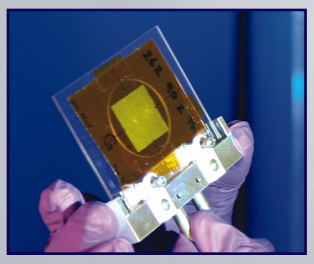
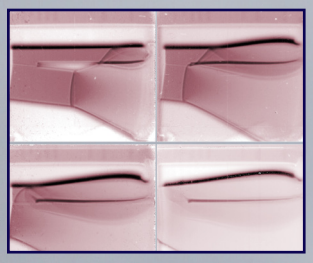
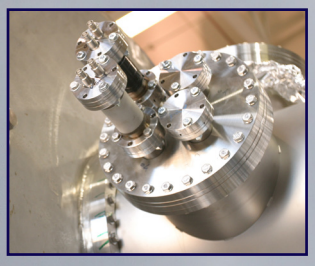






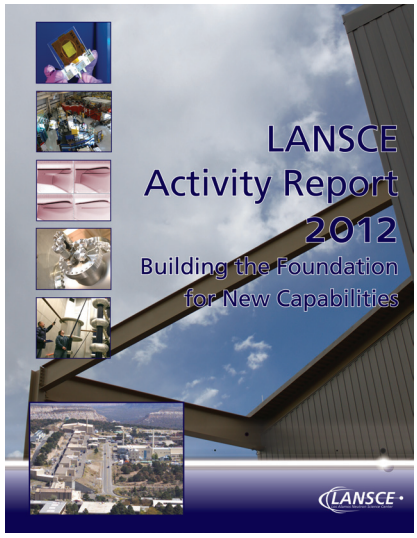
LANSCE Activity Report 2012

Building the Foundation for New Capabilities

LANSCE
Los Alamos Neutron Science Center

About the Cover

The Los Alamos Neutron Science Center (LANSCE) is building new foundations for new capabilities. The running theme of blocks throughout this report echoes the building blocks of capabilities, which lead to collaborations and discoveries. Featured is the new Weapons Neutron Research facility building—a cornerstone for cutting-edge science.



Los Alamos
NATIONAL LABORATORY
EST. 1943

LANSCE Activity Report 2012

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

Abstract

The "LANSCE Activity Report 2012" describes scientific and technological progress and achievements at LANSCE during calendar year (CY) 2012. This report includes LANSCE research highlights, accelerator operations highlights, and user program demographics. Of special emphases for the CY2012 report are LANSCE's collaborative efforts, and new capabilities—with a focus on the Weapons Neutron Research facility.

This report is available online:
http//lansce.lanl.gov.

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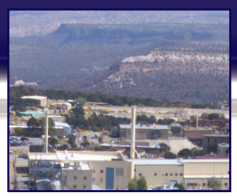


Foreword

Colleagues,

We present to you the 2012 LANSCE Activity Report. This year was busy and interesting for LANSCE. The overall beam reliability at all facilities topped 89%. Collaborations and new capabilities further enabled LANSCE's world-class science and enhanced its contributions to international science and national security.

The experimental capabilities of the Weapons Neutron Research facility were increased by the completion of its new experimental area. The Proton Radiography Facility team celebrated its 500th shot in support of national security. Our active user program, national security work, and accelerator-based actinium-225 production at the Isotope Production Facility are all great examples of how LANSCE continues to serve the nation. Because of the continuing National Nuclear Security Administration support, great progress was made related to the LINAC Risk Mitigation.

In the summer of 2012, LANSCE served as the technical host for the National User Facility Organization Annual Meeting. This meeting was attended by representatives from major user facilities in the US and focused on university relations, industry, and user access in general.

The year 2012 was also challenging. The user community was impacted by the technicium-99 incident. Some operations at the Lujan Center were suspended during the clean up process and were successfully resumed upon completion of the decontamination.

In 2012 the first Rosen Scholar fellowship was awarded. This fellowship was equally shared between Professor Richard Casten, Department of Physics, Yale University; and Professor Markus Roth, Institut für Kernphysik, Technische Universität Darmstadt, Germany. During their fellowship, both scholars made seminal contributions that increased our scientific outreach and experimental capabilities.

We hope you enjoy reading about our highlights and new capabilities for 2012.

- Alex Lacerda and Kurt Schoenberg

Alex H. Lacerda
Deputy Director, LANSCE

Kurt F. Schoenberg
Director, LANSCE

Contents

Foreword iii

Los Alamos National Laboratory vi

Los Alamos Neutron Science Center 1

LANSCE at a Glance 2

Capabilities and Collaborations 4

- Capabilities and Collaborations at a Glance 5
- Highlights 6

Isotope Production Facility 18

- IPF at a Glance 19
- Highlights 20

Lujan Neutron Scattering Center 24

- Lujan Center at a Glance 25
- Highlights 26

Proton Radiography 50

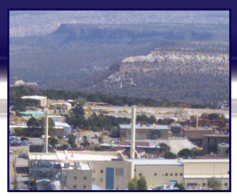
- pRad at a Glance 51
- Highlights 52

Weapons Neutron Facility 58

- WNR at a Glance 59
- Highlights 60

User Program 70

- User Program at a Glance 71
- User Demographics 72



Accelerator Operations Technology 76

AOT at a Glance 77

LANSCE Risk Mitigation 78

LANSCE Beam Facts 80

Beam Reliability 81

Conferences, Workshops and Tours 82

Conferences and Workshops at a Glance 83

Tours 91

News and Celebrations 94

News and Celebrations at a Glance 95

Acknowledgments 108

Los Alamos National Laboratory

Los Alamos National Laboratory's (LANL's) mission is to develop and apply science and technology to ensure the safety, security, and reliability of the United States (US) nuclear deterrent; reduce global threats; and solve other emerging national security and energy challenges.

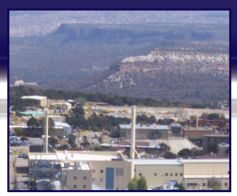
LANL has a proud history and heritage of almost 70 years of science and innovation. The people of LANL work on advanced technologies to provide the best scientific and engineering solutions to the nation's most crucial security challenges.

Located 35 miles northwest of Santa Fe, New Mexico, LANL lies on 36 square miles of DOE-owned property and contains more than 2000 individual facilities, including 47 techical areas.

As a premier national research and development (R&D) laboratory, LANL collaborates with universities and and industry. LANL personnel play leading roles worldwide in basic and applied scientific research and technology.

Discoveries, developments, advancements, and inventions pouring from LANL make America—and the world—a better and safer place and bolster national security.

LANL's main site.



Los Alamos Neutron Science Center

Five state-of-the-art facilities operate simultaneously at the Los Alamos Neutron Science Center (LANSCE), contributing to national security, nuclear medicine, materials science and nanotechnology, biomedical research, electronics testing, fundamental physics, and many other areas. During the run cycle, when the linear accelerator (LINAC) 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. LANSCE provides the scientific community with intense sources of neutrons and protons and with the capability of performing experiments supporting civilian and national security research.

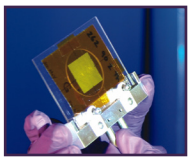
The LINAC's capability to reliably deliver beam current is the key to the LANSCE's ability to perform research—and thus the key to meeting NNSA's and DOE's mission deliverables.

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 and the products we use in our daily lives by supporting materials science and technology.

LANSCE site.

LANSCE at a Glance

Isotope Production Facility

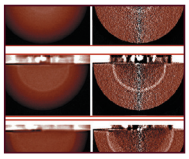


LANL produces radioactive isotopes for medicine and research. The Isotope Production Facility (IPF) at LANSCE supplies a wide range of radioisotopes to medical researchers all over the world and has been a leader in developing and producing new and unique isotopes for R&D.

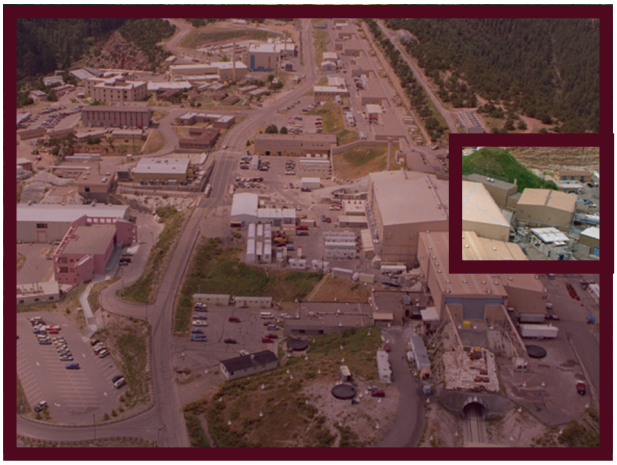
Lujan Neutron Scattering Center

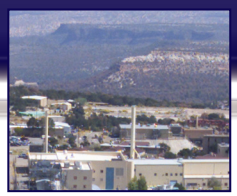
The Lujan Neutron Scattering Center (Lujan Center) uses a pulsed spallation neutron source equipped with time-of-flight spectrometers for neutron scattering studies. Neutron scattering is a powerful technique used for materials science, engineering, condensed matter physics, chemistry and biology, and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

Proton Radiography Facility



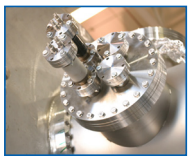
The Proton Radiography Facility (pRad) and project use the 800-MeV protons provided by the LANSCE accelerator to diagnose more than 300 dynamic experiments in support of national and international weapons science and stockpile stewardship programs.





LANSCE at a Glance

Ultra-Cold Neutron Facility



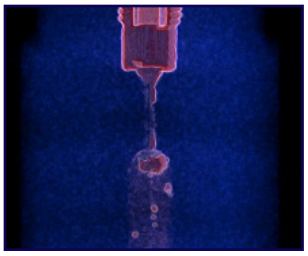
An international collaboration of researchers working at LANSCE and eight other member institutions use the Ultra-Cold Neutron Facility (UCN) for experiments that could answer questions about the fundamental constants of nature and aid in the quest for new particles. The ultra-cold neutron extraction port at UCN delivers the most intense source of ultra-cold neutrons in the world.

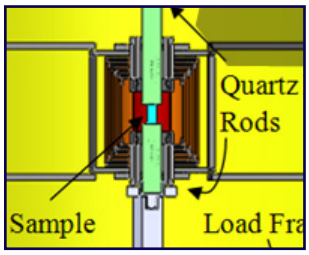
Weapons Neutron Research Facility

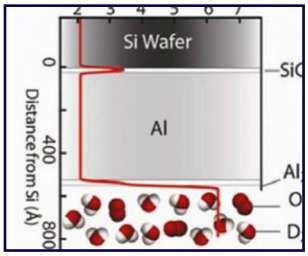
The Weapons Neutron Research Facility (WNR) provides neutron and proton beams for basic, applied, and defense-related research. Neutron beams with energies ranging from about 0.1 MeV to more than 600 MeV are produced in Target 4 (an unmoderated tungsten spallation source) using the 800-MeV proton beam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

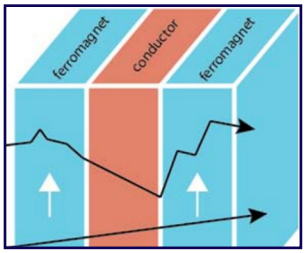
User Program

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









Capabilities and Collaborations 2012

LANSCE
Los Alamos Neutron Science Center

Capabilities and Collaborations

Capabilities
New capabilities at LANSCE provide the technology and tools that not only open new paths for our valued partners, but attract new collaborators.

Sample New Capabilities for 2012:

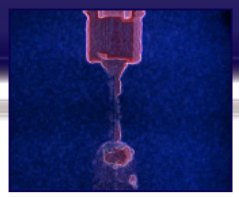
- New neutron tomography station
- Furnace for in situ, high-temperature deformation and creep experiments at LANSCE
- Development of a high-pressure-temperature (P-T) cell to study interface processes

Collaborations
Working together to serve the common purpose of creating and producing science, LANSCE with its collaborators and their contributions are leading the way to new discoveries.

Sample Collaborations for 2012:

- Development and demonstration of neutron computer tomography
- Effect of interface-induced exchange fields on cuprate-manganite spin switches
- Unique laser systems set world record for neutron beam generation

Image (right): Workers collaborate on a safety check for the Cockcroft-Walton Generator's capabilities.



New Neutron Tomography Station Studies High-Pressure CO_2 in Porous Media

LANL researchers have developed a new tomography station at LANSCE using Flight Path 5B, located 60 m from the neutron source. The project was inspired by research in multiphase flow and reaction in carbon dioxide (CO_2)-brine systems for understanding the geological storage of CO_2. The first experimental results show a tomographic image of the injection of water into a glass-bead-filled, gas-cell apparatus filled with CO_2 at approximately 200 bars (figure right). The tomogram easily resolves the 500-µm-diameter glass beads, some of which contain strongly absorbing metals and display as distinct spheres. The image comes close to achieving the theoretical resolution of 150 µm. Contrary to initial predictions, the injected water forms an irregular mass at the top of the cell and does not penetrate the bead pack. Flight Path 5b will eventually house a new triaxial coreflood system for in situtomographic imaging of multiphase flow through geomaterials under both confining and axial loads. The coreflood system will enable detailed investigations of the behavior of multiple fluid phases in porous media and the development and flow of fluids through fractures.

This new imaging capability supports LANL's Energy Security mission and the Materials for the Future science pillar by enabling the investigation of multiphase interactions in porous media with applications in conventional and nonconventional fossil fuel, geothermal energy, environmental contamination, and nuclear waste repository science. The tomography capability also supports materials characterization, with applications ranging from the weapons program to fuel cells.

The team includes B. Carey and D. Newell (Earth Systems Observations, EES-14), A. Lopez, J. Hunter, W. Ward, and T. Claytor [Applied Engineering Technology (AET)-6]; and J. Zhu (Lujan Center), with assistance from R. Nelson (WNR).

Laboratory Directed R&D (LDRD) and LANL's Small-Scale Instrument Program (G&A Reinvestment through Principal Associate Directorate Science, Technology and Engineering (PADSTE) funded different aspects of the research.

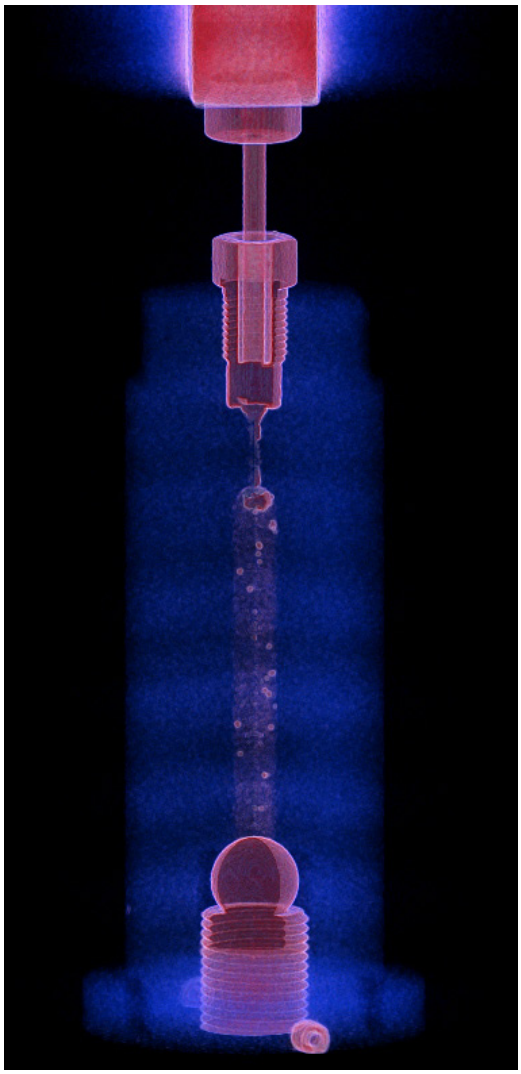
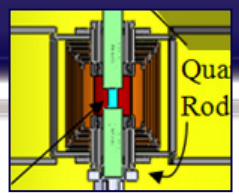


Figure: Tomographic image of the injection of water into a glass-bead-filled, gas-cell apparatus filled with CO_2 at approximately 200 bars.



Furnace for In Situ, High-Temperature Deformation and Creep Experiments at LANSCE

For material scientists and engineers working on optimizing material properties, it is crucial to understand and ultimately predict the microstructural evolution of metals and alloys during thermo-mechanical treatment. The orientation distribution of all crystals (i.e., texture) strongly influences the material properties of the polycrystalline aggregate. The ability to study the distinct influences of elevated temperatures and uniaxial stress on the texture, temperature-dependent lattice strains, and phase transformation kinetics of a material in situ provides unique insight into variant selection during phase transformations or deformation mechanisms active during creep. Sven C. Vogel (Lujan Center) and H. Matthew Reiche [New Mexico State University (NMSU) and the Lujan Center] led the development of a novel sample environment at the Lujan Center, which extends the capabilities for in situ studies in support of neutron diffraction users. The journal *Review of Scientific Instruments* published the work.

The researchers designed and commissioned a resistive furnace that enables the acquisition of neutron diffraction data while the centimeter-sized specimen is under uniaxial stress (≤2700 N) at elevated temperatures (≤1000°C). Additional rotation (≤80°) around the vertical compression axis of the sample enables texture measurements in the High-Pressure-Preferred Orientation (HIPPO) diffractometer at LANSCE. This apparatus revealed quantitative insights on the development of texture- and lattice-plane-dependent strains throughout deformation and phase changes (at approximately 860°C), which simulated thermomechanical processing steps of Zr-2.5wt%Nb, an alloy used for pressure tubes in Canada deuterium uranium (CANDU) nuclear reactors. The scientists confirmed sample composition and texture via comparisons with room temperature results from a known sample environment. Temperature-dependent lattice parameters agree with published results of conventional furnaces and literature values.

Researchers can use this apparatus to separate the texture and strain changes introduced by temperature change, phase transformation, and uniaxial deformation. The data could help refine models that predict material properties after the processing. The novel instrument apparatus provides new opportunities to study the individual influences of elevated temperatures and uniaxial stress on the texture and lattice parameters of sample materials. In addition to Reiche and Vogel, Eric Larson (Lujan Center) provided design support, and collaborators included Paula Mosbrucker and Mark Daymond (Queen's University in Kingston, Canada).

Reference: "A Furnace with Rotating Load Frame for In Situ High Temperature Deformation and Creep Experiments in a Neutron Diffraction Beam Line," *Review of Scientific Instruments* **83**, 053901 (2012).
doi: 10.1063/1.4708619.

This research benefits from the Lujan Center at LANSCE, which the DOE's Office of Science, Basic Energy Sciences (BES) funds, and the Natural Sciences and Engineering Research Council (NSERC) Industrial Research Chair in Nuclear Materials at Queen's University.

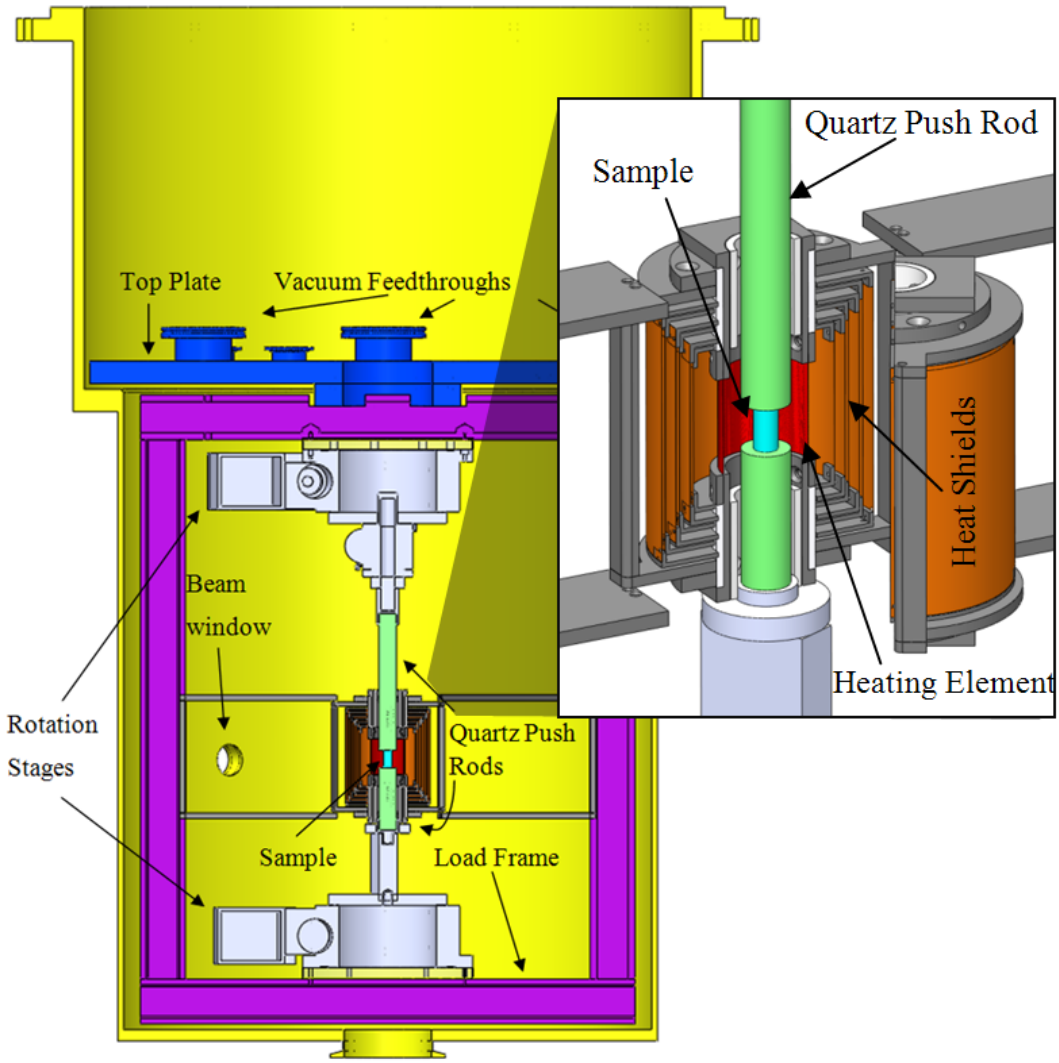


Figure: Schematic of 1.3-m-tall sample environment, accommodating load frame (purple), rotation stages (grey), and furnace core (inset). The schematic depicts vanadium heat shields (orange), the heating element (red), and the sample (light blue).

Development of a High-Pressure-Temperature Cell to Study Interface Processes

Solid-liquid interactions control the success or failure of many attempts to engineer Earth's subsurface for energy and/or environmental applications. These interactions are not well understood, nor can they be optimized effectively, except using Edisonian approaches. Interactions at solid/fluid interfaces at elevated P-T control mineral growth or dissolution and well-bore corrosion at geologic carbon sequestration sites, corrosion and scaling in nuclear reactors and geothermal systems, and hydrocarbon extraction from conventional and unconventional oil and gas reservoirs. Maintaining or restricting porosity to extract hydrocarbons in deep-gas fields, stimulating geothermal reservoirs, and maintaining porosity and seals in geologic carbon sequestration reservoirs require accurate predictions of the dissolution and precipitation of solids in dense, often supercritical, mixed-volatile fluids. Investigations at high P-T, the critical regime for many energy applications, are limited. The growing importance of research at extreme conditions demands the development of appropriate experimental apparatus to withstand high P, T, and extreme environmental conditions (e.g., radiation field, mechanical stress, pH, and ion saturations) while providing high-spatial-resolution capabilities. LANL researchers and a collaborator have developed the first neutron reflectometry (NR) P-T cell specifically for the interrogation of geologic and materials science samples. The cell provides the greatest combined P-T capabilities for NR currently available. The work is in press in the *European Journal of Physics–Plus*.

