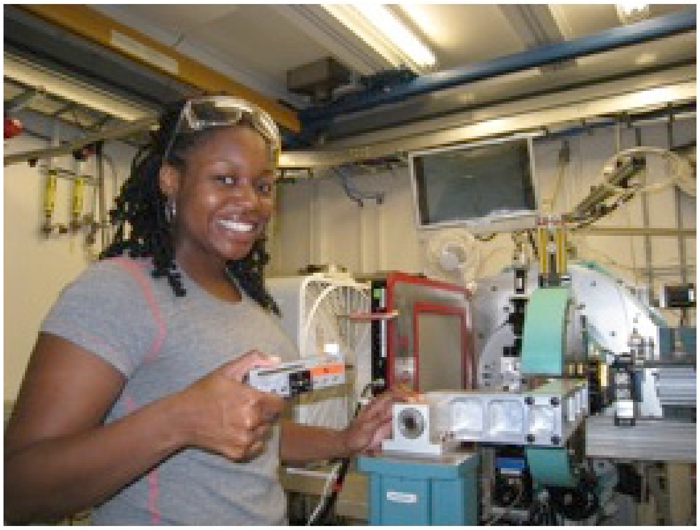
2011

LANSCE
Los Alamos Neutron Science Center

Celebrating and Applauding the Outstanding Accomplishments of LANSCE Users, Staff, Students, Researchers, and Contributors

Summer Student Wins LANL Student Symposium Award
NNSA summer student Breaunnah Bloomer won a LANL Student Symposium 2011 award in the Materials Science Category. Breaunnah is a Junior chemistry major at Howard University and is looking forward to graduate school, possibly in analytical chemistry, following her bachelor's program.

Her talk was "Following Geopolymerization Synthesis: In Situ X-Ray Pair Distribution Function Analysis." Breaunnah was mentored in the total scattering group by NPDF instrument scientist Katharine Page and Lujan Center/CNLS Postdoc Claire White.



Breaunnah Bloomer in the lab.

Katharine Page Receives Award at Los Alamos Postdoc Research Day
Katharine Page (Lujan Center) is the recipient of a poster award at the recent Los Alamos Postdoc Research Day for her work on "Probing Atomic Structure in Functional Thin Films and Nanoparticles."

Katharine Page.

Katharine Page Joins Lujan Center Staff
In January 2011, Katharine was hired at the Lujan Center as the NPDF Instrument Scientist and Total Scattering Team Leader. Page is an expert in pair distribution function methods.

Rosenfest

The Rosenfest Lectures were held on May 18 -- 20, 2011, at the historic Fuller Lodge in Los Alamos, New Mexico. In honor of Louis Rosen, the Father of the LANSCE, Rosenfest covered Rosen's early life, career, and influence at LANL on nuclear science and international relations. Lectures were presented on the past, present, and future of LANSCE and its world-class research; and the Matter-Radiation Interactions in Extremes (MaRIE) experimental facility, LANL's proposed next-generation signature science complex, was described.

To help ensure that LANL remained a premier science institution, Rosen led the way in developing the world's most powerful linear accelerator. His efforts culminated in the construction of the Los Alamos Meson Physics Facility (LAMPF), which is known today as LANSCE. From its dedication in 1972 until 1985, Louis Rosen served as director.

Rosen continued to work at LANSCE until 2 days before his death in August 2009 at the age of 91.

In conjunction with the Rosenfest Lectures, a public tour of the LANSCE accelerator attracted over 300 visitors.

Louis Rosen: The Father of LANSCE 1918-2009

LANL Senior Fellow Emeritus Louis Rosen may have been small in stature, but he was a giant among nuclear physics researchers.

Louis was the driving force behind the conception, funding, design, and development of LAMPF, for decades the largest and most powerful linear accelerator in the world.

He had plenty of incredibly talented, devoted, and similarly driven confederates to help him realize his vision (e.g., Laboratory Director Norris Bradbury and fellow scientists Edward Knapp, Donald Hagerman, and Darragh Nagel), but everyone involved then and now in the life of LANSCE will agree that Louis Rosen was truly the "Father of LANSCE."

Rosen's Vision of Nuclear Science

Rosen's vision was born of an epiphany he had in 1959 while on a LANL- and Guggenheim Memorial Foundation-sponsored sabbatical in Paris. This vision was keenly focused on the future of nuclear science at both the Laboratory and in the nation.

Rosen believed that LANL could not remain the cornerstone of national security without achieving international scientific excellence (the so-called "deterrence through competence" argument) and meeting the broad challenges of national security required to solve problems in areas such as energy security, medicine, environmental stewardship, and nuclear nonproliferation.