The ability of neutrons to penetrate high-P-T cells and to interrogate buried structures, combined with their sensitivity to H/deuterium in hydrocarbon-rich fluids, make NR a powerful technique to examine fluid properties within a few nanometers of interfaces. The time-of-flight Surface Profile Analysis Reflectometer (SPEAR) at LANSCE provides state-of-the-art NR capabilities to study solid-liquid interfaces. Researchers developed an NR cell to conduct experiments at moderately elevated P-T (200 MPa and 200° C). This cell allows for the study of 2-in.-diameter disks of minerals and other materials in contact with a variety of fluids, including CO_2-saturated liquids. Initial applications focused on the corrosion of aluminum (Al) at elevated P-T and on calcite/fluid interfaces.

The scientists conducted a preliminary experiment at roughly half the cell's design pressure capability. Their goal was to measure the growth of Al corrosion when Al is in contact with aerated deuterated water (D_2O) at elevated P and T. The surface oxide (Al_2O_3) that forms on the Al has a higher scattering length density (SLD) than pure Al, providing neutron scattering contrast between the two materials. NR measures the change in the distribution of the SLD over time. Material growth or dissolution, density and composition changes, and interface roughening can be probed in situ with NR in elevated P-T conditions. The experiment demonstrates the importance of performing in situ measurements because features such as surface morphologies, intra- and interlayer expansion or distortion, and fluid structuring in high-P-T conditions may be unquenchable. Therefore, the features cannot be investigated with other technology via ex situ or extremely slow measurements.

The team concluded that the ability to reach high P and T while controlling the sample environment with regard to dissolved species and gas content, coupled with the near atomic-level resolution of NR, will extend NR into new fields. This capability could be applied to a range of LANL mission areas where high-P-T solid/fluid interface interactions are important, including deep-gas extraction, high-P-T corrosion of nuclear fuels and cladding, performance of waste forms in repositories, and the understanding and controlling of a range of engineered geosystems in extreme P-T environments.

Reference: "High Pressure and High Temperature Neutron Reflectometry Cell for Solid-Fluid Interface Studies," *European Physics Journal–Plus*, **127**: 26, 2012.
http://dx.doi.org/10.1140/epjp/i2012-12076-0

Researchers include P. Wang, M. Taylor, and J. Majewski (Lujan Center); A.H. Lerner and D. Hickmott [Earth and Environmental Sciences (EES)]; A. Misra and J. Baldwin [Materials Physics Applications (MPA)—Center for Integrated Nanotechnologies (CINT)]; A. Voter, D. Perez, and C-Y. Lu (Physics and Chemistry of Material, T-1); and R. Grubbs [Sandia National Laboratories (SNL)].

LDRD sponsored the work. The research benefited from the use of the SPEAR neutron time-of-flight spectrometer at Lujan Center, which the DOE's Office of Science, BES funds.

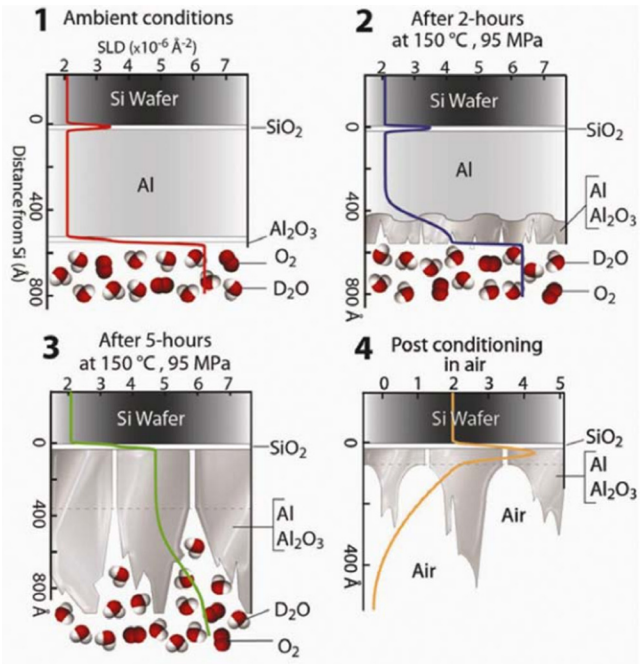


Figure: Schematic of the evolution of the Al film during the course of the P-T condition based on interpretations of NR reflectivity modeling (superimposed real-space SLD profiles). The altered layer is an Al/Al_2O_3 mixture, and the open areas are D_2O-filled pits.

Development and Demonstration of Neutron Computer Tomography

A collaboration between the Nondestructive Testing and Evaluation Group (AET-6) and WNR developed and demonstrated neutron computed tomography (CT) at LANSCE on Flight Path 5. The nondestructive characterization of material samples and experimental systems has the driven development of computed tomography techniques, dominantly using x-ray radiation. Using neutrons in a similar fashion to x-rays provides additional nondestructive evaluation capability.

A limited set of facilities, such as WNR, provides neutrons with well-defined characteristics and collimation. LANL researchers focus development and application demonstrations on highly specialized experiments for components with unique aspects that can be investigated within facility-specific schedules. These recent developments have established the neutron tomography capability at LANSCE. Researchers interested in applications of this inherently collaborative work should contact James Hunter (AET-6) and the WNR team.

Proof-of-principle studies characterized complex parts. The researchers imaged a Mac mini computer, a motor assembly, and a fluid experiment involving water injection into a porous cell filled with liquid CO_2. The results demonstrated good penetration, strong contrast between plastic and metal components, excellent resolution, and minimal streaking. These tests also involved the comparison of five scintillators for brightness and quality.

Reconstruction and imaging using neutrons are functionally identical to x-ray CT. They leverage the extensive expertise, reconstruction, and computational capabilities in AET-6. In comparison to established x-ray radiography, neutrons do not attenuate in the same fashion; this results in radically different attenuation coefficients and creates the potential for measuring physical quantities other than attenuation.

Reconstruction and imaging using neutrons is functionally identical to x-ray-computed tomography. Neutron imaging leverages the extensive expertise in image reconstruction and computational capabilities in AET-6. In comparison to established x-ray radiography, neutrons do not attenuate in the same manner, being sensitive to properties of the atomic nucleus rather than the atomic electrons. This sensitivity results in radically different attenuation coefficients and creates the potential for measuring physical quantities other than x-ray attenuation due to atomic properties. As an example, neutrons penetrate many heavy elements much more than x-rays. The neutron attenuation properties enable specific characterization applications, such as identifying light elements and materials like plastic and water inside metal components. This ability is an advantage in specific applications, for example, in evaluating items like solder on circuit boards or plastic parts embedded in heavy metal containers. Due to typically lower source intensities and lower detection efficiencies for neutrons compared to x-rays, longer scans are required to obtain good images.

Reference: *CT Systems and Applications Development at LANL* ASNT 22nd Research Symposium 2013 Memphis, TN 18-21 March 2013.

Researchers include J. Hunter, W. Ward, A. Lopez, T. Claytor, D. Summa, and T. Ickes (AET-6); and F. Tovesson and R. Nelson (WNR). B. Carey and J. Zhu (EES-14) are the Principal Investigators on the CO_2 sequestration project.

A PADSTE small-equipment grant and NNSA Campaign 8 funded the capability development.

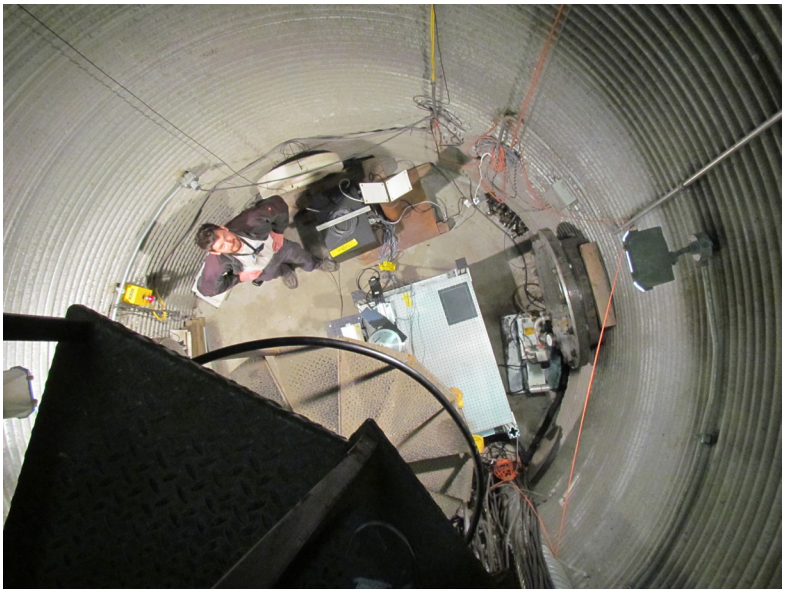


Image: James Hunter (AET-6) standing at the Flight Path 5, 60-m station, as viewed from above. This station is located 9 m underground, with access provided by a spiral staircase. The current Neutron CT system setup is in front of him, and the neutron beam enters via the pipe on the right side of the image. The large neutron beam spot available in this station enables better imaging of larger objects than at the closer stations.

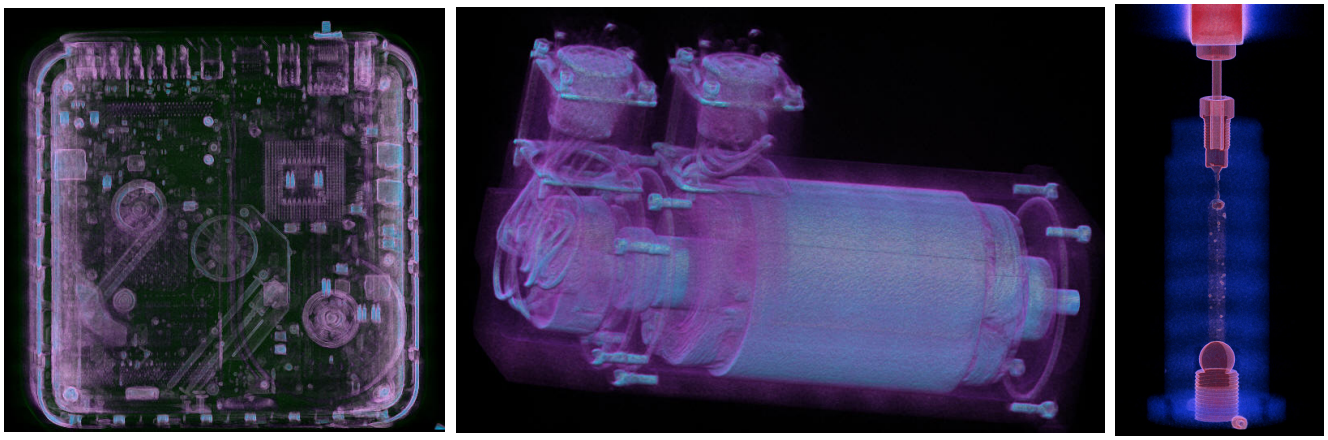


Figure: (Left to right): Neutron CT false color interpretation images of a Mac-mini, motor assembly, and a 1-in., internal-diameter Al cell filled with glass beads and liquid CO_2 as water is injected.

Effect of Interface-Induced Exchange Fields on Cuprate-Manganite Spin Switches

Scientists from Argonne National Laboratory (ANL); Universidad Complutense de Madrid, Spain; and LANL used the Asterix polarized neutron reflectometer at the Lujan Center to elucidate the mechanism of inverse spin switching in ferromagnetic/superconducting heterostructures. *Physical Review Letters* published the research.

In a conventional spin-valve system, the orientation of two transition element ferromagnetic films sandwiching a conducting layer directly determines whether spin scattering of one or both electron spin states takes place (figure top). The resistivity of the spin valve (i.e., whether the resistivity is high or low) is the means to translate data stored in nanometer-sized magnetic domains into electrical signals such as the 1's and 0's that computers use.

However, the situation is very different when the ferromagnetic films are complex oxides and the conductor is a high-temperature cuprate superconductor. Researchers examined the anomalous inverse spin switch behavior in $La_{0.7}Ca_{0.3}MnO_3$(LCMO)/$YBa_2Cu_3O_{7-\delta}$(YBCO)/LCMO trilayers by combined transport studies and PNR. They observed nearly the opposite behavior (and thus the name inverse spin switch). Many theories have been sought to explain the inverse switch phenomena in terms of the orientation of ferromagnetic layers. The research team found compelling evidence that the orientation of the ferromagnetic layers does not directly affect the resistivity of the superconductor. The conventional explanation based on the scattering of electron spins is not applicable. Rather, the ferromagnetic layers induce a magnetic field in the superconductor via exchange (figure bottom a). When the exchange field opposes the applied field, the superconductivity of the YBCO layer is maximized (figure bottom 6b).

Superconductivity is suppressed when the exchange field augments the applied field. This work highlights the importance of induced magnetization in complex oxides and the possibility of detecting minute magnetic fields using a potentially more sensitive technology. Because the inverse spin switch is governed by interfacial electronic reconstruction and not shape-dependent micromagnetic effects, the scientists expect it to survive miniaturization to the nanoscale.

Reference: "Effect of Interface-Induced Exchange Fields on Cuprate-Manganite Spin Switches," *Physical Review Letters* **108**, 207205 (2012). doi:10.1103/PhysRevLett.108.207205.

Researchers include M.R. Fitzsimmons and M. Zhernenkov (Lujan Center); Y. Liu, L.Y. Zhu, A. Hoffmann, and S.G.E. te Velthuis (ANL); and C. Visani, N.M. Nemes, J. Tornos, M. Garcia-Hernandez, C. Leon, and J. Santamaria (Universidad Complutense de Madrid, Spain).

The DOE's Office of Science, BES funded the LANL portion of the research and the Lujan Center, a national user facility.

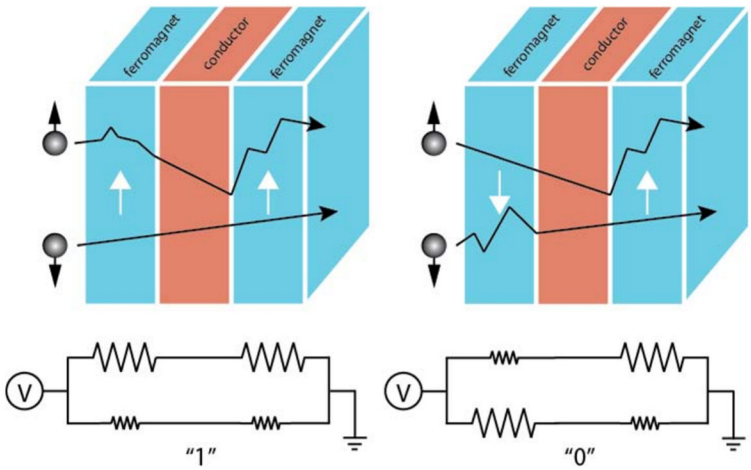


Figure Top: Trajectories (top) of electron spins, up and down, as they traverse the ferromagnet/conductor trilayer. Kinks in the trajectories indicate scattering of the electron and increased resistivity. (Bottom): Electrical circuits representing electron scattering as resistance. The low resistance circuit is depicted as a "1".

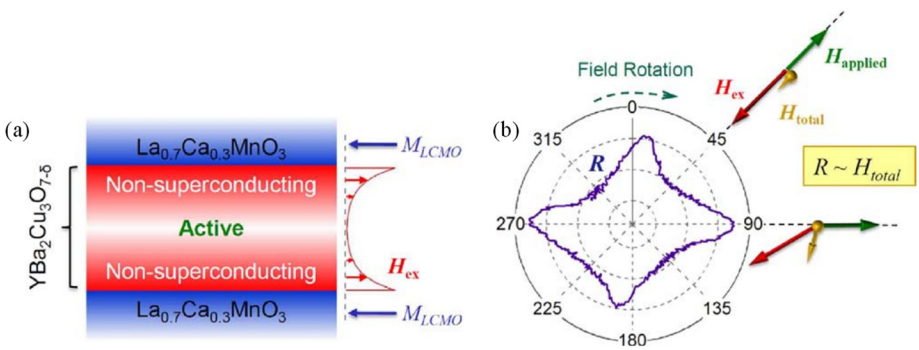


Figure Bottom: (a) Schematic picture of the exchange field induced in YBCO by proximity to LCMO. The exchange field decays with distance from the interface. The superposition of the exchange field from each side of YBCO can either cancel or augment the applied field, thus affecting the strengthening or suppressing the superconducting properties of the YBCO, respectively. (b): Dependence of the resistance R on the orientation of the applied field. When the exchange field H_{ex} negates the applied field, superconductivity is strengthened.

Unique Laser Systems Set World Record for Neutron Beam Generation

Scientists used a one-of-a-kind laser system at LANL to create the largest neutron beam ever made by a short-pulse laser. Neutron beams are usually generated with particle accelerators or nuclear reactors and are used in a wide variety of scientific research, particularly in advanced materials science. Researchers from LANL, the Technischen Universität Darmstadt (TU-Darmstadt), Germany, and SNL focused high-intensity light from the Trident laser, a unique and powerful 200-trillion-watt, short-pulse laser, on an ultra-thin plastic sheet infused with deuterium [an isotope of hydrogen (H)].

The laser light—200 quintillion watts per square centimeter, equivalent to focusing all of the light coming from the sun to the earth (120,000 terawatts) onto the tip of a pencil—interacts with the plastic sheet, creating a plasma (an electrically charged gas). The plasma then accelerates large numbers of deuterons (the nucleus of the deuterium atom) into a sealed beryllium target, converting the deuterons into a neutron beam. A unique property of plasmas called relativistic transparency enables the deuterons to be accelerated in just 1 mm, rather than the many meters required by standard accelerator technologies. Only the Trident laser has implemented this new plasma acceleration mechanism. The neutrons are emitted along the direction of the initial laser beam and can reach very high energies (in excess of 50 MeV). The neutron image driven by the short-pulse laser demonstrated excellent agreement with numerical calculations. The new record is five times greater than the previous record and required less than a quarter of the laser energy.

This record neutron beam has the speed and energy range that makes it an ideal candidate for radiography and a wide variety of high-energy-density physics studies. Neutrons are useful probes to examine fundamental properties of the universe and advanced materials. Potential applications include actively interrogating cargo containers, monitoring for clandestine nuclear explosives at border crossings, and being used as a test bed for fusion-relevant neutron diagnostics. Short-pulse lasers for the production of neutrons can open the field of neutron research to universities and a broader research community.

This project combined the expertise of LANSCE's neutron science group with Physics Division's plasma physicists, Trident laser scientists, and scientists developing neutron detection diagnostics to be fielded at the National Ignition Facility. SNL researchers provided neutron yield and nuclear activation measurements.

Markus Roth (TU-Darmstadt) a 2012 Rosen scholar at the LANSCE, led the project.

Researchers include D. Jung, K. Falk, J. Fernandez, D. Gautier, M. Geissel, B. Manuel Hegelich, R. Johnson, T. Shimada, and G. Wurden (Plasma Physics, P-24); N. Guler, F.E. Merrill, J. Tybo, and C. Wilde (Neutron Science and Technology, P-23); M. Devlin, R. Haight, T. Taddeucci, and S. Wender (WNR); A. Favalli (Safeguards Science and Technology, NEN-1); C. Hamilton (Polymers and Coatings, MST-7); K.F. Schoenberg (Experimental Physical Sciences, ADEPS); G. Schaumann and O. Deppert (TU-Darmstadt); and M. Schollmeier (SNL).

Reference:
https://www.lanl.gov/newsroom/news-releases/2012/July/07.10-world-record-neutron-beam-at-lanl.pdf

The Rosen Scholar funding, NNSA, and LDRD sponsored different aspects of the research.

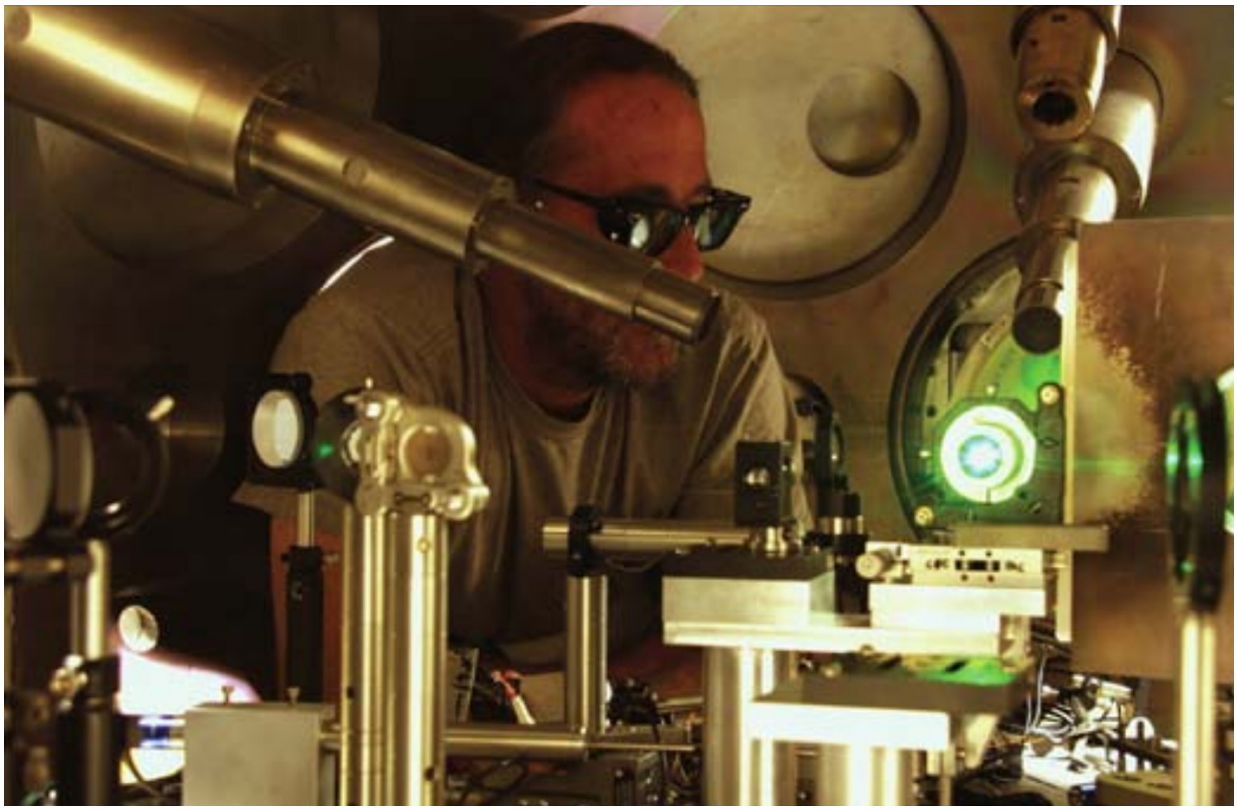
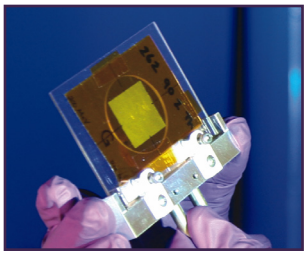
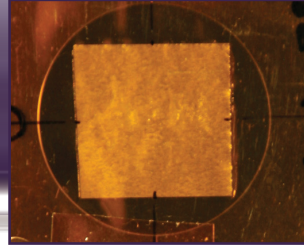


Image: Donald Gautier (Plasma Physics, P-24) works in Trident's north target chamber.



Isotope Production Facility 2012

LANSCE
Los Alamos Neutron Science Center



IPF

The Office of Nuclear Physics administers the nation's isotope program for the Office of Science.

The national isotope program has three main objectives:

- Produce and distribute radioactive and stable isotopes that are in short supply, as well as associated by-products, surplus materials, and related isotope services.
- Maintain the infrastructure required to produce and supply isotope products and related services.
- Conduct R&D on new and improved isotope production and processing techniques.

The LANL Isotope and Applications Program is a leader in developing and producing new and unique isotopes for R&D.

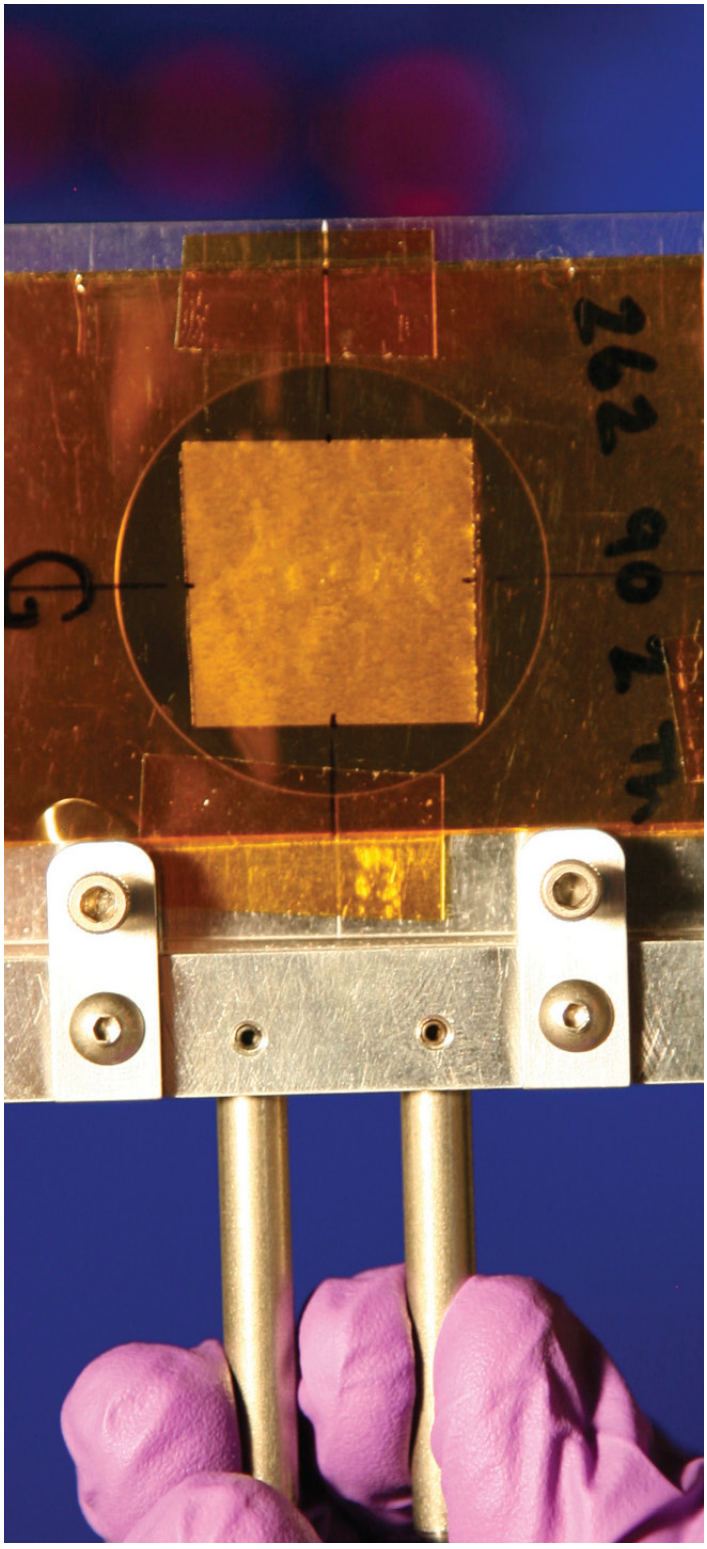
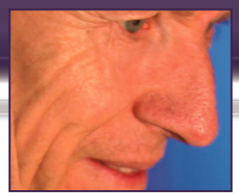


Image (right): A thorium foil test target for proof-of-concept ^{225}Ac production.



Cancer Therapy Gets a Boost from a New Isotope

The LANL Isotope Program completed a successful R&D project to explore the accelerator-based production of the isotope actinium-225 (^{225}Ac). The isotope is a promising cancer therapeutic agent to attack cancer cells through the emission of alpha radiation. Its alpha particles are energetic enough to destroy cancer cells but are unlikely to move beyond a tightly controlled target region and destroy healthy cells. Alpha particles are stopped by 1 to 2 in. of air or a layer of skin. President Obama recognized the development of new cancer therapies such as ^{225}Ac in his 2012 State of the Union Address: "Today, the discoveries taking place in our federally financed labs and universities could lead to new treatments that kill cancer cells but leave healthy ones untouched."

One of the primary barriers to the wider use of ^{225}Ac has been the lack of an economically viable supply. Actinium-225 has historically been produced in a volume of 600–800 millicuries per year via the natural decay of thorium-229 (^{229}Th) from uranium-233 (^{233}U). However, the current need for ^{225}Ac far outstrips the supply possibilities from this method of production, and annual demand potentially could reach 50,000 millicuries by 2014. If we consider the current clinical demand coupled with increasing difficulties associated with ^{233}U safeguards, it is clear that new sources are needed to meet our national need for this isotope. The Nuclear Science Advisory Committee—Isotope (NSACI) focus group recently cited the gap between production and demand, saying that we should "invest in new production approaches of alpha emitters with highest priority for ^{225}Ac."

LANL's work to address the NSACI recommendation has focused on the production of research-scale quantities of ^{225}Ac via the irradiation of thorium target foils using the 100-MeV proton beam supplied by LANSCE's accelerator to IPF and the 200- to 800-MeV beam supplied to WNR.

Preliminary experiments provide a promising indication that accelerator-based production will be viable at the scales required to support clinical applications. The LANL proof-of-concept work received international recognition at an International Atomic Energy Agency consultant's meeting in 2011, where Meiring Nortier (Inorganic Isotope and Actinide Chemistry, C-IIAC) presented details on ^{225}Ac production using accelerators and described the nuclear data needs for medical isotope production (http://www-nds.iaea.org/publications/indc/indc-nds-0591/).

The ^{225}Ac effort is now shifting to the development of high-power targetry and bulk-scale radiochemical processing technology to enable production of the medical isotope routinely. LANL is pursuing this goal in conjunction with research teams at Oakridge National Laboratory (ORNL) and Brookhaven National Laboratory (BNL). The research indicates that it will be possible to match current annual worldwide production of ^{225}Ac in just 2 to 5 days of operations using the accelerator at LANL and analogous facilities at BNL. The scientists estimate that 2 to 3 years of production scale-up and process development are needed before ^{225}Ac could be routinely produced.

The ^{225}Ac research is a first and important step for LANL toward creating therapeutic isotopes, in addition to the successful imaging isotopes.

The DOE's Office of Science funded the project via an award from the Isotope Development and Production for Research and Applications subprogram in the Office of Nuclear Physics. LANL's Isotope Program has generated isotopes since the 1970s. Larger-scale production began in 2005 with the construction of IPF, which provides medical imaging isotopes (such as strontium-82) for positron emission tomography (PET).

Image: Meiring Nortier holds a thorium foil test target for the proof-of-concept ^{225}Ac production experiments, as displayed in Times Square, New York City, New York.

New Cancer Fighting Isotopes Developed at IPF

IPF uses the accelerator at LANSCE to investigate proof-of-concept production of the radionuclides ^{225}Ac and radium-233 (^{223}Ra) for exploratory cancer treatment research. Appropriate radioactive alpha emitters potentially have great advantages over beta emitters for use in cancer therapy due to higher effectiveness and the limited range of alpha particles in tissue. Alpha is better than beta at destroying cancer and leaving healthy tissue untouched. However, these alpha emitters have been in such short supply that the medical community has been unable to conduct sufficient clinical trials or begin to test their effectiveness for treatments. Recently, however, work at LANL and elsewhere suggests a means of increasing availability and improving the radiochemistry of alpha-particle-emitting nuclides. This is an encouraging boost for their use in radioimmunotherapy.

The isotope ^{225}Ac has a half-life of 10 days, emits four alpha particles in its decay chain, and has great potential in the treatment of metastatic cancer. Actinium-225 can also be used as a generator for ^{213}Bi, another shorter-lived alpha emitter (half-life of 45.6 minutes) under study for targeted alpha therapy. Until now, the widespread use of ^{225}Ac and ^{213}Bi in radiotherapy has been restricted by their limited availability. These isotopes have been almost exclusively supplied via a complex separation process from products that were created in molten salt breeder reactors in the 1960s. The challenging and nonrenewable supply has been a significant barrier to research. A second radionuclide of interest, ^{223}Ra, has a half-life of 11.4 days, emits four alpha particles in its decay chain, and has promise for the treatment of bone cancer and as a generator for the production of lead-211 (^{211}Pb). Similar to ^{225}Ac, the supply of ^{223}Ra is limited because of its production method.

The LANL work explored the use of proton beam energy at both 800 MeV and below 200 MeV supplied from LANSCE to produce these nuclides. This work is part of a wider evaluation of high-energy accelerator production routes using intense 100-, 200-, and 800-MeV proton beams and natural thorium targets for the large-scale production of therapy isotopes. Such beams are available at LANL and BNL. Researchers made the first measurements of cross sections for the production of ^{223}Ra, ^{225}Ra, ^{227}Th, and ^{227}Ac from the bombardment of a natural thorium target with the LANSCE beam. Calculations, based on these preliminary irradiation experiments, predict that the ^{225}Ac yield from a single production-scale run is nearly 20 times the current annual worldwide production. A single production run for ^{223}Ra could produce a yield of 6.5 Ci. Curie amounts of the parent isotopes ^{225}Ra and ^{227}Th are also produced, enabling the production of additional curies from the resulting generators. The lower energy (below 200 MeV) is important for other facilities, such as the Brookhaven Linac Isotope Producer, which lacks the capacity for an 800-MeV beam.

The scientists will focus on refining both the production process and the isotope separation process. The IPF team at LANL plans to produce sufficient ^{225}Ac to begin offering it as a scientific research isotope as well, such as for establishing a nuclear cross-section measurement capability at LANL.

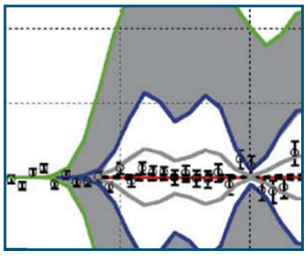
References: "^{225}Ac and ^{223}Ra Production via 800 MeV Proton Irradiation of Natural Thorium Targets,"*Applied Radiation and Isotope* 70, 2590 (2012).
doi:org/10.1016/j.apradiso.2012.07.003.

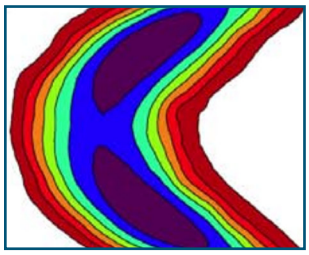
"Proton-Induced Cross Sections Relevant to Production of and in Natural Thorium Targets below 200 MeV, "*Applied Radiation and Isotope* 70, 2602 (2012).
doi:org/10.1016/j.apradiso.2012.07.006.

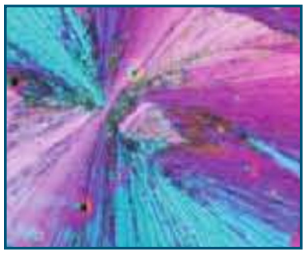
Researchers include J.W. Weidner, E.R. Birnbaum, M.E. Fassbender, G.S. Goff, L.E. Wolfsberg, and F.M. Nortier (Inorganic, Isotope and Actinide Chemistry, C-IIAC); S.G. Mashnik (Monte Carlo Codes, XCP-3); K.D. John and W. Runde (Science Program Office-Office of Science, SPO-SC); B. Ballard (Actinide Processing Support, MET-1); L.J. Bitteker, A. Couture, and J.L. Ullmann (WNR); R. Gritzo (Information Security, CIO-IS); and F.M. Hemez (XTD Primary Physics, XTD-3).

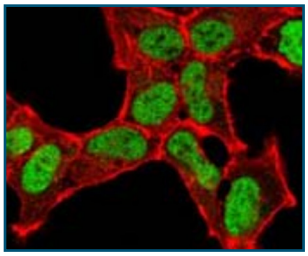
The DOE's Office of Science funded the research via an award from the Isotope Development and Production for Research and Applications subprogram in the Office of Nuclear Physics.

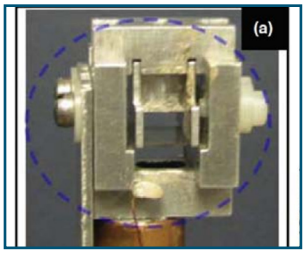
Image: John Weidner (C-IIAC) handling a target assembly in full protective gear.











Lujan Neutron Scattering Center

2012

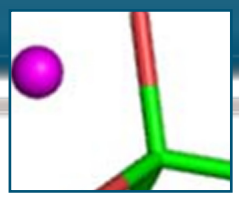
LANSCE
Los Alamos Neutron Science Center

Lujan Center

The Lujan Center is a national user facility funded by the DOE's Office of Science, BES. The Lujan Center provides pulsed neutron beams for basic and applied research, serving a national and international user community in the fields of materials science, earth science, chemistry, engineering, nuclear energy, pharmaceutical research, industry, biology, nuclear physics, and national security. Special accommodations can be made for classified and proprietary research.

Due to the highly versatile neutron target, a modern suite of specialized and diverse neutron scattering instruments populates the Lujan Center experimental hall. Users have access to a range of temperature, pressure, corrosion, and stress environment capabilities, including very low temperatures, high magnetic fields, and an extensive high-pressure capability.

Image (right): Lujan Center experimental hall.



First Neutron Diffraction Structure of a Clinical Drug Bound to Its Human Target Enzyme

A new article describing work by LANL researchers and colleagues from the University of Florida (UF) in the *Journal of the American Chemical Society* reports the first neutron structure of a clinical drug, acetazolamide (AZM), which is bound to its human target enzyme, human carbonic anhydrase (HCA) II. Scientists collected neutron and x-ray diffraction data for this study at the Protein Crystallography Station (PCS) at LANSCE. AZM is a sulfonamide drug that has been used for decades to treat a variety of diseases, such as glaucoma, altitude sickness, and epilepsy. Despite the availability of several high-resolution, x-ray crystal structures of this protein and inhibitor complex, the atomic details of drug binding have been largely unknown because of the lack of information on H-atom positions and H-bonding. AZM has three possible protonation states when it is dissolved. X-ray structures do not reveal which charged form of AZM actually binds to HCA II. Neutrons offer a unique insight into these details.

Carbonic anhydrases (CAs) are ubiquitous metalloenzymes that use a zinc-hydroxide mechanism to catalyze the reversible hydration of CO_2 to form bicarbonate and a proton. This reaction is important for many physiological processes throughout the body, including respiration, fluid secretion, and pH regulation. CAs have isoforms (proteins having amino acid sequences that differ slightly but having general activity that is very similar). In humans, 15 expressed isoforms of CAs exist in diverse tissues throughout the body, and isoforms are also involved with disease states. The similarity of the CA isoforms leads to a significant amount of cross reactivity and side effects when CA inhibitors are used as drugs to target a particular disease-associated CA. Many side effects could be avoided with the design of isoform-specific drugs. Precise information on H-bonding between targets and drugs is required to improve these compounds for targeted binding and enhanced affinity. For example, the HCA IX isoform, which is expressed only when solid tumors become hypoxic, is a prominent target for cancer therapy. The similarity of the structure and sequence of HCA IX to other human CAs has hampered drug design efforts for cancer treatment.

Many drug-binding interactions are mediated through H-atoms [either through H-bonds or water (H_2O)]. Because of the electron-poor nature of the H-atom, x-ray methods cannot inform on (1) the charged state of the drug (important for solubility, membrane permeability, absorption in the body, and how it interacts with the enzyme); (2) water-mediated binding of the drug to the enzyme; or (3) how the drug H-bonds to the protein. Neutrons offer the direct observation of the charged state of compounds when they are bound to their targets. This information yields clues for optimizing specific chemistries involved with binding.

The LANL researchers and collaborators used neutron diffraction to examine HCA II bound to a clinical drug, AZM. This neutron diffraction example is the first of a clinically used inhibitor bound to a human enzyme target. This study reveals explicit details about the charged form of the drug that binds to HCA II, the H-bonding to the target that occurs, the water that is displaced when AZM binds to the enzyme, and hydrophobic interactions that play a key role in binding. The structure demonstrates that when AZM binds to the enzyme's active site, it displaces four water molecules that had been bound to either the zinc or H-bonded to other water molecules in the active site. A detailed understanding of the water patterns and H-bonding in the active site provides a new avenue for rational structure-based drug design research to create anti-CA inhibitors for specific HCA isoforms.

Reference: "Neutron Diffraction of Acetazolamide-Bound Human Carbonic Anhydrase II Reveals Atomic Details of Drug Binding" *Journal of the American Chemical Society* **124**, 14726 (2012). doi:10.1021/ja3068098.
Publication Date (Web): August 28, 2012.

Researchers include S.Z. Fisher and M.J. Waltman (Bioenergy and Environmental Science, B-8); A.Y. Kovalevsky (formerly B-8, currently ORNL); and R. McKenna, D. Silverman, and M. Aggarwal (UF).

The DOE's Office of Biological and Environmental Research funds the PCS at LANSCE. S.Z. Fisher received partial support through an LDRD Early Career Award.

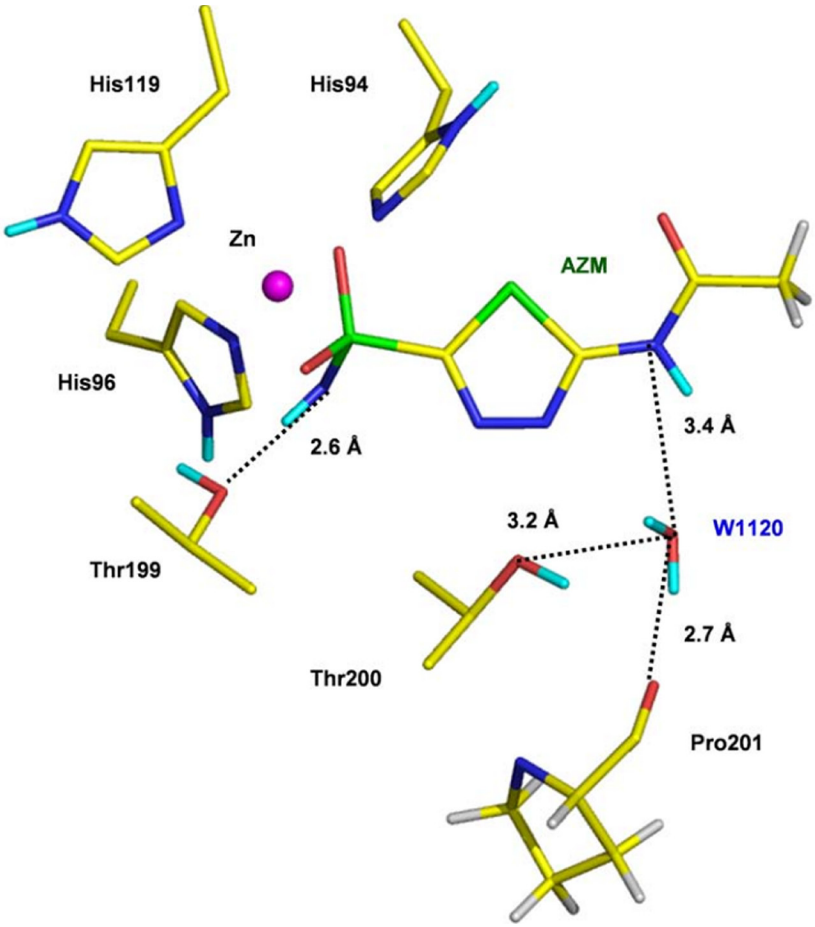
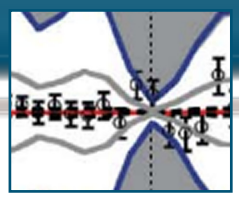


Figure: The active site of HCA II with AZM bound as determined by joint neutron and x-ray crystallography. Active-site amino acid residues are shown in yellow ball sticks and zinc (Zn) as a magenta sphere. H-bonds are indicated as dashed lines, with H-bond, donor-acceptor distances indicated. Deuterium atoms are shown in cyan, and H-atoms are shown in white.



Emergent Magnetism Measurements at $LaAlO_3/SrTiO_3$ Interfaces Set Bounds on Theory

LANL researchers and collaborators used PNR at the Lujan Center to measure the neutron-spin-dependent reflectivity from four $LaAlO_3/SrTiO_3$ superlattices. They observed important restrictions on theories that imply a strongly enhanced magnetism at the interface between $LaAlO_3$ and $SrTiO_3$. *Physical Review Letters* published the work. Improvements in sample fabrication capabilities have enabled the growth of increasingly complex materials with crystalline quality; this has allowed us to observe exotic behavior, such as the electronic confinement of a two-dimensional electron gas at the interface between two nominally insulating materials ($LaAlO_3$ and $SrTiO_3$). The conductivity can be strongly affected by magnetic fields, despite neither being magnetically ordered. Bulk magnetometry measurements of $AlO_3/SrTiO_3$ bilayer samples have reported magnetization exceeding 10kA/m if attributed to the interface. However, bulk magnetometry cannot identify whether the magnetic signal originates from the interface, substrate, film bulk, or contamination on the sample or in the magnetometer. The Lujan Center's Asterix polarized neutron reflectometer is intrinsically sensitive to interfacial magnetism. Therefore, LANL scientists used Asterix to examine magnetism at a $LaAlO_3/SrTiO_3$ interface.