Rosen understood that nuclear science played a key role in solving each of these challenges. His vision was to build the world's most advanced nuclear science facility based on the world's most powerful, high-intensity-proton linear accelerator. This accelerator would be capable of producing Pi mesons at intensities up to 10,000 times over anything then in use, making LAMPF a kind of Pi-meson factory. These mesons would be used to probe the structure and function of the nucleus and would keep LANL at the forefront of nuclear physics for decades.

LANSCE: Continuing to Honor Rosen's Vision

Today, LANSCE strives to maintain a balance between the fundamental and applied nuclear, materials, biological, and defense sciences to help meet the complex challenges of national security. Even after retirement, Rosen continued to work at LANSCE, where he served as an inspiration and mentor to students, scientists, and Laboratory management.

Rosen is remembered by family members, coworkers, students, political leaders, and the world's nuclear scientific community for his tireless efforts, scientific achievements, humor, and compassion. He lives on in the hearts of all who had the privilege to know him.

Rosenfest 2011

Dr. Louis Rosen: "The Father of LANSCE"

Daniel Shoemaker Wins Graduate Award

Daniel Shoemaker, a University of California-Santa Barbara (UCSB) graduate student and Lujan Center researcher, was awarded the Graduate Student Gold Award by the Materials Research Society (MRS) at the society's annual fall meeting. Shoemaker, a UCSB/Institute for Multiscale Materials Studies (IMMS) fellow, earned the award for his research in total scattering descriptions of local and cooperative Jahn-Teller distortions in the $CuXMg_{1-x}Cr_2O_4$ solid solution. He received a cash award and a presentation plaque.

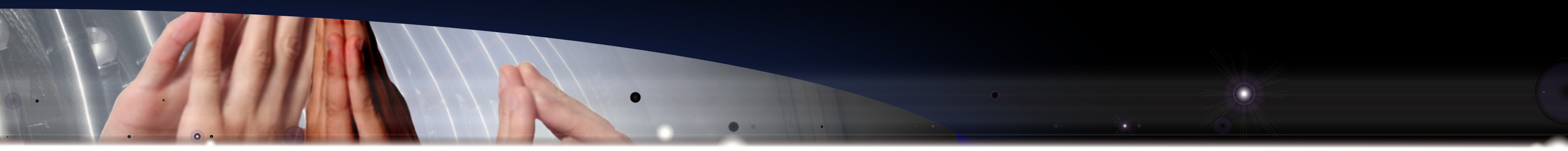
Shoemaker came to the Lujan Center in 2007, initially as a user and later as an IMMS fellow mentored by Anna Llobet and Thomas Proffen from the Total Scattering team in the Lujan Center. His research, directed by Ram Seshadri (UCSB), uses neutron total scattering to describe structure-property relations in disordered, magnetic, and functional oxides. This research includes least-squares refinement and reverse Monte Carlo simulations of the real-space pair distribution function. In the research for which he won the award, Shoemaker showed that Cu^{2+} forms significantly more distorted coordination environments than Mg^{2+} on the same crystallographic site, even in compounds that are a single crystalline phase as determined by Rietveld refinement. Local distortions remain prevalent in cases where long-range orbital ordering produces a cooperative Jahn-Teller distortion. He defended his thesis in September 2010 and began a postdoctoral appointment at Argonne National Laboratory.

The MRS is an organization of materials researchers from academia, industry, and government that promotes communication for the advancement of interdisciplinary materials research to improve the quality of life.

MRS Graduate Student Awards are intended to honor and encourage graduate students whose academic achievements and current materials research display a high level of excellence and distinction. MRS seeks to recognize students of exceptional ability who show promise for significant future achievement in materials research. A panel of judges chose the graduate student award winners based on their oral presentations and application materials.

AOT and LANSCE - The Pulse, February 2011.
LALP-11-017

Daniel Shoemaker.



Daniel Shoemaker Named 23rd Rosen Prize Winner

Daniel P. Shoemaker, a postdoctoral fellow at Argonne National Laboratory, is the winner of the 23rd Rosen Prize.

The prize, established in honor of Louis Rosen, the Father of LANSCE, is awarded for the most outstanding Ph.D. or M.S. thesis based on experimental or theoretical research performed at LANSCE. Criteria include the originality and scientific impact of the research and the student's contribution to the research.

Shoemaker's winning Ph.D. thesis is titled "Understanding Atomic Disorder in Polar and Magnetic Oxides."

His thesis focused on creating and characterizing large-box models of materials that cannot be described using traditional crystallographic tools due to disorder on the nanoscale. For example, local dipoles from Bi displacements in $Bi_2Ti_2O_7$ are geometrically frustrated and form an electronic analog of spin ice. These techniques can also provide insight into phase transitions, such as V-V dimerization across the VO_2 metal-insulator transition. His study of local and cooperative Jahn-Teller distortions in the $Cu_xMg_{1-x}Cr_2O_4$ solid solution revealed that Cu^{2+} forms more distorted coordination environments than Mg^{2+} on the same crystallographic site, even in compounds that are a single crystalline phase. This localized orbital ordering represents a strong interplay between structural, electronic, and magnetic degrees of freedom.