Data of the neutron beam spin asymmetry obtained from two superlattice samples at 11 T and 1.7 K are shown in the figure. The solid curves and region between them represent the range over which the data should have been observed if the magnetization measured by bulk magnetometry been produced by the $LaAlO_3/SrTiO_3$interface. The neutron data are inconsistent with this explanation and instead establish an upper limit of less than 2 kA/m to magnetism for the $LaAlO_3/SrTiO_3$ interface. These results place strong constraints on theories of magnetism in $LaAlO_3/SrTiO_3$ heterostructures.

Reference: "Upper Limit to Magnetism in $LaAlO_3/SrTiO_3$ Heterostructures," *Physical Review Letters*, **107**, 217201 (November 2011). doi:10.1103/PhysRevLett.107.217201.

Researchers include M.R. Fitzsimmons, N.W. Hengartner, S. Singh, and M. Zhernenkov (Lujan Center). Collaborators: A. Brinkman, M. Huijben, and H. Molegraaf (University of Twente, The Netherlands); F.Y. Bruno and J. Santamaria (Universidad Complutense de Madrid, Spain); and J. de la Venta and Ivan Schuller (University of California–San Diego).

The DOE's Office of Science, BES funded the LANL portion of the research and the Lujan Center, a national user facility.

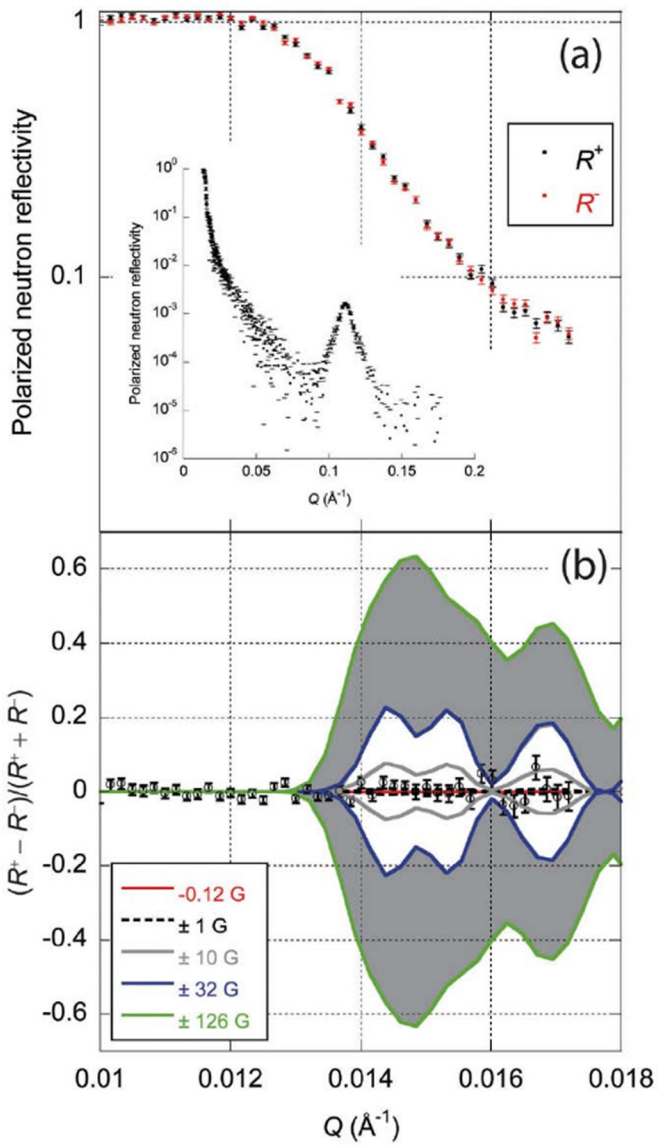
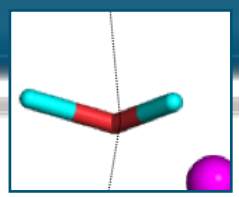


Figure: (a) PNR from one superlattice sample and (inset) R^+ from a second superlattice sample over a broader range of wave vector transfer Q.

(b) Spin asymmetry of the neutron reflectivity (1 sigma errors). Curves show the spin asymmetry anticipated for some values of magnetization.



Hydrogen-Bonded Water Network "Switch" Observed in Carbonic Anydrase

HCA II is a human enzyme found in red blood cells and secretory tissues, where it catalyzes the reversible hydration of CO_2 and HCO_3^-. HCA II serves as a relatively simple model enzyme for the study of long-range proton transfer mechanisms in more complex systems, such as adenosine triphosphate (ATP) synthase, bacteriorhodopsin, and cytochrome coxidase. Industrial interest also is increasing in using engineered CA for the extraction of CO_2 from flue gas and for the use of algae-based biofuel production. LANL scientists collaborated with the UF to publish a study in the journal *Biochemistry,* revealing important details of the proton transfer in HCA II that should improve our understanding of the enzyme's mechanism. The Lujan Center at LANSCE provided crucial structural information for the research. These results are the basis of ongoing re-engineering of the CA active site for biofuel applications.

The joint x-ray and neutron structures of wild-type HCA II at pH 10.0 and 7.8 have been determined to 2.0 Å resolution with data collected at the Lujan Center's Protein Crystallography Station. Detailed structural analysis and comparisons between the structures revealed the first observation of a "pH switch." At high pH, the water network is arranged such that proton transfer is not possible. The structure at the physiological pH of 7.8 reveals a crucial rearrangement of the water network to establish a complete H-bonded network. The data also elucidated the protonation states of two very catalytically important amino acid residues (Tyr7 and His64) as protonated and neutral, respectively. The scientists concluded that changes in charge compared with high pH probably drive the rearrangement of the water structure. This report is the first of a complete and functional H-bonded network in the active site of CA. This study also suggests that a particular water, W2, may be the one that directly interacts with His64. Scientists had not observed this previously. The results have led to further NMR spectroscopy experiments to obtain dynamic data on the H/deuterium exchange of some of the active-site amino acid residues.

Reference: "Neutron Structure of Human Carbonic Anhydrase II: A Hydrogen-Bonded Water Network 'Switch' Is Observed between pH 7.8 and 10.0," *Biochemistry*, **50**, 9421 (October 2011). doi:10.1021/bi201487b.

Scientists include S.Z. Fisher, A.Y. Kovalevsky, R. Michalczyk, and M. Mustyakimov (Bioenergy and Environmental Science, B-8); P. Langan (formerly B-8, currently ORNL); and D. Silverman and R. McKenna (UF).

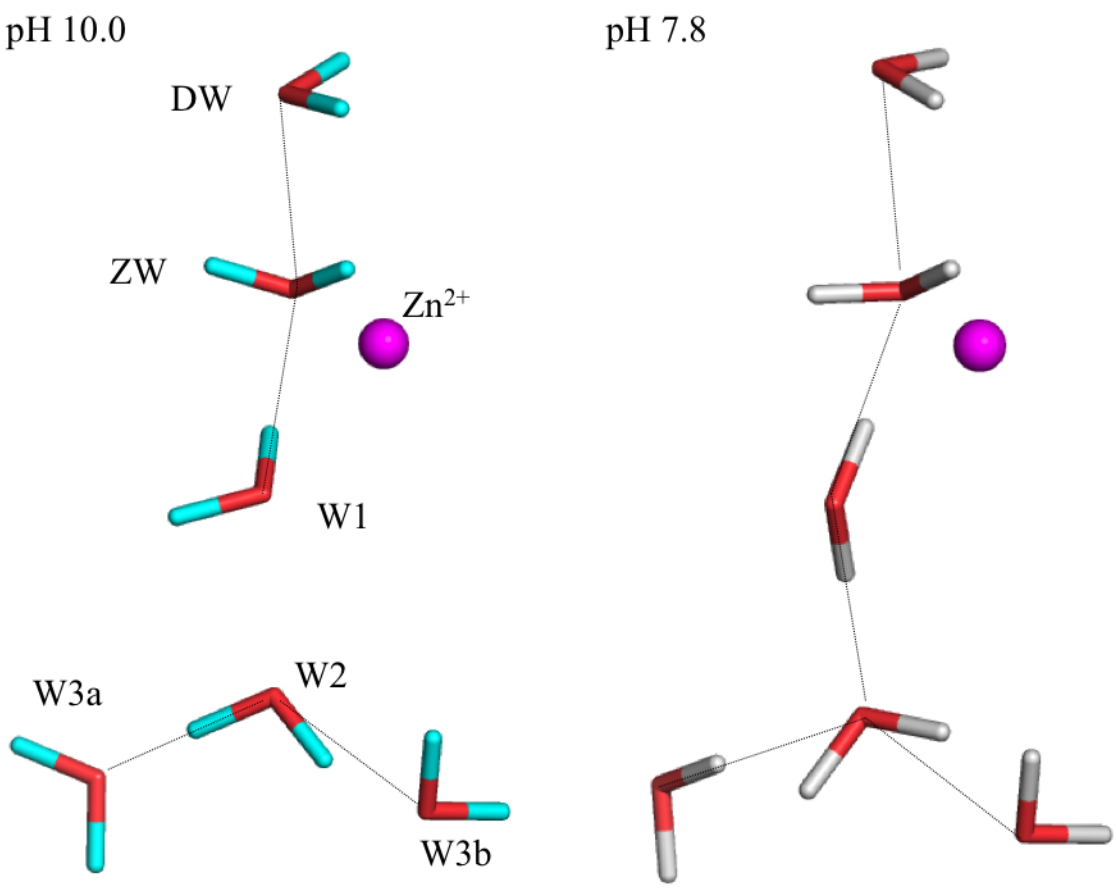


Figure: Comparison stick diagram of the water networks in the active site of HCA II determined by neutron crystallography at pH 10 (left) and 7.8 (right). The Zn cation is included for reference, and waters (W) are labeled. Observed H-bonds are shown as black lines, and active-site amino acid residues have been omitted for the sake of clarity.

Insight into the Mechanism of Toxicity of the Alzheimer's-Disease-Related Tau Protein

Alzheimer's disease is a progressive, degenerative disorder that attacks the brain's nerve cells (neurons), resulting in loss of memory, thinking and language skills, and behavioral changes. It is the most common form of dementia, affecting as many as 5.1 million Americans. From a molecular standpoint, the disease is characterized by neurofibrillary tangles (NFTs) and amyloid plaques found in the brains of affected patients. The extracellular amyloid plaques consist of deposits of the amyloid-β peptide, and the intracellular NFTs are composed of aggregates of the hyperphosphorylated tau protein. In addition to Alzheimer's disease, NFTs have also been linked to the pathogenesis of more than 20 other neurodegenerative disorders that are collectively termed tauopathies. Tau's role in the development of neurodegenerative diseases is still unclear, but a link between pathological tau aggregation and cognitive impairments has been shown. Moreover, the identification of multiple tau gene point mutations that result in hereditary tauopathies is evidence that tau malfunction alone is sufficient to cause neurodegeneration. However, two key features of tau pathology are still unclear: (1) the molecular basis of the early aggregation events, such as the structural fluctuations that trigger the aberrant accumulation of tau into NFTs rich in β-sheets *in vivo*; and (2) the mechanism by which tau aggregation causes neuronal dysfunction. In a paper accepted for publication in the journal *Biochemistry*, a collaboration between University of New Mexico (UNM), Max Planck Institute, The German Center for Neurodegenerative Diseases, and the Lujan Center at LANSCE shows that highly charged and soluble tau protein is very surface active and selectively inserts into model membranes (anionic lipid monolayers), inducing membrane morphological changes.

The scientists used complementary neutron and x-ray scattering techniques to resolve molecular-scale structural details of human tau protein (hTau40) associated with lipid model membranes. The neutron scattering experiments assessing lipid bilayer structural integrity before and after the addition of the hTau40 revealed that tau selectively disrupts anionic lipid bilayers, even at lipid packing densities higher than those of a cell membrane. However, hTau40 leaves neutral lipid bilayers intact. The results suggest that electrostatic interactions play an important role in modulating tau-membrane interactions, with hTau40 displaying a strong affinity toward the anionic membrane. Moreover, both air/water and anionic lipid membrane interfaces induce the disordered tau protein to adopt a more compact conformation, with a density similar to that of a folded protein. The results demonstrate the structural plasticity of the tau protein and the multiple mechanisms that can induce the structural compaction accompanying disordered-to-ordered transitions in the protein to render it aggregation-competent. The research provides some structural insights into the dual roles that the lipid membrane plays in catalyzing tau misfolding and aggregation and in serving as a target for tau aggregates to exert toxicity via membrane destabilization. Interactions with the tau protein disrupt lipid membrane structure, both on a molecular scale of disrupting lipid packing and on a morphological scale of completely disrupting the integrity of lipid bilayers.

These findings suggest possible membrane-based mechanisms of tau aggregation and toxicity in neurodegenerative diseases. Because anionic membranes are known to induce tau fibrillization, this lipid-membrane-induced structural compaction may render the otherwise soluble and stable tau aggregation competent, or proaggregant, and seed the assembly of tau into fibrils. The inner leaflet of the neuronal cell membrane contains several anionic lipid species. Upon the detachment of tau from microtubules

due to hyperphosphorylation that occurs early on during the pathogenesis of Alzheimer's disease, association of free tau with anionic lipids in the plasma membrane could seed the formation of the paired helical filaments found in the brains of Alzheimer's victims. Furthermore, tau's interaction with anionic lipid membranes disrupts lipid packing and compromises membrane structural integrity, providing a potential mechanism of protein aggregate-induced toxicity in diseased cells.

Reference: "Interaction of Tau Protein with Model Lipid Membranes Induces Tau Structural Compaction and Membrane Disruption," *Biochemistry,* **2012**, *51* (12), pp. 2539–2550. doi:org/10.1021/bi201857v.

Researchers include E.M. Jones, P. Camp, B. Vernon, and E. Chi (University of New Mexico); J. Biernat and E. Mandelkow (Max Planck Institute and the German Center for Neurodegenerative Diseases); and M. Dubey and J. Majewski (Lujan Center).

This research benefited from the use of the Lujan Center at LANSCE funded by the DOE's Office of Science, BES.

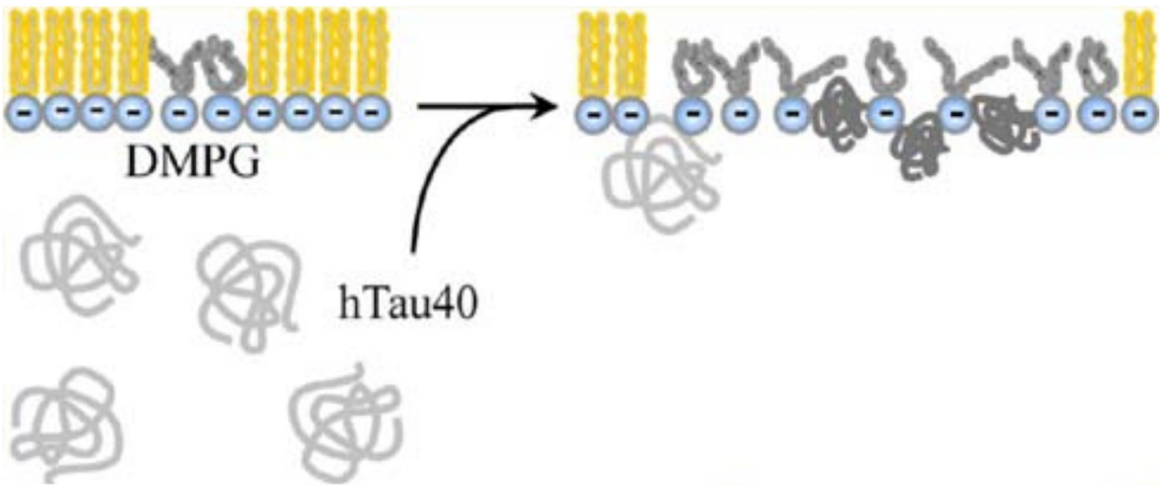
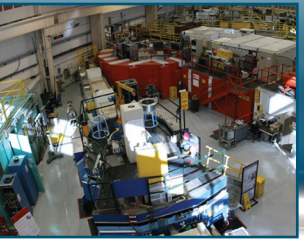
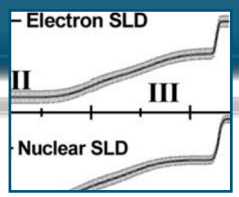


Figure: Schematic illustration of adsorption of human tau protein (hTau40) to the anionic lipid monolayer (DMPG) at the air/water interface, which causes damage to the lipid packing order.





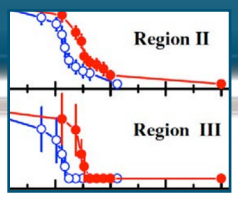
Polarized Neutrons Probe the Chemical Uniformity of Manganite Films

Doped bulk perovskite manganites, such as $(La_{1-x}Pr_x)_{1-y}Ca_yMnO_3$, exhibit a rich variety of magnetic, electronic, and structural phenomena and phases that are closely coupled to atomic structure and strain. The coupling produces potentially useful nonlinear responses to the environment, including colossal magnetoresistance and colossal elastoresistance. Collective-charge, spin-orbital lattice interactions lead to the coexistence of different phases in which the minority phase domains range from nanometers to microns in size. The competition between the different phases is crucial to understanding macroscopic properties in bulk materials. The strain between the films of doped perovskites and substrate adds complexity and influences magnetic ordering and electronic transport. Because manganite thin films exhibit nonlinear response, such as colossal magnetoresistance near the metal insulator transition, they have the potential for a variety of applications, including magnetic sensors and tunnel junctions. The high spin polarization of magnetite thin films at the Fermi level should make the thin films attractive as spin injectors. However, the unexpectedly low values of tunneling magnetoresistance for magnetic tunnel junctions composed of manganite films are problematic for applications. LANL researchers and collaborators used PNR to measure the neutron-spin-dependent reflectivity from a single crystalline manganite thin film. They observed (1) coexistence of magnetic phases as a function of depth and (2) correlation of the coexistence with a variation of the chemical composition with depth. The research highlights a concern about the degree of chemical uniformity needed for developing applications of manganite films. *Physical Review Letters* published the work.

Improvements in sample fabrication capabilities have enabled the growth of increasingly complex materials with crystalline quality; this has allowed observation of exotic behavior, such as the coexistence of phases. Commonly, the behavior is assumed to occur in chemically uniform material. However, given the small length scales over which coexistence occurs (typically tens or hundreds of nanometers), it is challenging to prove chemical uniformity over this length scale.

The scientists used the Lujan Center's Asterix polarized neutron reflectometer, which is intrinsically sensitive to interfacial magnetism, to examine the magnetism occurring across the thin dimension of a $(La_{1-x}Pr_x)_{1-y}Ca_yMnO_3$-$\delta$($x$ = 0.52±0.05, y = 0.23±0.04, δ = 0.14±0.10) single-crystal film. The researchers measured the depth dependence of the chemical and magnetic structures in the film. They found that the magnetic nonuniformity across the film's thickness is related to its nonuniform chemical depth profile. X-ray reflectivity and PNR measurements indicate a change of chemistry near the film's surface and buried interface. These regions have lower magnetization than the film bulk. The magnetization of the film bulk is uniform over length scales of nanometers. The scientists determined that the thermal evolution of the saturation magnetizations for the surface and buried interface (regions I and III) are different from the film bulk (region II). Thus, different regions have different ordering temperatures. The thermal hysteresis of the magnetization indicates a first-order transition, and the magnitude of the hysteresis is different for the surface and buried interface compared with the film bulk. The chemical nonuniformity across the depth can lead to a modified effective coupling that can influence the ordering temperature and hysteresis.

The researchers concluded that the variation of the depth-dependent chemical, electronic, and magnetic properties should be considered for understanding the phase coexistence or separation in manganites and in interpreting data acquired from characterization between different regions of the sample. Suppression of the saturation magnetization M is important for



understanding the origin of poor tunnel magnetoresistance of these films. The research provides insight into the materials requirements to enable successful applications.

Researchers include S. Singh and M.R. Fitzsimmons (Lujan Center), T. Lookman (T-4, Physics of Condensed Matter and Complex Systems), and J.D. Thompson (Condensed Matter and Magnet Science, MPA-CMMS). Collaborators are H. Jeen, A. Biswas (UF), M.A. Roldan (Universidad Complutense de Madrid, Spain), and M. Varela (ORNL).

Reference: "Magnetic Nonuniformity and Thermal Hysteresis of Magnetism in a Manganite Thin Film," *Physical Review Letters* **108**, 077207 (2012). doi:10.1103 PhysRevLett.108.077207.

The DOE's Office of Science—BES supported the LANL portion of the research and the Lujan Center, a national user facility.

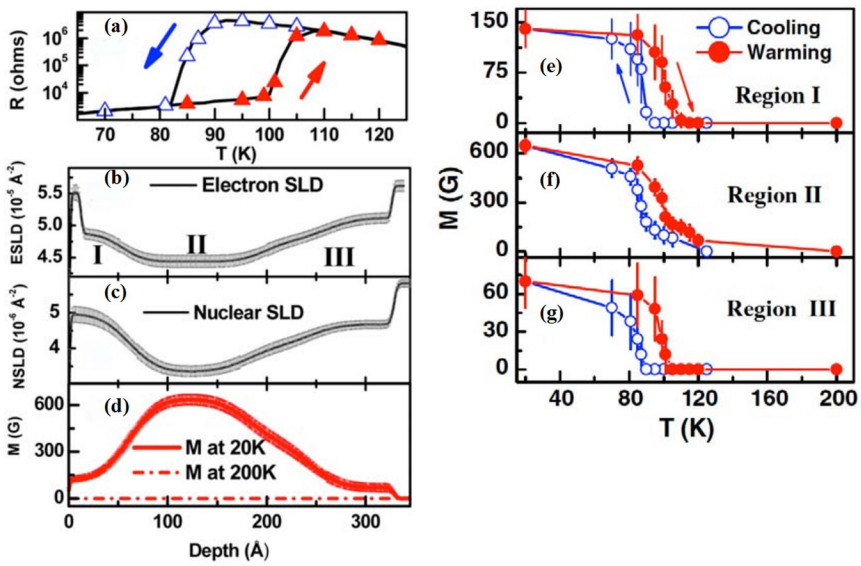
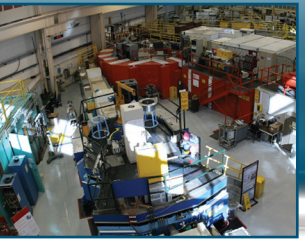


Figure: (a) Resistivity of the sample measured during the experiment showing the metal-insulator transitions. (b) and (c) Electron and nuclear scattering length density depth profiles obtained from the x-ray and neutron reflectivities, respectively. The results reveal regions with different chemical and nuclear compositions. (d) The saturation magnetization M depth profile. (e–g) Curves for the different regions during cooling (blue) and warming (red). (f–g) Measurement of M as a function of temperature reveals the dependence of the curie temperature of the film (and thus the phase coexistence of magnetism) on depth.