His research, directed by Ram Seshadri (UCSB), uses neutron total scattering to describe structure-property relations in disordered magnetic and functional oxides.

Shoemaker received his Ph.D. from the Materials Department at UCSB. He defended his thesis in September 2010 and was awarded a Graduate Student Gold Award by the Materials Research Society in 2010.

AOT and LANSCE - The Pulse, October 2011.
LALP-11-017

LANSCE Former Student Selected to Attend 61st Lindau Nobel Laureates Meeting

The Lindau meeting, which is dedicated to physiology and medicine, takes place from June 25 to July 2 in Lindau, Germany. Attendance at the 61st Lindau Nobel Laureates Meeting is highly competitive, with 500 attendees accepted from over 20,000 applicants. The annual meetings provide a forum for the transfer of knowledge between Nobel Laureates and young researchers. Lectures of the Nobel Laureates reflect current scientific topics and future research areas and address basic research and application-orientated themes. In panel discussions, seminars, and social events, young researchers from more than 60 countries interact with the Nobel Laureates. The researchers are nominated by a global network of Academic Partners and then carefully evaluated by a review panel. Mike Jablin and Dominique Price were selected to attend the meeting.

Mike Jablin (Lujan Center) is a former undergraduate student of Jarek Majewski (Lujan Center). Both investigated model biomembranes. Jablin gave an invited talk describing their work on the structure and composition of lipid domains in cell biomembranes at the International Student Workshop on Lipid Domains, held at the Weizmann Institute of Science in Israel. He is examining the influence of beta-cyclodextrin on the structure, composition, and reorganization of model membranes composed of mixed sphingomyelin/cholesterol bilayers. During the LANL student symposium, Jablin presented neutron scattering studies of radiation resistant materials. Currently, he is a graduate student at Carnegie Mellon University. Jablin continues to collaborate with Majewski and other LANL researchers on the physics of biomembranes, including a first-author article in Physical Review Letters in March 2011.

Michael Jablin.

AOT and LANSCE - The Pulse, April 2011.
LALP-11-017

Lujan Center User Ellen Moons Receives Swedish National Prize for Scientific Achievement

Lujan Center user Ellen Moons, associate professor of Materials Physics at Karlstad University in Sweden, was awarded the Göran Gustafsson Prize in physics for her achievements in furthering the development of organic and hybrid solar cells. The Göran Gustafsson prize is awarded annually by the Royal Swedish Academy of Sciences for outstanding scientific achievement in physics, chemistry, mathematics, medicine, and molecular biology, The prize, which is named after a Swedish businessman, is considered the most prestigious prize for young scientists in fundamental science disciplines at universities in Sweden. Moons will receive 4.5 million Swedish Crowns ($700,000) in research funding and a personal prize of $15,000. She plans to use part of the research grant for building a polymer solar cell device lab at Karlstad University. King Carl XVI Gustaf of Sweden presented Moons with the award at the awards ceremony at the Royal Academy of Science in Stockholm on March 31, 2011.

Moons used the neutron surface profile analysis reflectometer (SPEAR) at the LANSCE Lujan Center to understand the properties of polymer-fullerene thin films used for light harvesting systems. In collaboration with Lujan Center scientist Jarek Majewski, she studied bulk heterojunction structures, in which an electron-donating component intermingles with an electron-accepting component. This concept has proven its importance for low-cost organic polymer/fullerene solar cells. In such a solar cell, an exciton is formed in the polymer upon absorption of light and is separated at the interface between polymer and fullerene into an electron and a hole.

According to the model, the electron-accepting fullerene derivative transports the electron to the metal electrode, and the electron-donating polymer transports the hole to the indium tin oxide (ITO) electrode. The need for efficient absorption gives rise to criteria regarding the polymer material and the film thickness, while the optimal film morphology in the solar cell is a trade off between the criteria for efficient charge generation and charge transport. Despite the significant body of research in the area of polymer-fullerene blends, the organization of these structures and the interplay between the fullerenes and the polymer is not fully understood. Because of the sensitivity to low-Z elements, neutron reflectometry provides an excellent tool to probe the structure of these systems.

AOT and LANSCE - The Pulse, June 2011.
LALP-11-017

King Carl VI Gustaf of Sweden presents Moons with the Göran Gustafsson Prize in physics.