Spin and Orbital Ordering in $Y_{1-x}La_xVO_3$

Many important technological devices are based on transition-metal oxide materials. These materials often possess strongly correlated electrons that give rise to highly desirable physical properties, such as high-T_c superconductivity in layered cuprates, colossal magnetoresistance in perovskite manganites, and the coexistence of magnetism and ferroelectricity (termed multiferroicity). Understanding how to manipulate strongly correlated electron systems enables scientists to develop new and better tunable, functional materials that are stable under high temperatures and chemically extreme conditions. In research published in *Physical Review B*, A. Llobet (Lujan Center) and collaborators (Ames Laboratory and Iowa State University) examined $Y_{1-x}La_xVO_3$ compounds to understand the interplay between the strongly correlated spin-orbital-lattice degrees of freedom.

The orthorhombic RVO_3 perovskites [R = rare earth or yttrium (Y), V = vanadium, O = oxygen)] are a family of compounds in which all atoms have the same configuration of electrons, regardless of which atom occupies the R site. In the V^{3+} ions ($t_{2g}^2e_g^0$), a preferential occupation of the electron orbitals can lead to a distortion of the VO_6 octahedra (Jahn-Teller distortion), where some of the V–O bonds elongate and others shorten. When a particular arrangement of the octahedral distortion coherently propagates through the crystal, an orbital ordered (OO) state emerges. All RVO_3 members show multiple orbital orderings and ordering of the magnetic spins. Orbital orderings and ordering of the magnetic spins provides a unique opportunity to study the spin-orbital-lattice coupling of π-bonding *t*-orbital electrons. To distinguish competing effects, the team focused on the $Y_{1-x}La_xVO_3$ system because (1) the La^{3+} and Y^{3+} ions carry no magnetic moment either to obscure the magnetic behavior of the VO_3 array or to interact with it and (2) $LaVO_3$ and YVO_3 have a different sequence of spin and orbital ordering.

In addition to examining the magnetic properties, thermal conductivity, and specific heat, the scientists investigated the corresponding crystal-strucutre changes associated fluctuations with the spin and orbital ordering. They used a variety of techniques, including neutron powder diffraction performed at the High Intensity Powder diffractometer (HIPD) at LANSCE. These extensive characterizations led to understanding the evolution of spin and orbital ordering and a full description of the phase diagram for all values of x in $Y_{1-x}La_xVO_3$.

Figure 4(a) summarizes the results, where the phase diagram of $Y_{1-x}La_xVO_3$ as a function of the R^{3+}-ion average ionic radius (IR) or doping substitution x is shown. This diagram is compared with the phase diagram of the RVO_3 system (R = rare earth and Y) depicted in Figure 4(b). Magnetization and neutron powder diffraction measurements point to the coexistence below the magnetic order temperature T_N of the two magnetic phases in the compositional range $0.4 < x < 0.738$. Samples in the compositional range $0.20 < x \leq 1.0$ revealed an additional suppression of a glasslike thermal conductivity in the temperature interval $T_N < T < T^*$ and a change in the slope of the temperature dependence of the magnetic susceptibility. The findings show that T^* represents a temperature below which spin and orbital fluctuations couple via spin-orbit coupling [transition between disordered orbital state I and disordered orbital state II in Figure 4(a)]. The team concluded that for $0.20 \leq x \leq 1.0$, competitive orbital ordering could introduce short-range orbital fluctuations of orbitally ordered regions that suppress the thermal conductivity by phonons (disordered state II).

The dramatic difference between the two-phase diagrams in the figure (right) is in sharp contrast to the strong similarity between the phase diagrams for $RTiO_3$ and $Y_{1-x}La_xTiO_3$ (previously published). This contrast can be traced to the different effect of the bias by the intrinsic site distortions, which causes a different orbital and magnetic ordering competition in vanadate vs titanate perovskites. This study reveals the way in which an intrinsic site distortion of orthorhombic perovskites

biases the development orbital ordering and unveils the development of short-range orbital fluctuations of orbitally ordered regions that suppress the thermal conductivity by phonons in $Y_{1-x}La_xTiO_3$.

Reference: "Spin and Orbital Ordering in $Y_{1-x}La_xVO_3$," *Physical Review B* **84**, 214405 (December 2011). doi:10.1103/PhysRevB.84.214405.

Researchers include J-Q. Yan (Ames Laboratory); J-S. Zhou, J.G. Cheng, and J.B. Goodenough (University of Texas–Austin); Y. Ren (ANL); A. Llobet (Lujan Center); and R. J. McQueeney (Ames Laboratory and Iowa State University).

The DOE's Office of Science, BES, Division of Materials Sciences and Engineering, sponsored the research. This work has benefited from the use of HIPD at the Lujan Center, funded by the DOE's Office of Science, BES.

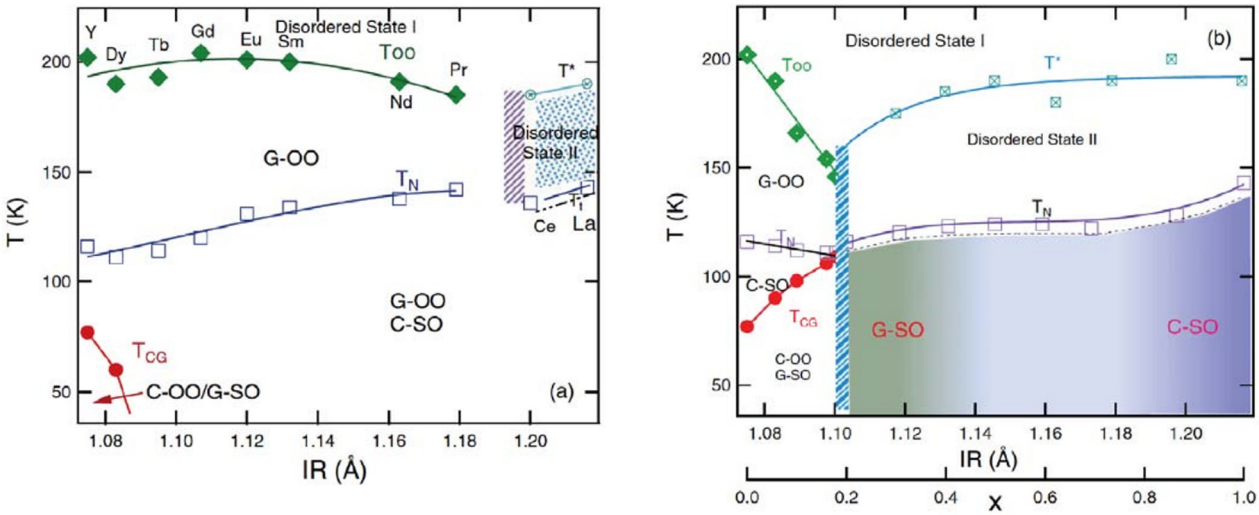


Figure: (a) Spin and orbital-ordering phase diagram for $Y_{1-x}La_xTiO_3$. (b) Spin and orbital-ordering phase diagram for RVO_3 (R = rare earth and Y) perovskites. *G/C*-type orbital ordering is labeled as *G/C-OO*, *G/C*-type atomic force microscopy (AFM) magnetic spin order is labeled as *G/C*-SO. G-OO/C-SO and C-OO/G-SO states are schematically represented in (a).

Neutron Scattering Aids Understanding of Pharmaceutical Tablet Formation

Pharmaceutical powder engineering often involves forming interfaces between the drug and a suitable polymer to improve the compaction properties of the resulting tablets. The structure at the interface plays a critical role for the properties and performance of the composite material. However, interface structures have not been well understood due to a lack of a suitable characterization tool. LANL researchers and a collaborator used the spectroscopic techniques of ellipsometry and NR (Lujan Center) together to characterize the structure of such interfaces in detail. Ellipsometry provides a quick estimate of the number of layers and their thicknesses, whereas NR describes richer structural information, such as density, thickness, roughness, and intermixing of different layers. The combined information allowed the scientists to develop an accurate model of the layered structure and reveals information about the intermixing of different layer components. These results yield useful information for engineering particle properties through the control of the interfacial chemistry and an approach for understanding structure-processing relationships. The journal *Molecular Pharmaceutics* published the research.

Poor tabletability (the ability to form stable tablets) of granulated drug powders is a serious problem in pharmaceutical manufacturing. Coating the granules with a biocompatible polymer binder from a solvent (wet agglomeration) may improve tabletability, but many tablets fracture under everyday handling. For example, acetaminophen (e.g., Tylenol) is a large pill because the drug powder does not compress easily and requires large amounts of binder. Fracture of a tablet before ingestion has implications ranging from quality control in manufacturing to efficacy or drug release rate. Poor tablet design stems from common trial-and-error approaches in the industry. Whether the drug form is solid granules or drug-polymer mixtures, chemical interactions at the interface between the pharmaceutical ingredient and the binder can be important, especially when considering solubility and stability (e.g., shelf life).

A group of researchers led by J. Yeager (Shock and Detonation Physics, WX-9) used NR at the Lujan Center to develop accurate models of wet, agglomerated, polymer-drug interfaces. The scientists had previously developed a methodology of two spectroscopic techniques (ellipsometry and NR) to characterize the structure at the interface of an acetaminophen-poly (esterurethane) Estane 5703 molecular composite that had application to plastic-bonded explosives. The researchers applied this methodology to study the interfaces of pharmaceutically relevant model systems created by a simulated wet agglomeration.

The combined information enables the development of an accurate model about the layered structure and provides information about the intermixing of different layer components. NR shows that the drug-binder interface depends on the materials and the presence of the polymer solvent. For example, a stable 5-nm-thick layer of mixed acetaminophen and binder is formed when ethanol solvent is used in the wet agglomeration process, but the layer is not formed when methanol is used as solvent. The systematic use of these characterization techniques on several model systems suggests that the nature of the polymer has a small effect on the interfacial structure, whereas the solvent used in the polymer coating has a larger effect. The choice of polymer in engineered composites is more likely to be dependent on the desired bulk properties, and the choice of solvent is more likely to depend on the desired interfacial structure. The researchers learned that the structure at the interface plays a critical role for the properties and performance of the composite. In pharmaceuticals, composite microstructure affects the mechanical stability and drug release rate. These results provide useful information for engineering particle properties through the control of the interfacial chemistry. Moreover, neutron scattering provides a powerful characterization tool to link formulation processing to nanoscale structure, assisting in the design and formulation of pharmaceuticals and other composites.

Reference: "Probing Interfaces between Pharmaceutical Crystals and Polymers by Neutron Reflectometry," *Molecular Pharmaceutics*, web publication date: 04 June 2012. doi:10.1021/mp2006517.

Researchers include J. Yeager, K. Ramos, and D. Hooks (Shock and Detonation Physics, WX-9); S. Singh, M. Dubey, and J. Majewski (Lujan Center); and C. Sun (University of Minnesota).

This work was performed, in part, at CINT, a DOE BES user facility, and at the Lujan Center, funded by the D0E's BES. The DOE/Department of Defense (DoD) Joint Munitions Project and the Explosives Science project of the NNSA Campaign 2 funded the work. An Agnew National Security Fellowship sponsors Yeager.

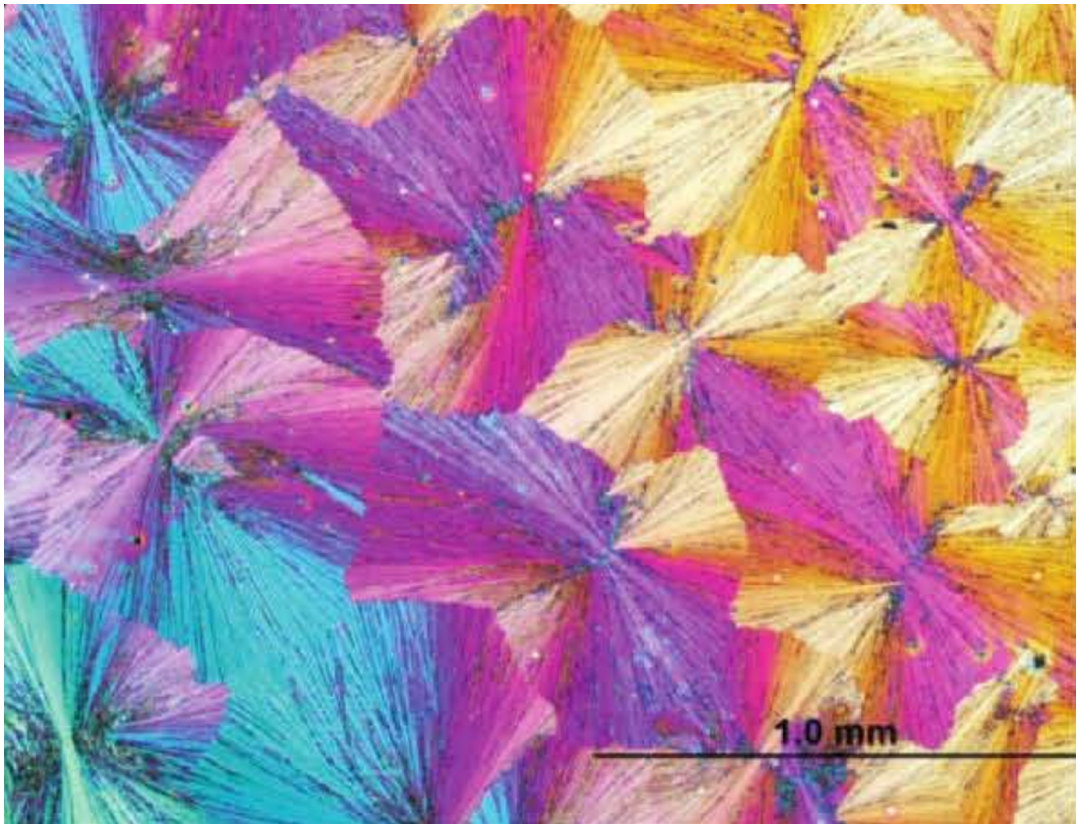
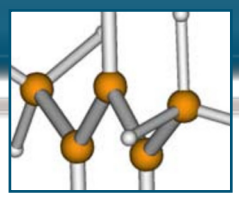


Figure: Thin film of acetaminophen obtained by dip-coating a silicon wafer in an ethanol solution. Coloration in the film is a result of thickness variation. The researchers used similar films in neutron scattering investigations.



Proton Transfer Investigated Using Neutrons

Lujan Center researchers and collaborators performed an experimental and theoretical study on short, strong H-bonding in tetraacetylethane (TAE), a model system for proton transfer. Proton transfer is one of the most important reactions in biology and biochemistry. Proton-driven machines populate cell membranes and are necessary for biological processes. Proton transfer reactions are of central importance in redox systems, ionic reactions, and chemical catalysis. Numerous proton transfer mechanisms are possible and are still poorly understood, despite years of study. Modeling the structures and dynamics of protons and of proton transfer with ab initio techniques requires difficult and costly quantum chemical calculations, few of which have been validated experimentally in detail. The team's research, which appears in the *Journal of Physical Chemistry A*, highlights a novel mechanism for facilitating proton transfer or stabilizing H-bond geometry mediated by the dynamics of adjacent functional groups in a very short, strong H-bond; these are possible intermediates in enzyme catalysis, where such a process would have enormous complexity. This complexity would be difficult to unravel with anything like the detail possible with the team's model system.

H-bonding occurs when H is shared between electronegative atoms located on different parts of the same molecule (intramolecular) or on different molecules (intermolecular). An H-atom bound to an electronegative atom can interact strongly with another electronegative atom or even be transferred between atoms. H-bonding plays an important role in biochemistry because it occurs in proteins and nucleic acids. Between single strands of DNA, it stabilizes the double helix. H-bonding strongly influences the structure and dynamics of materials. Therefore, model systems with short, strong H-bonds are of great interest to scientists in various fields.

TAE $[(CH_3CO)_2CH{=}CH(COCH_3)_2]$ is a highly symmetric molecule with short, strong, intramolecular H-bonds. The researchers performed periodic density functional theory (DFT) calculations of the structure and the dynamics of crystalline TAE, as well as molecular dynamics simulations. They validated the results against experimental neutron scattering data. The team derived potential energy surfaces for the H-bond to determine the factors that govern proton transfer. The methyl groups (CH_3 groups) on each "side" of the TAE molecule form weak intermolecular H-bonds in the solid to the oxygen atom (of the intramolecular H-bond) of a neighboring molecule. The researchers showed experimentally that the movement of the methyl groups (mainly rotation) strongly correlates with the position of the proton between the oxygen atoms and vice versa. This phenomenon supports or hinders the proton transfer process. A mechanism that interferes with proton transfer had not been recognized previously.

The scientists could study the proton in the H-bonds and the methyl group dynamics easily because incoherent inelastic neutron scattering (IINS) is particularly sensitive to H-atom motion. Although the computational determination of the electronic structure of H-bonded systems is difficult, the neutron vibrational spectrum can readily be obtained from such computational studies. The simplicity of the neutron-nucleus interaction permits the calculation of the position and intensity of the vibrational modes for direct comparison with the experimental neutron vibrational spectrum. This tool is powerful for the validation of ab initio calculations, which have become an indispensable part of spectroscopic studies.

The researchers used experiments and computations to determine the correlations between the movement of the various parts of the system with that of the bridging H-atom on its potential energy surface. Calculations on a fully periodic system representing the crystal reveal the important effect of the intermolecular interactions on the potential energy surface of the H-bond, as compared with the result for an isolated molecule (bottom right).

The team collected incoherent inelastic neutron scattering data on the Filter Difference Spectrometer (FDS) at the Lujan Center.

Reference: "Methyl Dynamics Flattens Barrier to Proton Transfer in Crystalline Tetraacetylene," *Journal of Physical Chemistry* **A116**, 2283 (2012).
doi:org/10.1021/jp210212q

Researchers include G. Kearley (Australian Nuclear Science and Technology Organization), J. Stare (National Institute of Chemistry, Slovenia), R. Kutteh (University of Sydney), L. Daemen and M. Hartl (Lujan Center), and J. Eckert [University of South Florida (USF).

DOE's Office of Science, BES funded the LANL research.

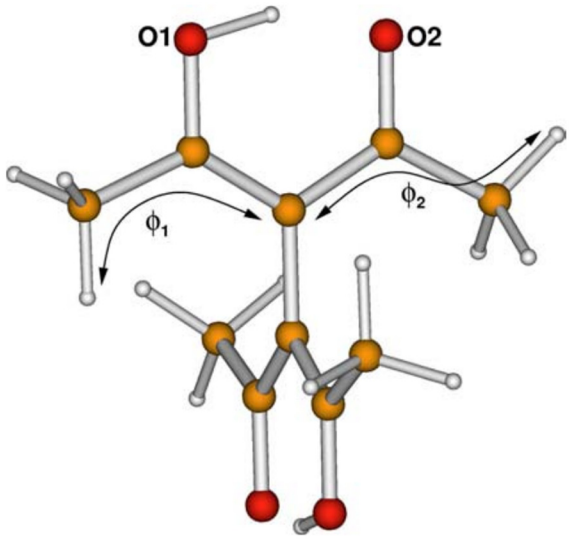
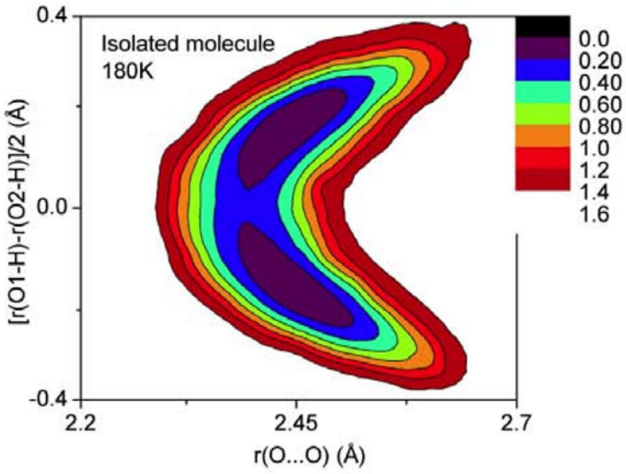


Figure Top: Ball-stick representation of an isolated molecule of TAE in the lowest-energy conformation.



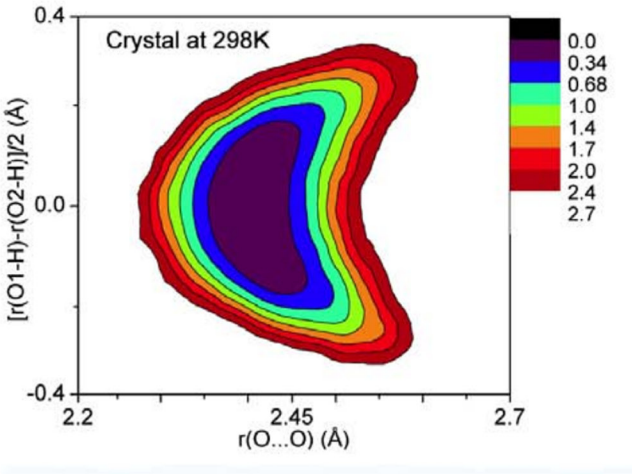
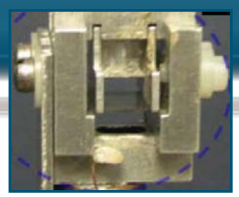


Figure Bottom: Potential energy surface of the H-bond in an isolated molecule (left) and in a crystal (right). The well in the crystal is 0.1 Å wide in the O...O coordinate (energy < 0.34 Kcal mol) and 0.4 Å along the approximate O...H coordinate. At low temperature, the reorientation of the methyl groups leads to a preferred O-atom for the bridging proton. The amplitude of methyl torsions becomes larger with increasing temperature so that the free-energy minimum for the proton becomes flat, in contrast with the isolated molecule case.



Role of Elastic Bending Stress on Magnetism of a Manganite Thin Film

LANL researchers and collaborators used PNR at LANSCE to measure the neutron-spin-dependent reflectivity from a single crystalline (La1-xPrx) 1-y Cay MnO3-δ (x = 0.52±0.05, y = 0.23±0.04, δ = 0.14±0.10) thin film as functions of applied stress and temperature. They demonstrated that the application of elastic bending stress to the manganite film strengthens the ferromagnetic phase. Remarkably, 0.01% compressive strain produces a 20% increase of the saturation magnetization. This result suggests a means to improve the magnetic properties of complex oxide films and a methodology to investigate a broad range of materials. The journal *Physical Review B* published the research.

Improvements in sample fabrication capabilities have enabled the growth of increasingly complex materials with crystalline quality; this has allowed observation of exotic behavior, such as the coexistence of ferromagnetic metallic, orthorhombic antiferromagnetic charge-ordered insulating and pseudo-cubic paramagnetic insulating phases. Because the ground state energies of these phases are very nearly degenerate, magnetic fields, temperature, or stress can favor one ground state over another; this leads to nonlinear response—a hallmark of complex materials.

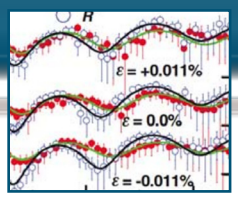
Scientists used the Lujan Center Asterix polarized neutron reflectometer, which is intrinsically sensitive to interfacial magnetism, to examine the magnetism occurring across the thin dimension of a (La1-xPrx)1-yCayMnO3-δ single-crystal film. To apply elastic stress, the scientists developed a four-point bending jig especially designed for NR (figure top). The jig enables simultaneous measurement of the resistance and the neutron reflectivity of the sample as functions of temperature, applied magnetic field, and stress. The magnetic depth profile can be evaluated as functions of these parameters. Tensile (ε>0) or compressive (ε<0) strain of the thin film can be realized by placing the film in contact with or opposite to the inner supports of the jig, respectively. The researchers obtained data corresponding to the two polarization states of the neutron beam at selected temperatures [figure bottom (upper)]. From these data, the team determined the saturation magnetization *M* depth profile [figure bottom (lower)]. The result shows that, independent of the film's chemical composition (which changes across its thickness), compressive strain increases the *M* by approximately 20%, whereas tensile strain decreases *M* by the same value.

The research clarifies a previously conflicting picture of the influence of stress on the magnetic properties of manganite films. The results suggest that long-range strain plays an important role across the metal-insulator transitions because applied stress changes both the metal-insulator transition temperature and the magnetization of the film. With the development and application of the four-point bending jig to neutron scattering, scientists have the opportunity to turn just the "elastic strain knob" for materials characterization. The jig and neutron scattering protocol could benefit studies of a broad range of important materials, including piezeomagnetic and multiferroic materials.

Reference: "Role of Elastic Bending Stress on Magnetism of a Manganite Thin Film Studied by Polarized Neutron Reflectometry," Physical Review B **85**, 214440 (2012).
doi: 10.1103/PhysRevB.85.214440.

Researchers include S. Singh and M.R. Fitzsimmons (Lujan Center); T. Lookman (Physics of Condensed Matter and Complex Systems, T-4); and collaborators H. Jeen and A. Biswas (UF), M.A. Roldan (Universidad Complutense de Madrid, Spain), and M. Varela (ORNL).

The DOE's Office of Science, BES sponsored the LANL portion of the research and the Lujan Center, a national user facility.



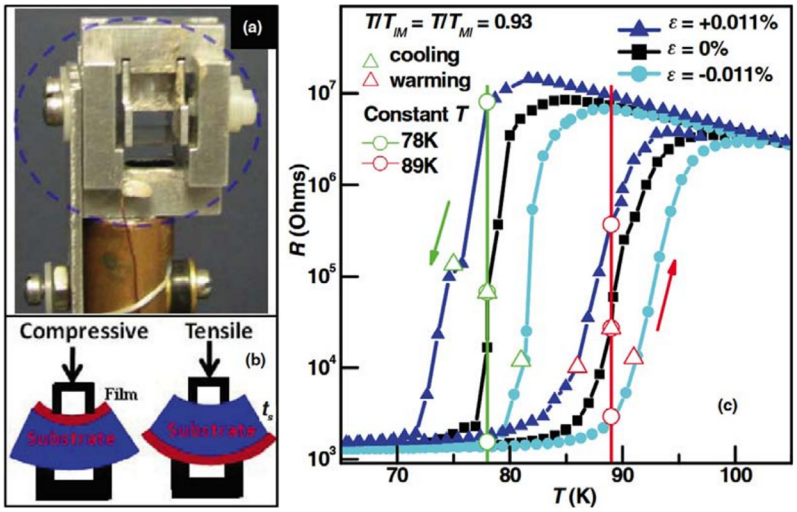


Figure Top: (a) End-view image of the four-point jig (circled) mounted on a cryostat, and (b) side-view schematic representation of applied bending stress. (c): Transport measurements of the film at different applied bending stress/strain, tensile (▲), compressive (◆) and no strain (■). Open circles and open triangles represent the constant T and constant T ratio ($T/T_{IM}=T/T_{MI}=$ 0.93) at which the scientists simultaneously measured the NRs.

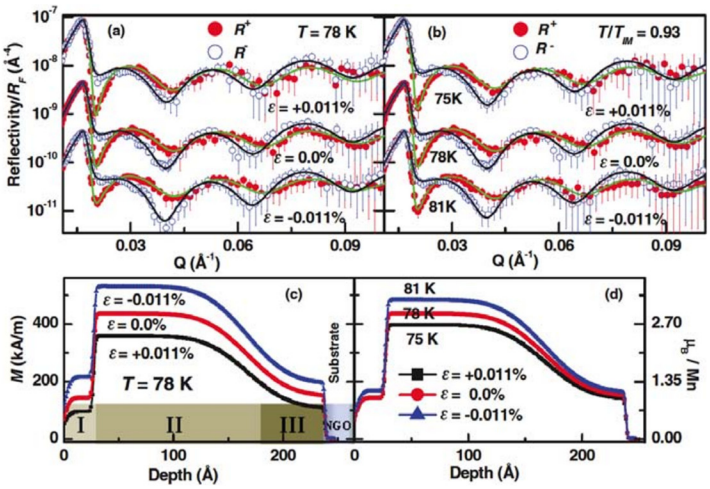
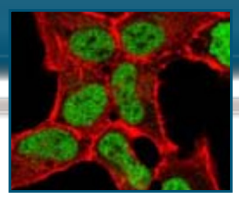


Figure Bottom: (a) PNR measurements from the film for different applied strain at constant temperature, and (b) constant T/T_{IM} while cooling. Reflectivity data at different applied stress/strain are shifted by a factor of 5 for the sake of clarity. (c) and (d) The magnetization (M) depth profile corresponding to (a) and (b), respectively.



Development of New Biocompatible Interfaces

Thin polyelectrolyte multilayer (PEM) films deposited by a layer-by-layer (LbL) self-assembly technique are used for a wide variety of applications, such as targeted drug delivery, water desalination, and biosensors. The LbL self-assembly technique enables the deposition of ultrathin films by sequential deposition driven by electrostatic interactions of charged polymers, nanoparticles, biological templates, or biologically active species. An inherently charged substrate, such as glass, is consecutively exposed to solutions of oppositely charged species (i.e., polycation and polyanion), which adsorb to the developing film at rates that enable nanometer-scale control of the film thickness. Combining different polycations and polyanions enables many useful applications. The facile deposition of polyelectrolyte nano-films, the ability to control the thickness with nanometer precision, and the possibility of tailoring the surface properties (e.g., wettability, surface charge, and roughness) make such films highly attractive for biomedical and other applications. LANL researchers used neutron scattering at LANSCE to understand the structural and biocompatible properties of polyelectrolyte films made of alternating layers of the strong polyethylene imine (PEI) and the strong polyanion polystyrene sulfonate (PSS). The journal *Soft Matter* published the research.

Ann Junghans, Saurabh Singh, and Jarek Majewski (Lujan Center); Mary J. Waltman (Bioenergy and Environmental Science, B-8); Amber Nagy (Biosecurity and Public Health, B-7); and Rashi Iyer (Systems Analysis and Surveillance, D-3) used NR to characterize the structures of PEM films in different environmental conditions. They then assessed the PEM films' ability to serve as an attachment support for two different cell lines: fibroblast (3T3) and human embryo kidney cells (HEK-293). The cells adhered to and spread on the PEM, revealing no evidence of toxicity. The team attributed the cytocompatibility of the films to the high hydration levels of the PEM. The primary cell culture benefited from the positively charged PEI's outer layer, which enhanced the ability of the cells to attach to culture plates. The team concluded that such multilayers could provide a suitable support for cell growth and for a potential biocompatible platform.

Reference: "Neutron Reflectometry Characterization of PEI-PSS Polyelectrolyte Multilayes for Cell Culture," *Soft Matter* (September 20, 2012).
doi:10.1039/C2SM26433A.

The research benefited from the use of the Lujan Center funded by the DOE's Office of Science, BES.

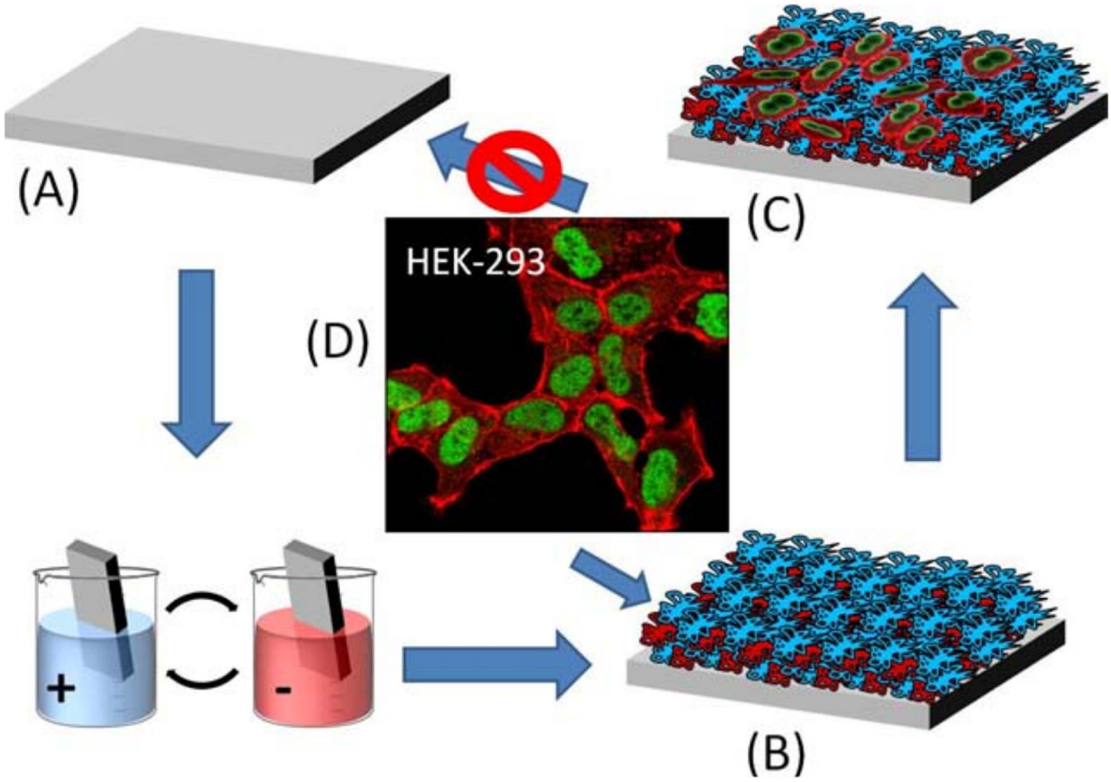


Figure: Schematic depicts PEM film deposition on a quartz substrate using an LbL self-assembly technique. (A) Flat quartz substrate. (B) Quartz coated with a PEI-PSS film. (C) Healthy proliferation of human embryo kidney (HEK) cells. (D) Microscopy image of the fluorescently labeled HEK-293 cells grown on a PEI-PSS modified quartz surface.

Design and Manipulation of Macroscopic Quantum States in Materials

Researchers from DOE's Institute for Quantum Matter at John Hopkins University collaborated with Anna Llobet (Lujan Center) to discover a new driving force for the emergence of highly entangled quantum states of matter: a mixed-valence-driven, heavy fermion state in KNi_2Se_2. The finding is relevant to a class of materials called "heavy-fermions," which are metals in which the conduction electrons behave as though they have a mass 10–1000 times that of a normal electron. This behavior occurs in systems where individual magnetic electrons become indistinguishable as a result of strong interactions with a bath of nonmagnetic conduction electrons. The result is an overall nonmagnetic state that is coherent across the material, causing deviations from traditional solid-state theory and behavior. The journal *Physical Review B* published the research.

The paper presents the discovery of a new class of heavy-fermion materials in which the fundamental interaction that gives rise to the emergent electronic state is electrostatically, rather than magnetically driven. The scientists used pair distribution function analysis of neutron total scattering data from the Lujan Center. The researchers first observed a local distortion in KNi_2Se_2 that disappeared on cooling the sample—a highly unusual and rare structural trend. This distortion, an aperiodic charge density wave (CDW), reflects the fluctuations of nearly localized charges. The disappearance is accompanied by the formation of a "heavy" electronic mass state, which indicates a quantum mechanical hybridization of the electronic states. Superconductivity emerges from the heavy-mass state at a temperature of 0.80(1) K. This discovery is important in the quest for new exotic states of matter because it demonstrates a new strategy for the design and manipulation of large-scale quantum states and energy harvest and conservation.

Reference: "Mixed-Valence-Driven Heavy-Fermion Behavior and Superconductivity in KNi_2Se_2," *Physical Review B* **86**, 054512 (2012).
doi: 10.1103/PhysRevB.86.054512.

Researchers include J.R. Neilson, A.V. Stier, L. Wu, J. Wen, Z.B. Tesanovic, N.P. Armitage, and T.M. McQueen (Johns Hopkins University); A. Llobet (Lujan Center); and J. Tao and Y. Zhu (BNL).

The DOE's Office of Science, BES, Division of Materials Science and Engineering, funded the LANL work, which benefited from the use of the HIPD and the neutron powder diffractometer (NPDF) at LANL's Lujan Center. Scientists performed a portion of this research at the National High Magnetic Field Laboratory (Tallahassee, Florida), which the National Science Foundation (NSF), the State of Florida, and the DOE sponsor.

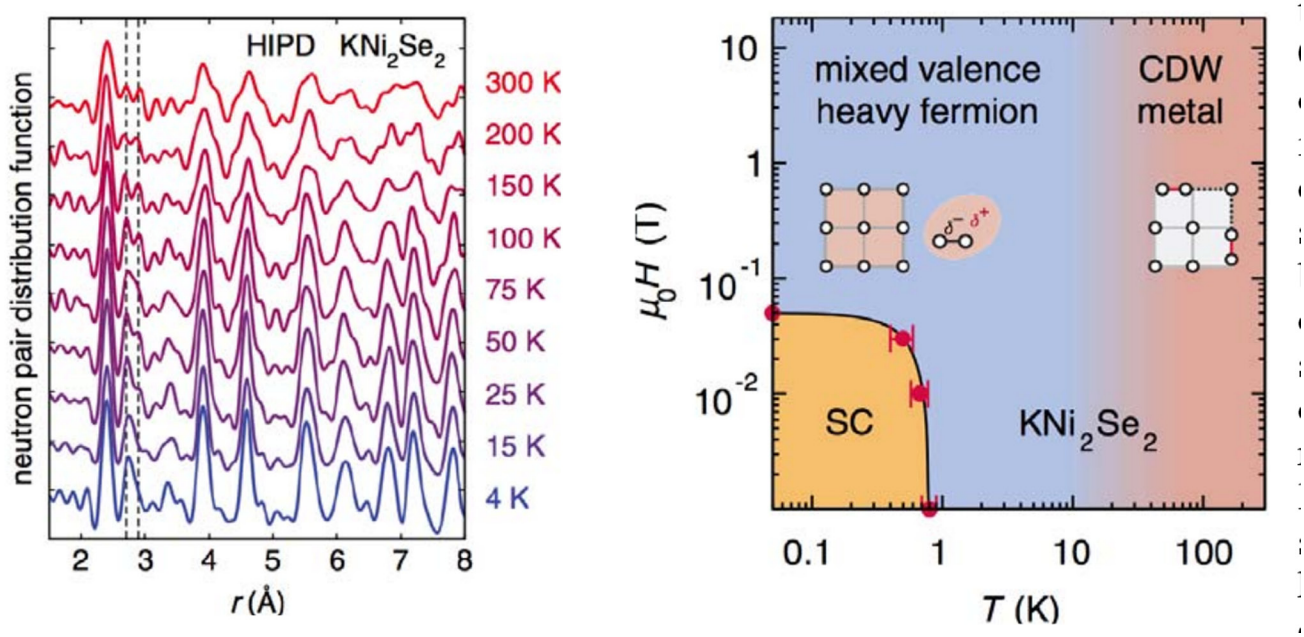
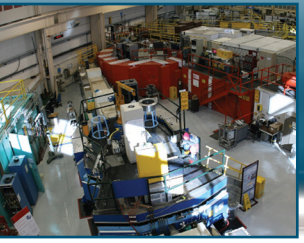


Figure: (Left):Temperature-dependent pair distribution function analysis of KNi2Se2 reveals multiple nickel (Ni)-Ni distances at *T*=300 K (dashed lines at r~2.7 Å and 2.9 Å), yet only one Ni-Ni distance at *T*=4 K. The loss of multiple Ni-Ni distances occurs between *T*=25 K and *T*=15 K.

(Right): The temperature/field phase diagram shows the superconducting, field-independent, mixed-valence, heavy-fermion, and incipient CDW metal states of KNi_2Se_2.



Technicium-99 Incident

On August 24, 2012, unexpected surface contamination was discovered in Experimental Room 1 at the Lujan Center.

The contamination was caused by the inadvertent spreading of Technicium-99 (^{99}Tc), which is a beta emitter. Betas are low-energy electrons that can travel through several feet of air but that are generally stopped by clothing and skin. Beta emitters occur naturally in the environment, and this incident involved approximately the same radiation levels that occur naturally in bricks or stone flooring in the Southwest. Decontamination involves washing with soap and water.

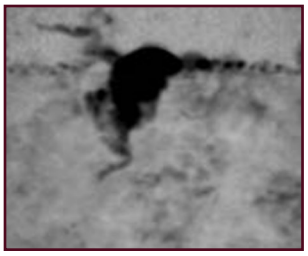
Some Lujan Center operations were put on temporary hold during the cleanup. However, normal beam delivery continued to IPF, WNR Target 4, pRad, and UCN, and the 2012 LANSCE School on Neutron Scattering ran as scheduled.

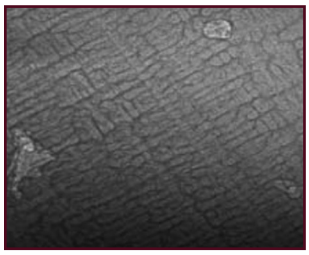
In December 2012, resumption of the User Program and related activities was authorized for the Lujan Center.

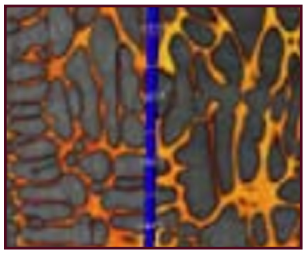
Reference:
http://www.lanl.gov/newsroom/news-stories/2012/September/lanl-responds-to-radiological-incident.php.

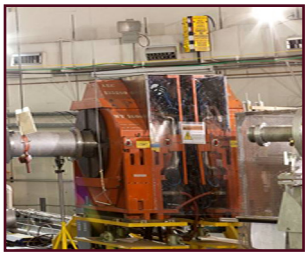
Image: Flight-Path 4 after decontamination. In background: Radiological Control Technician (RCT) preparing to survey the data acquisition system following initial startup.

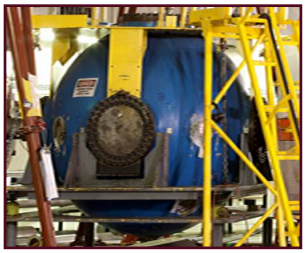
Image: Reorganized workbench after decontamination.





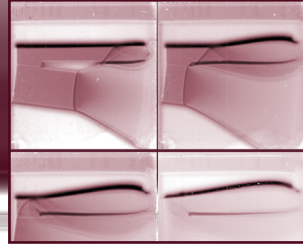






Proton Radiography 2012

LANSCE
Los Alamos Neutron Science Center



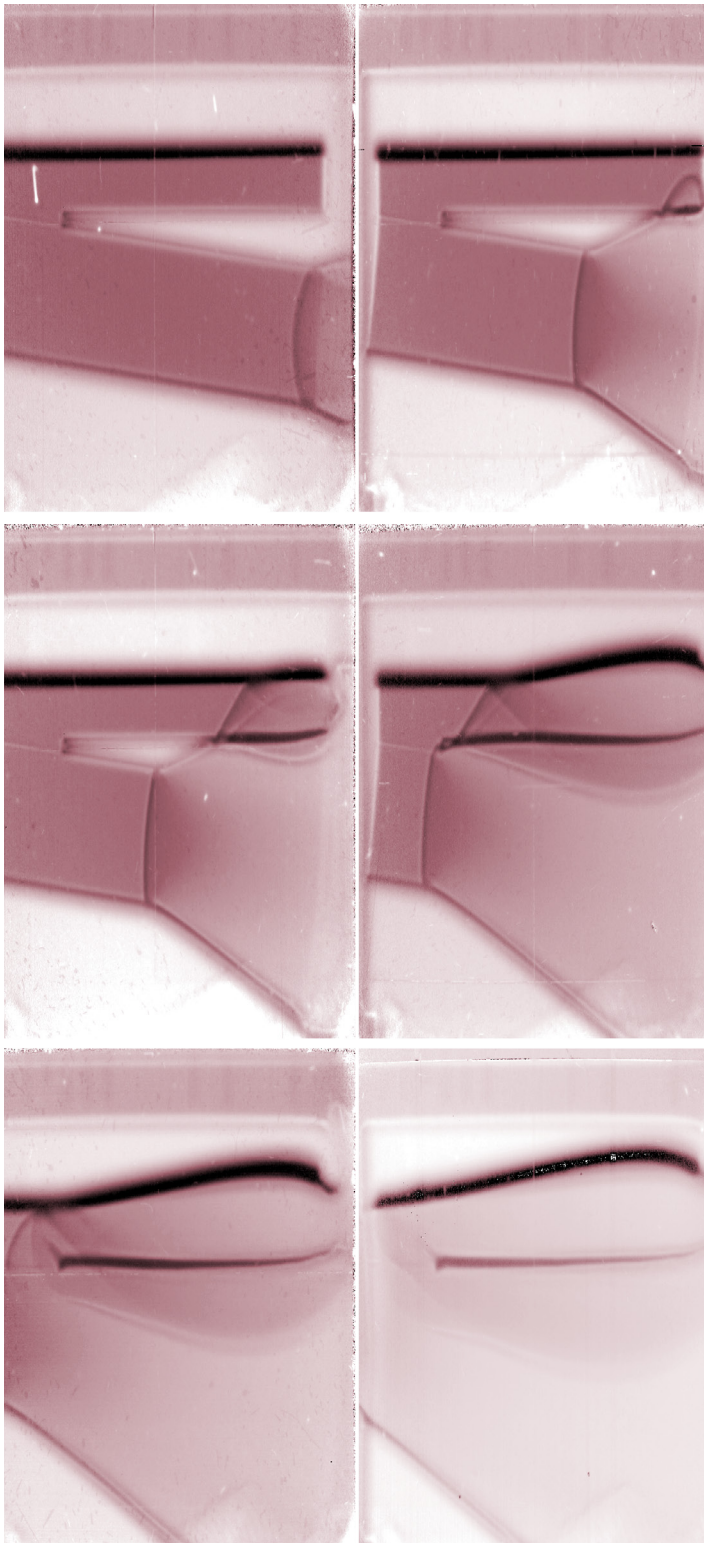
pRad

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

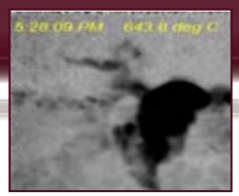
The proton radiography effort at LANSCE has operated as a user facility since 2003 and has recently been designated as one of the three DOE user facilities at LANSCE. Each year, a proposal call is distributed and the submitted proposals are reviewed by a program advisory committee.