Photo credit: Markus Marcetic/©KVA

LANL Communicators Recognized with APEX Awards for Publication Excellence

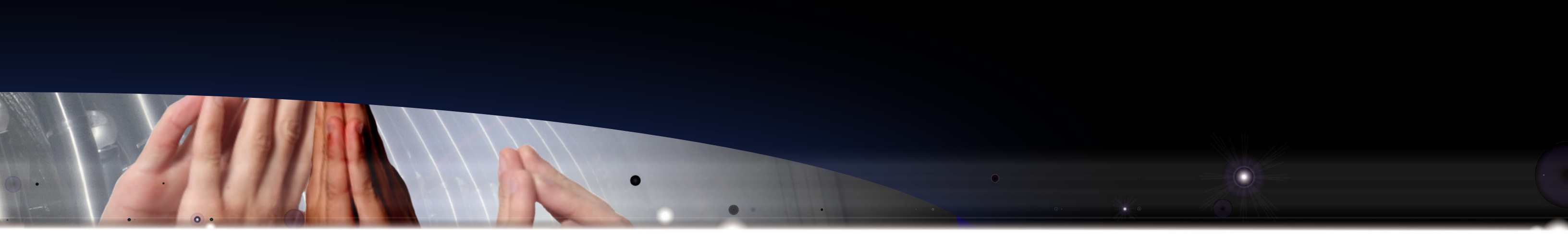
LANL communicators Elena Fernández (LANSCE-DO) and Clay Dillingham and Barbara Maes (Communication Arts and Services, IRM-CAS) received 2011 APEX Awards for Publication Excellence for products highlighting LANSCE.

Fernández was recognized for her work on promotional materials related to the 2011 LANSCE School on Neutron Scattering. The award, in the Special Purpose Campaigns, Programs & Plans category, was awarded for the school's website, poster, and brochure related to the annual event and supported by the National Science Foundation and the DOE Office of Basic Energy Sciences.

Dillingham and Maes were honored for their work on the LANSCE Activity Report 2007-2009, which is dedicated to Louis Rosen, "The Father of LANSCE," and highlights not only Louis's legacy but the ongoing endeavors and accomplishments at LANSCE. Six Awards of Excellence were given out of 105 entries in the category of Annual Reports - Print. Dave Van Etten (IRM-CAS) received an award in the Microsites & Individual Web Pages category.

APEX Awards, sponsored by the editors of *Writing That Works: The Business Communications Report*, are presented to communications professionals around the globe and are based on excellence in graphic design, editorial content, and the ability to achieve overall communications effectiveness and excellence. For 2011, there were more than 3,300 entries in 11 major categories.

http://www.apexawards.com/A2011_Win.List.pdf



Taylor Hood Receives Distinguished Scholars Award

Taylor Hood, a summer student at LANSCE last year, has won a Distinguished Scholars Award from the Thurgood Marshall College Fund. Part of her citation of achievement was being published in the *Journal of Applied Crystallography* in January 2011. She completed the work at the Lujan Center.

While in a National Nuclear Security Administration program for the summer, Hood attended experiments at the Advanced Photon Source, assisted with measurements at the Neutron Powder Diffractometer Facility (NPDF), and explored nanoparticle pair distribution function measurements. As part of a research team with Katharine Page, Thomas Proffen (both Lujan Center), and Reinhard Neder (Institute for Physics and Condensed Matter, Germany), she described complex finite structures using tools that have not been available previously. The scientists used the DISCUS simulation package to examine the buildup of internal atomic structure (including defects, chemical ordering, and other types of disorders) and nanoparticle size, shape, and architecture (including core-shell structures, surface relaxation, and ligand capping). DISCUS (discus.sourceforge.net) is still under development. Using the DIFFEV software package, the researchers demonstrated the structure refinement of a complete nanoparticle system, based on neutron pair distribution function data. DIFFEV uses a differential evolutionary algorithm to generate parameter values. These methods are a valuable addition to other tools appropriate for nanomaterials, adaptable to a diverse and complex set of materials systems, and extendable to additional data-set types.

Hood, a member of the 2012 class at Alabama A&M University, is studying chemistry, with a concentration in forensic science. She plans to seek a master's degree in analytical chemistry and enter the field of forensic toxicology and crime-scene analysis.

Reference: "Building and Refining Complete Nanoparticle Structures with Total Scattering Data," *Journal of Applied Crystallography* **44**, 327 (2011); doi: 10.1107/S0021889811001968.

Taylor Hood.

Acknowledgments

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This report is the tenth in this series.

Back Cover

Cockcroft-Walton Generator

After pre-acceleration out of an ion source, H- ions are further accelerated by the 670,000-volt electric field created by a Cockcroft-Walton Generator.

In the image here, a voltage-rectifier and multiplier ladder steps up an initial 56,000 volts to 670,000 volts, completing the first acceleration stage of the H- ions.

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Los Alamos Neutron Science Center

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