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

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



Images (right): The "Wedge Relight" series of pRad experiments to investigate the complicated processes of high-explosives detonation around obstacles within the high explosives. This data set provides detailed information on the location of detonation fronts and their convergence through and around an embedded Al wedge.



In Situ Monitoring of Dynamic Phenomena during Solidification

The creation of microstructures by design with application-tailored properties requires directed synthesis and processing. LANL scientists and collaborators are developing methods to monitor dynamic phenomena directly during phase transformations at nonambient temperatures using novel imaging techniques. Monitoring the processes during solidification will enable the control of microstructure evolution, will allow for the validation and advancement of science-based theories, and will enable predictive model development over the length scale relevant for phase transformations and microstructure evolution.

Metallurgy (MST-6) and the pRad Team completed the first in situ examinations of melting and solidification in Al-indium (In), gallium (Ga)-bismuth (Bi), tin (Sn)-Bi, and Al-copper (Cu) alloys using 800-MeV proton radiography. Proton radiography, a unique capability at LANSCE, probes dynamic material phenomena. In this new application of proton radiography for materials studies, the researchers image the heating and cooling of bulk metal alloy sections ranging from 2 to 6 mm in thickness (figure top). These images highlight liquid-liquid phase separation at elevated temperatures and solid-liquid interface movement. Advantages of proton radiography for these experiments include time-resolved imaging of dynamic phenomena (e.g., localized fluid flow and solute segregation during solidification) and microstructure evolution, examination of a large field of view in millimeter-thick samples (relevant to casting) that enables bulk materials analysis, and the ability to examine high-density materials.

The scientists also monitored alloy melting and solidification using synchrotron x-ray radiography at ANL's Advanced Photon Source. Figure bottom shows example radiographs captured just after continuous heating and slow or fast cooling of a 100-micron-thick Al-Cu sample. The images reveal that the cooling rate influences the length scale of the microstructure. Synchrotron x-ray radiography affords 1- to 2-micron spatial resolution. The post-mortem solidification microstructure of an Al-Cu alloy shown at the far right in figure bottom was obtained using x-ray tomography at LANL. This image highlights the wealth of information about three-dimensional (3D) microstructure evolution during processing that will be possible with in situ imaging techniques.

This work demonstrates that proton radiography and synchrotron x-ray radiography are complementary techniques for in situ observations and for the control of solidification behavior and microstructure evolution. The in situ methods will enable tomographic studies of 3D microstructure evolution during processing. The monitoring techniques will help achieve transformational advances in the creation of microstructures by design, which has been identified as a key grand challenge for synthesis and processing in materials science. Moreover, this work will help to define key Matter-Radiation Interactions in Extremes (MaRIE) capabilities needed for future process-aware solidification studies at LANL.

Researchers include A. Clarke, J. Cooley, T. Tucker, R. Field, R. Aikin, D. Korzekwa, D. Hammon, K. Clarke, J. Foley, R. Trujillo, S. Quintana, P. Kennedy, B. Folks, T. Beard, T. Wheeler, R. Hudson, R. Edwards, M. Paffett, J.D. Montalvo, A. Kelly, and D. Knowlton (MST-6); P. Dunn (MST-6, now Intelligence Analysis and Technology, IAT-DO); T. Ott, J. Hill, M. Barker, F. O'Neill, and M. Emigh (MST-6 summer students); F. Merrill, B. Hollander, C. Morris, F. Mariam, C. Munson, and the pRad Team; M. Maez (Prototype Fabrication–Fabrication Services, PF-FS); B. Patterson (Polymers and Coatings, MST-7); D. Teter (Materials Science and Technology, MST-DO); D. Thoma (Institutes, INST-OFF); W. Lee (BNL); and K. Fezzaa and A. Deriy (ANL).

LDRD sponsored this work.

Reference: Conference: MDI Summer Research Group Workshop: Advanced Manufacturing; 2012-07-25–2012-07-26; Los Alamos, New Mexico, US.

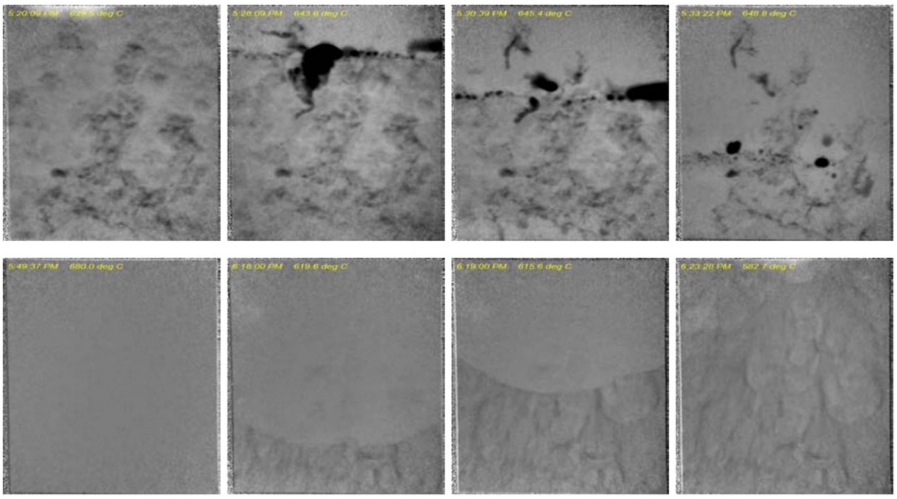


Figure Top: Example of time-resolved pRad images obtained during melting from the top downward (upper-row images) and directional solidification from the bottom upward (lower row images) of a bulk 6-mm-thick Al-In sample. The field of view is ~44 x 44 mm^2. The darker regions observed during melting are In-rich liquid, consistent with the liquid-liquid phase separation anticipated at elevated temperatures for this alloy system.

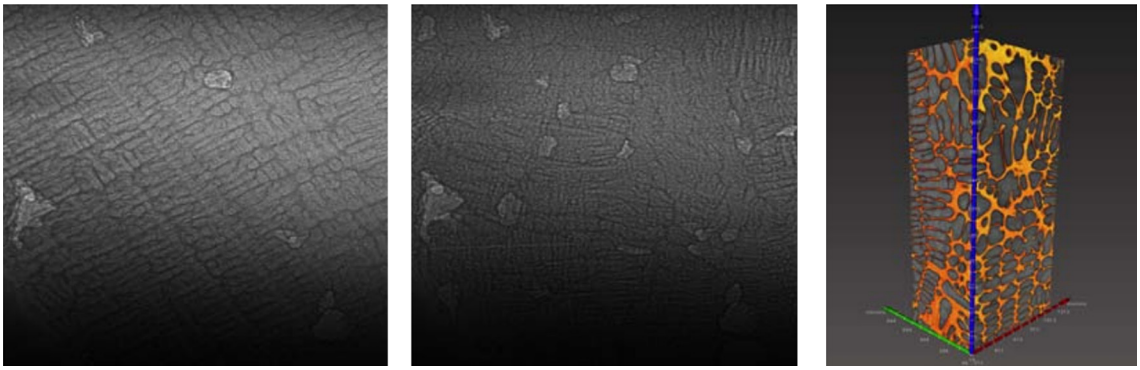
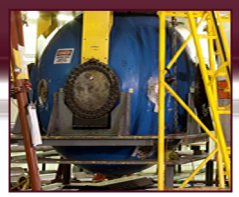


Figure Bottom: Synchrotron x-ray radiography images obtained during continuous heating and slow cooling (left) or continuous heating and fast cooling (center) of a 100-micron-thick Al-Cu sample. The light, branched structures in the radiographs correspond to Al-rich dendrites. The field of view is approximately 1.4 x 1.4 mm^2. A post-mortem X-ray tomography result (far right) of an Al-Cu alloy highlights the 3D nature of the dendritic (gray) and interdendritic (orange) regions. The volume is ~0.7 x 1.1 x 2.4 mm^3.



pRad Fires 500th Shot

Proton radiography, invented at LANL, uses a high-energy proton beam to image the properties and behavior of materials driven by high explosives. On January 23, 2012, the pRad team fired pRad shot number 500. This landmark shot was the second member of the "High Explosive (HE) Gaps" experiment series, which E. Ferm [Dual-Axis Radiographic Hydrodynamic Test Facility (DARHT) Physics and Pulse Power, WX-5] and J. Cooley (XTD Primary Physics, XTD-3) lead. The series examines the initiation of insensitive HE across a vacuum- or matter-filled gap.

The first proton radiography shot was conducted on April 15, 1997, in Beam Line B at LANSCE. In the intervening time, the team has recorded 45,111 proton pulse chains into 41,420 series of pictures, ranging from 4 pictures per series in the earliest days to as many as 2,000 pictures per series for the Moxie camera test shot and 5,000 for a typical cook-off experiment. The capability is 41 frames per series in typical modern running. Experiments have ranged in size from 100 mg to 10 pounds of high explosives and have contained uranium, plutonium, xenon, and many other elements, with densities ranging from a few milligrams per cubic centimeter to tens of grams per cubic centimeter. Secondary diagnostics have included (at least) the Velocity Interferometer System for Any Reflector (Visar), photonic doppler velocimetry (PDV); temperature probes; visual framing cameras; and piezo, optical, and voltage pins. In the coming weeks, the team will supplement the existing HE and powder gun drivers with the Precision High-Energy Liner Implosion Experiments (PHELIX) pulsed-power driver.

The team is proud to have been able to make 500 contributions to the weapons program and is eager to continue for the next 500.

The proton radiography core team consists of E. Campos, C. Espinoza, J. Fait, G. Hogan, B. Hollander, J. Lopez, F. Mariam, D. Morley, C. Morris, M. Murray, A. Saunders, A. Tainter, T.N. Thompson, and D. Tupa (Subatomic Physics, P-25); N. King, K. Kwiatkowski, F. Merrill, C. Munson, P. Nedrow, C. Schwartz, and J. Tybo (Neutron Science and Technology, P-23); D. Royer (DARHT Operations, WX-1); J. Heidemann, R. Lopez, and M. Marr-Lyon (Focused Experiments, WX-3); G. McMath and W. McNeil (DARHT Experiments and Diagnostics, WX-4); F. Trouw (Lujan Center); and H. Leffler, A. Meidinger, and N. Wilcox (NSTec).

Funding sources include the NNSA Science campaigns, LDRD, and work for others, including the Defense Threat Reduction Agency (DTRA), AWE, LLNL, SNL, and ORNL.

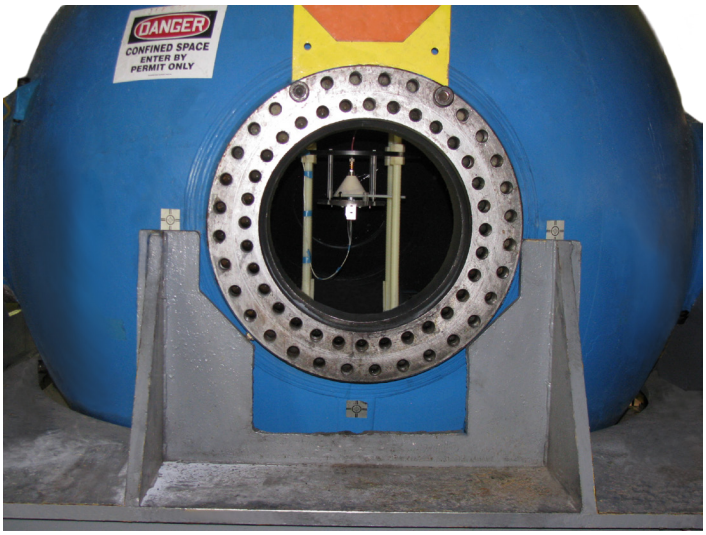
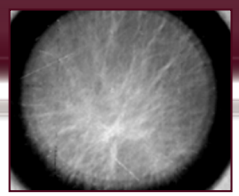


Image: The sealed vessel provides the safety envelope to study samples of hazardous materials.

Image: Magnets are used to maniuplate the proton beam.



Using Radiography to Study Thermal Explosions

LANL research on the use of pRad for imaging thermal explosions at high speeds yields a real-time look at how a thermal explosion unfolds and releases its energy. Understanding the thermal response of energetic materials to heating is a critical aspect of their proper engineering and use. Specifically, it is important to know the range of temperature over which ignition may occur and the subsequent power of the explosion. Dynamic radiography of explosives as they are heated through pre-ignition thermal decomposition and post-ignition burn propagation allows researchers to measure many phenomena involved in thermal explosions. These phenomena include the loss of solid before ignition due to thermal decomposition, cracking in the material after ignition, propagation of burning through the explosive by convection, and the consumption of explosive by conductive burning. Scientists have developed triggering techniques to synchronize the thermal ignition to a radiographic source. As a result, scientists have gained an understanding of the mechanism of a thermal explosion and have created a model capturing both the gas phase's convective and solid-state conductive components of a deflagration wave in a thermal explosion. This knowledge is important to enable the prediction of thermal explosions in HE systems. Two papers in the *Journal of Applied Physics* describe this research.

In related work, Bryan Henson and Laura Smilowitz (Physical Chemistry and Applied Spectroscopy, C-PCS) have made progress toward a "tabletop" dynamic radiography experiment. The experiment is a table-sized x-ray imaging apparatus that enables x-ray imaging of subsonic dynamic events, such as thermal explosions, on a routine basis.

Before this experiment was performed, the imaging experiments were done primarily at the pRad facility at LANSCE, which requires considerably more planning, lead time, and expense for a single experiment.

The small-scale aspect of both the experiment and the x-ray cinematography allows many more experiments to be performed, which helps map out experimental phase space. The approach provides a means to optimize experiments designed for larger radiographic facilities, such as proton radiography.

References: "The Evolution of Solid Density within a Thermal Explosion I. Proton Radiography of Pre-Ignition Expansion, Material Motion, and Chemical Decomposition," *Journal of Applied Physics* **111**, 103515 (2012).
doi: 10.1063/1.4711071.

"The Evolution of Solid Density within a Thermal Explosion II. Dynamic Proton Radiography of Cracking and Solid Consumption by Burning," *Journal of Applied Physics* **111**, 103516 (2012).
doi: 10.1063/1.4711072.

Coauthors include L. Smilowitz and B.F. Henson (C-PCS); B.W. Asay (Explosive Applications and Special Projects, WX-6); A. Saunders, C.L. Morris, F. Mariam, G. Hogan, M.M. Murray, and C. Espinoza (Subatomic Physics, P-25); F.E. Merrill, K. Kwiatkowski, and P. Nedrow (Neutron Science and Technology (P-23); G. Grim (Weapons Program, PADWP); W. McNeil (DARHT Experiments and Diagnostics, WX-4); P. Rightley (W76/W88); M. Marr-Lyon (Focused Experiments, WX-3); and J.J. Romero, C.L. Schwartz, T.N. Thompson, and J. Bainbridge.

Science Campaigns 1 and 2, the Surety Program, and the Joint Munitions Program administered by both the DOE and DoD funded the research.

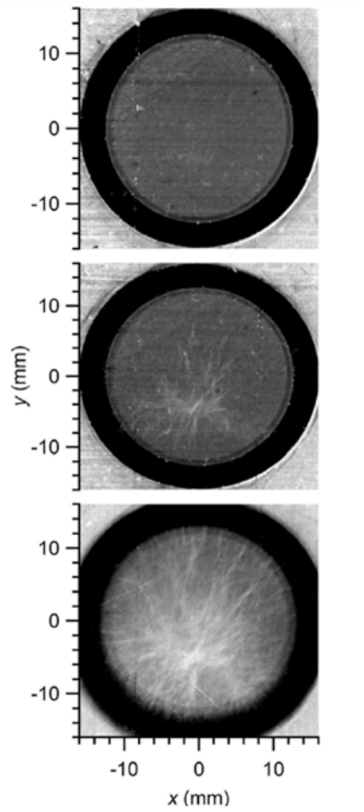


Figure Top: Proton transmission images (radial view) of an experiment with PBX 9501 (plastic bonded explosive). The time sequence begins from the top, with an interframe time of 20 µs.

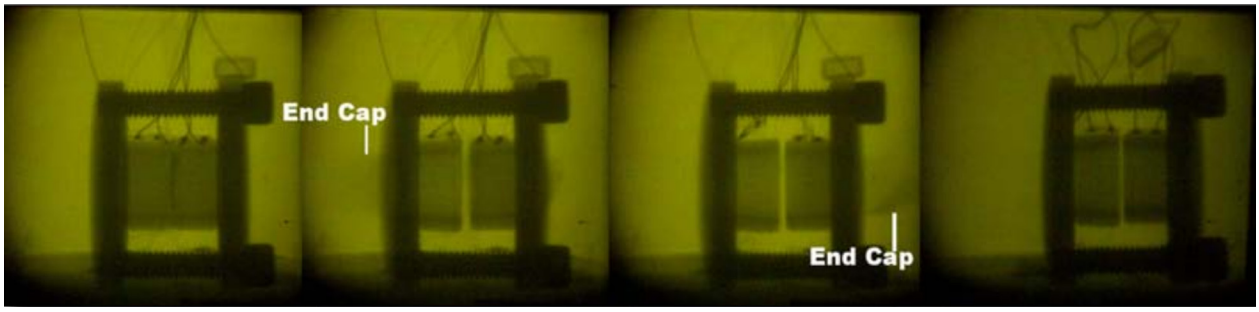
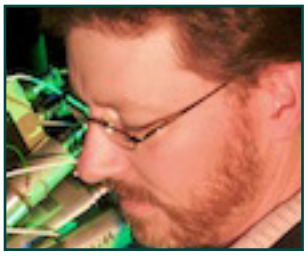
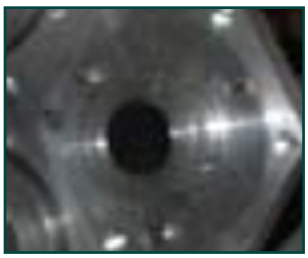


Figure Bottom: This image sequence taken with a tabletop x-ray experiment captures a spontaneous dynamic event (a thermal explosion). Because of the extremely fast nature of these events, the frame rate of the camera is about 50,000 frames per second. The images in the movies show a 1-in.-diameter radial thermal explosion experiment. The HE cylinders are encased in an Al case bolted together with steel screws. The x-ray movies show the final hundreds of microseconds as ignition is breaking out, and the burn is propagating and consuming the explosive. After about 10 frames, the end caps are punched out and fly out of the field of view and the case comes apart.





Weapons Neutron Research 2012

LANSCE
Los Alamos Neutron Science Center

WNR

The WNR facility provides intense, high-energy neutron and proton beams for nuclear science and engineering; semiconductor electronics quality testing; and a variety of defense, energy, and basic science experiments.

The facilities are open to qualified researchers from academia, industry, and laboratories worldwide.

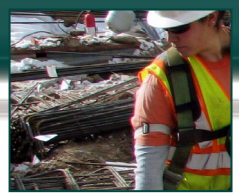
The WNR facilities consist of a high-energy spallation neutron source that is unique in the US, a proton irradiation area, and three low-energy neutron beam lines for nuclear science at the Lujan Center.

Together, these neutron sources cover the entire energy range of interest for many applications.

State-of-the-art instruments are available to measure properties of nuclear reactions, including fission, neutron capture, inelastic scattering, charged particle production, and total cross sections.

The WNR facility at LANSCE provides the neutron beams and instruments needed to measure fission and nuclear reaction properties for defense programs.

Image (right): The buttress of WNR's new building frames a window to the sky: a visual anecdote to the limitless potential of WNR's new facilities and capabilities.



Construction: Start to Finish

Construction of a new building to expand WNR's capabilities at the LANSCE/WNR Target-4 experimental area begin in CY2011. The building doubles WNR's capacity for neutron testing of semiconductor devices with the same neutron spectrum that currently exists at the Irradiation of Chips Electronics (ICE) House.

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

The new building covers the 15-Degree Right (15R) and Left (15L) Flight Paths, as well as parts of the 30R and 30L Flight Paths, and has a crane to move heavy shielding and equipment.

Contractors excavated in preparation for framing and pouring the foundation for the building. A detailed schedule was developed that combined the construction schedule with the installation of the flight paths.

Target-4 Flight Paths were brought up in a staged sequential manner: The 90L Time Projection Chamber (TPC) and the 60R GErmanium Array for Neutron Induced Excitations (GEANIE) Flight Paths were the first to receive beam because they were outside the building construction area.

The next flight paths to be brought on line were the 30-Degree Flight Paths (ICE House and ICE-II).

The last flight paths were 15R and 15L because they required the the most installation effort.

Images: Phase contruction of the foundation.
Clockwise from top left:
(1) excavating, (2) laying the foundation grid,
(3) pouring the slab, (4) completeing the foundation slab.

New Building, New Capabilities

The construction of the new WNR building has been completed (image).

The building is approximately 4,000 square feet, with a 5-ton crane capacity, and houses two flight paths: 15R and 15L.

The 15L Flight Path is designed for the Chi-Nu experiment and contains a 6-x-6-x-2-m-deep pit to reduce the background from scattered neutrons.

The goal of the Chi Nu experiment is to measure the neutron output spectrum from fission, especially below 0.5 MeV and above 5 MeV, where the existing data are sparse. The building and the installation of the 15L Flight Path for Chi-Nu opens up the 30R Flight Path for semiconductor testing by industry and universities.

Because the neutron spectrum at 30 degrees at WNR Target-4 mimics the cosmic-ray-induced spectrum, high demand exists for such a flight path to increase our capacity beyond what is currently available in the ICE House (30L).

With the new 30-Degree Flight Path, we have doubled our capacity to accommodate industrial users.

Image: Newly completed bulding.

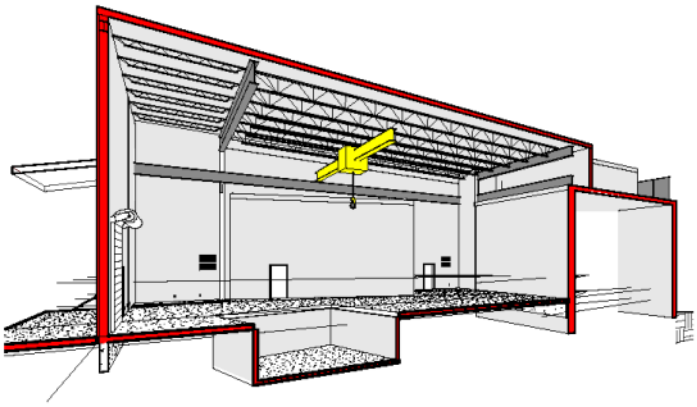
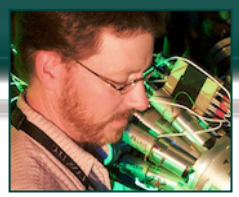


Figure: Schematic of Flight Path 15L (Chi-Nu) housing.



First Observations of Transitions Above the Previously Known 10+Isomers of Tin Isotopes

Tin is important in nuclear technology because it is used in the cladding of fuel rods in nuclear reactors and because the heavier tin isotopes are produced as fragments in the fissioning of actinides. Therefore, knowledge of rates of neutron induced reactions on tin isotopes is needed. Nuclear models in which nucleons occupy orbitals, much as the orbitals in atomic physics, are successful in explaining nuclear energy levels. Similar to atomic electron shells, nuclear theory predicts "magic numbers" of closed nuclear shells for both protons and neutrons. The tin isotopes have been a testing ground for such models and methods for many decades. The closed proton shell in tin isotopes makes them amenable to shell model calculations.

The researchers performed measurements of nuclear reaction rates by observing gamma rays emitted in neutron-induced reactions on the heaviest stable tin isotope ^{124}Sn (50 protons and 74 neutrons). They studied reactions where 1–8 neutrons are ejected from the recoiling nucleus. The scientists used the GEANIE spectrometer, comprising high-resolution germanium detectors (to detect gamma rays) and the pulsed neutron source of LANSCE's WNR facility, which provides neutrons over a wide energy range.

In the process of analyzing the data from this experiment, the researchers observed for the first time gamma-rays feeding the previously known long-lived states in ^{118,120,122}Sn (2.5-, 6.26- and 62-µs isomeric half lives, respectively). The deduced level schemes for these gamma rays are shown in the adjacent figure, in which the gamma ray energies are in keV, and the width of the arrows represent the relative intensities of the gamma rays. The similarities among these level schemes demonstrate that these isomers and the excited levels above them arise from a similar arrangement the neutrons in these nuclei.

These experimental results are in excellent agreement with predictions from shell model calculations. This work included data collected with the Gammasphere spectrometer at Lawrence Berkeley National Laboratory (LBNL), using heavy-ion reactions that complement the GEANIE data.

Reference: "States Built on the 10+ Isomers in 118,120,122,124Sn," by N. Fotiades, M. Devlin, and R.O. Nelson (WNR); J.A. Cizewski (Rutgers University); R. Krucken [Technische Universitat Munchen (TUM) and TRIUMF]; R.M. Clark, P. Fallon, I.Y. Lee, and A.O. Macchiavelli (LBNL); and W. Younes (LLNL). *Physical Review C* **84**, 054310 (November 2011).
doi: 10.1103/PhysRevC.84.054310.

The combination of the GEANIE spectrometer with the neutron source of the LANSCE/WNR facility has been used extensively to measure reaction rates and has contributed significantly to the knowledge of level schemes of isotopes. Measuring these reaction rates and comparing them with model predictions help improve the understanding of nuclear reactions and the structure of the nucleus, sustaining nuclear science in support of LANL's scientific and defense missions. One of the most notable accomplishments of the GEANIE spectrometer at LANSCE was the measurement of the ^{239}Pu($n,2n$)^{238}Pu reaction rate, which is an important diagnostic for Defense Program needs. The DOE Office of Science and NNSA Defense Programs fund GEANIE.

The work supports Energy Security and Nuclear Deterrence mission areas and the Materials for the Future and Science of Signatures science pillar.

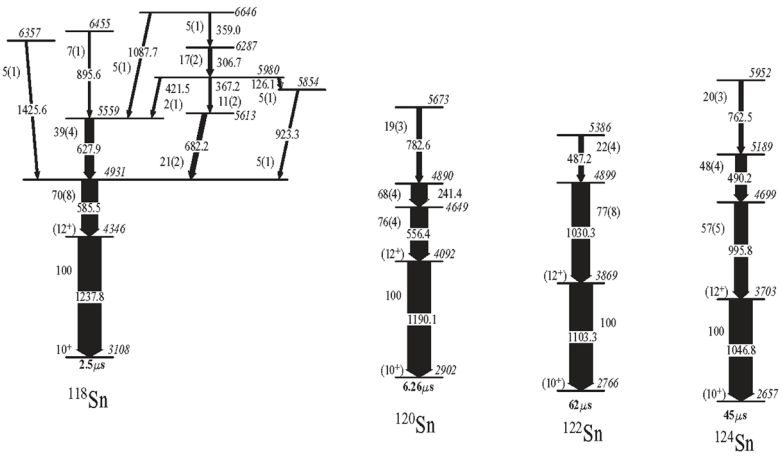


Figure: Schematic of the observed gamma-rays feeding isomers in Sn nuclei.

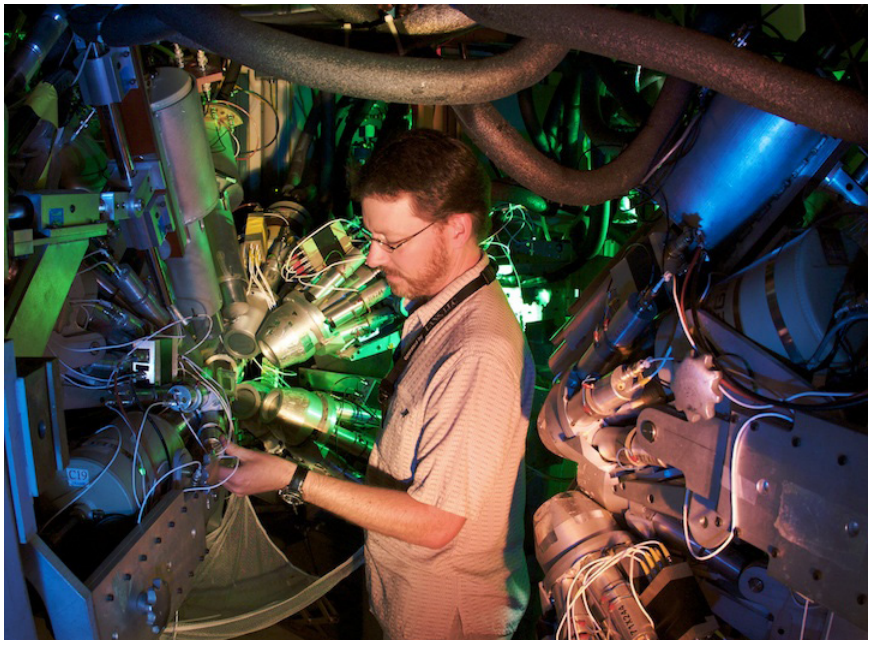


Image: Matt Devlin (WNR) works with the GEANIE spectrometer.

Experiments Hint That the Atomic Nucleus Still Holds Some Surprises

One of the highlights of nuclear physics is the description of highly excited states of a nucleus as being the epitome of random systems. The properties of such a system can be described simply by average statistical parameters, and a conceptually elegant description of these properties has been developed. Two papers based on experiments using the Detector for Advanced Neutron Capture Experiments (DANCE) at LANSCE have provided new information regarding these statistical properties.

The statistical parameters depend on a quantum-mechanical property of the excited nucleus called spin. Recently, a novel method for determining excited-state spins by counting the number of gamma rays emitted in a nuclear reaction has been developed. In a paper in *Physical Review C*, Bayarbadrakh Baramsai [North Carolina State University (NCSU) postdoctoral researcher, resident at LANSCE] and co-workers at NCSU, in collaboration with LANL and LLNL, presented an elegant technique to use DANCE as a "spin meter" through statistical pattern recognition techniques. When they tested the technique in a new and precise determination of excited-state properties in reactions on gadolinium-155 (^{155}Gd), they obtained results in substantial agreement with previous measurements. This method has advantages in that there is no need to select prototype resonances, the maximum amount of information is used, and a confidence level is obtained for the correctness of the spin assignment. These results demonstrate that the new pattern recognition method is a valuable addition to methods of determining the quantum numbers of resonances studied with the DANCE calorimeter. The scientists have planned measurements on nuclei where existing data are incomplete or contradictory.

Reference: "Neutron Resonance Parameters in ^{155}Gd Measured with the DANCE γ-Ray Calorimeter Array," *Physical Review C*, **85**, 024622 (2012).
doi:10.1103/PhysRevC.85.024622.

LANL coauthors include A. Couture, R.C. Haight, J.M. O'Donnell, and J.L. Ullmann (WNR); and T.A. Bredeweg, M. Jandel, A.L. Keksis, and R.S. Rundberg (Nuclear and Radiochemistry, C-NR).

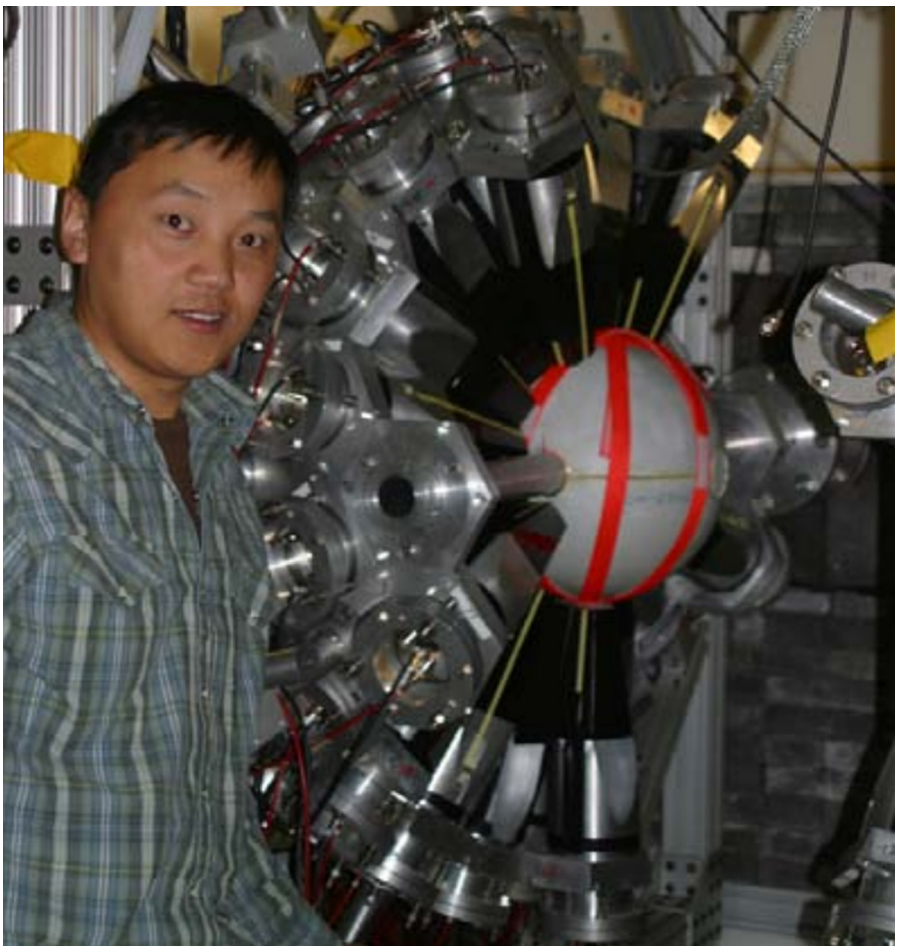


Image: Bayarbadrakh Baramsai (NCSU) with the DANCE detector.

Abrupt Change in Radiation-Width Distribution for ^{147}Sm Neutron Resonances

A paper published in *Physical Review Letters* by P.E. Koehler (ORNL), in collaboration with LANL researchers, hints that nature may still have some surprises. One of the consequences of the theory of random systems is that the average properties and their distribution should not change appreciably with small changes in excitation energy. The scientists used the DANCE detector and a spin-meter technique to make accurate measurements of the probability for gamma-ray emission following the capture of neutrons by samarium-147 (^{147}Sm). The results revealed abrupt changes in the average properties of highly excited states in the product nucleus ^{148}Sm for neutron energies above and below 300 eV. This result was not anticipated by the standard theory that underlies several models used to calculate nuclear reaction probabilities for applications in nuclear energy and defense. The new results indicate that the standard theory may be incomplete under certain conditions. Such effects could have important consequences for applications such as nuclear astrophysics and nuclear criticality safety, in which models often are used to calculate important quantities beyond the reach of measurement.

Reference: "Abrupt Change in Radiation-Width Distribution for ^{147}Sm Neutron Resonances," *Physical Review Letters* **108**, 142502 (2012).
doi:10.1103/PhysRevLett.108.142502.

LANL researchers include J.M. O'Donnell and J.L. Ullmann (WNR), R.S. Rundberg, D.J. Vieira, and J.M. Wouters (C-NR).

NNSA Defense Programs Science Campaigns fund the DANCE spectrometer.

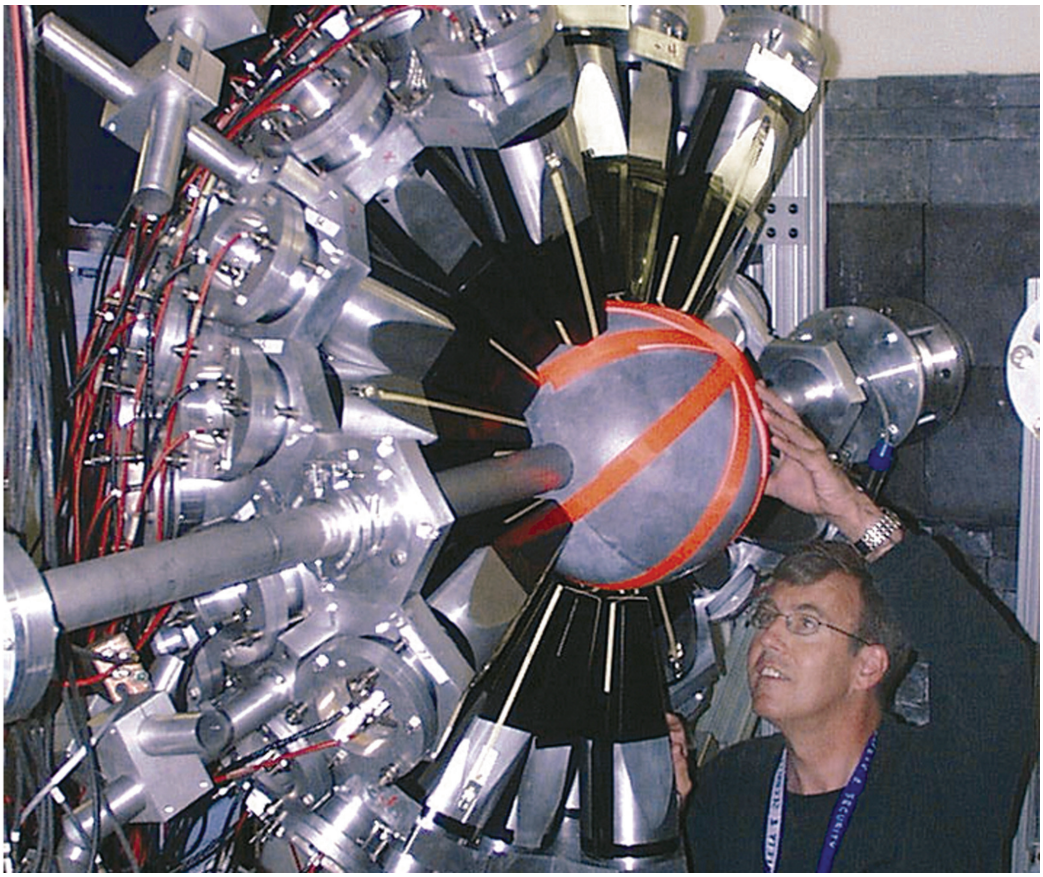
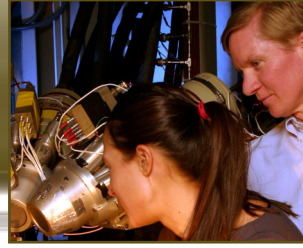


Image: Bob Rundberg (C-NR) prepares the DANCE detector.

User Program 2012

LANSCE
Los Alamos Neutron Science Center



User Program

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

DOES's designated national user facilities are the

- Lujan Center,
- pRad, and
- WNR.

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

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

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

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

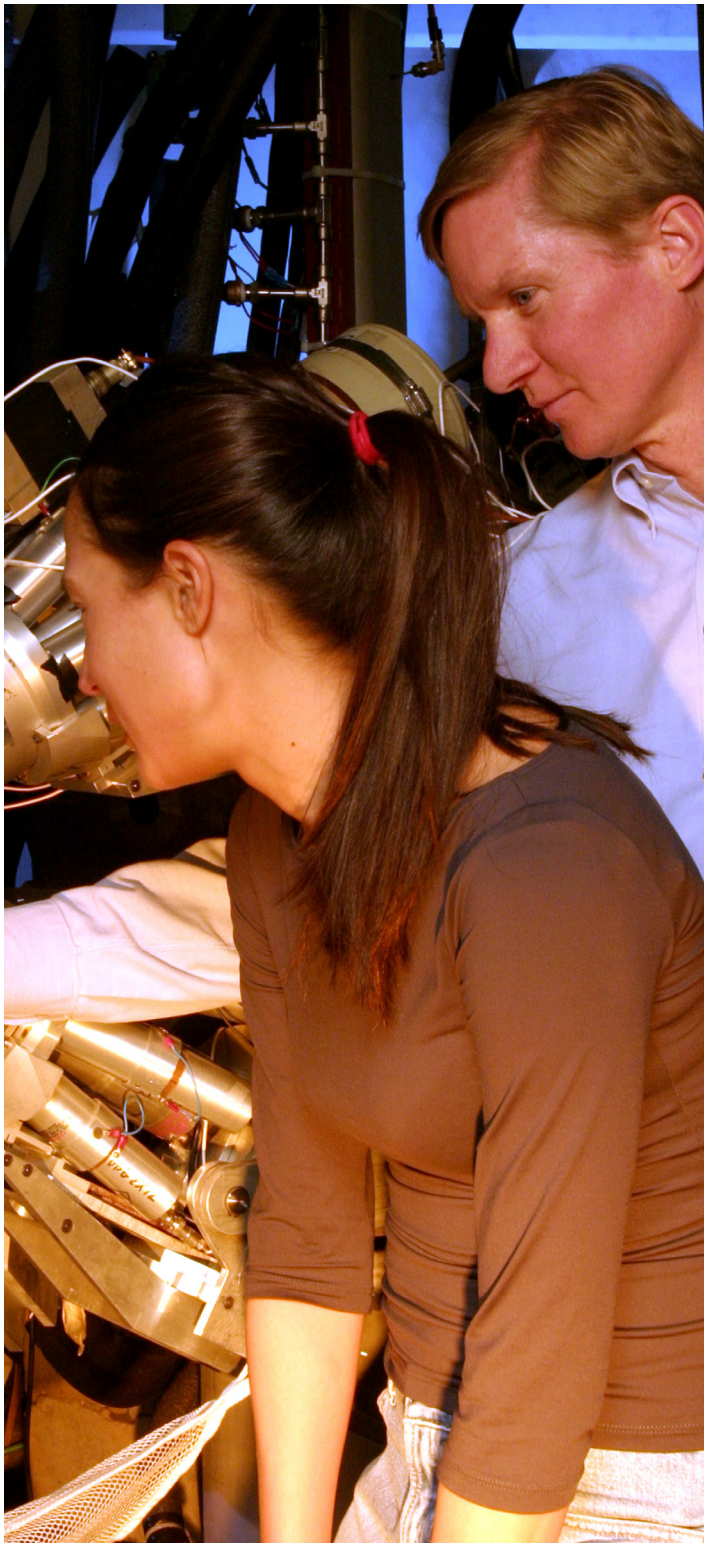
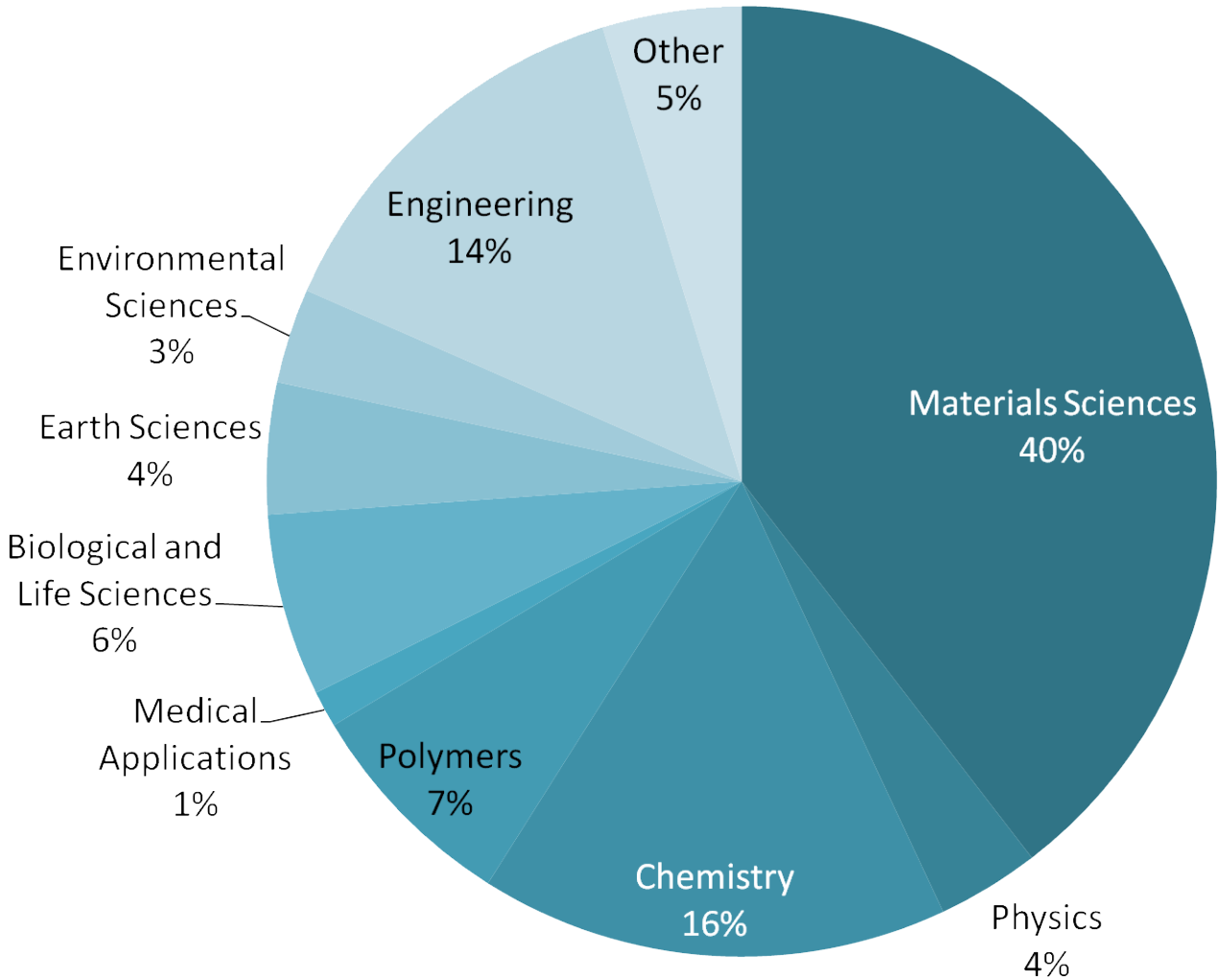


Image (right): Ron Nelson (WNR) demonstrates sample positioning to user Irene Beyerlin (T-3).

User Demographics

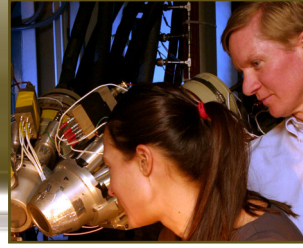
Materials Sciences
40%

Lujan Center

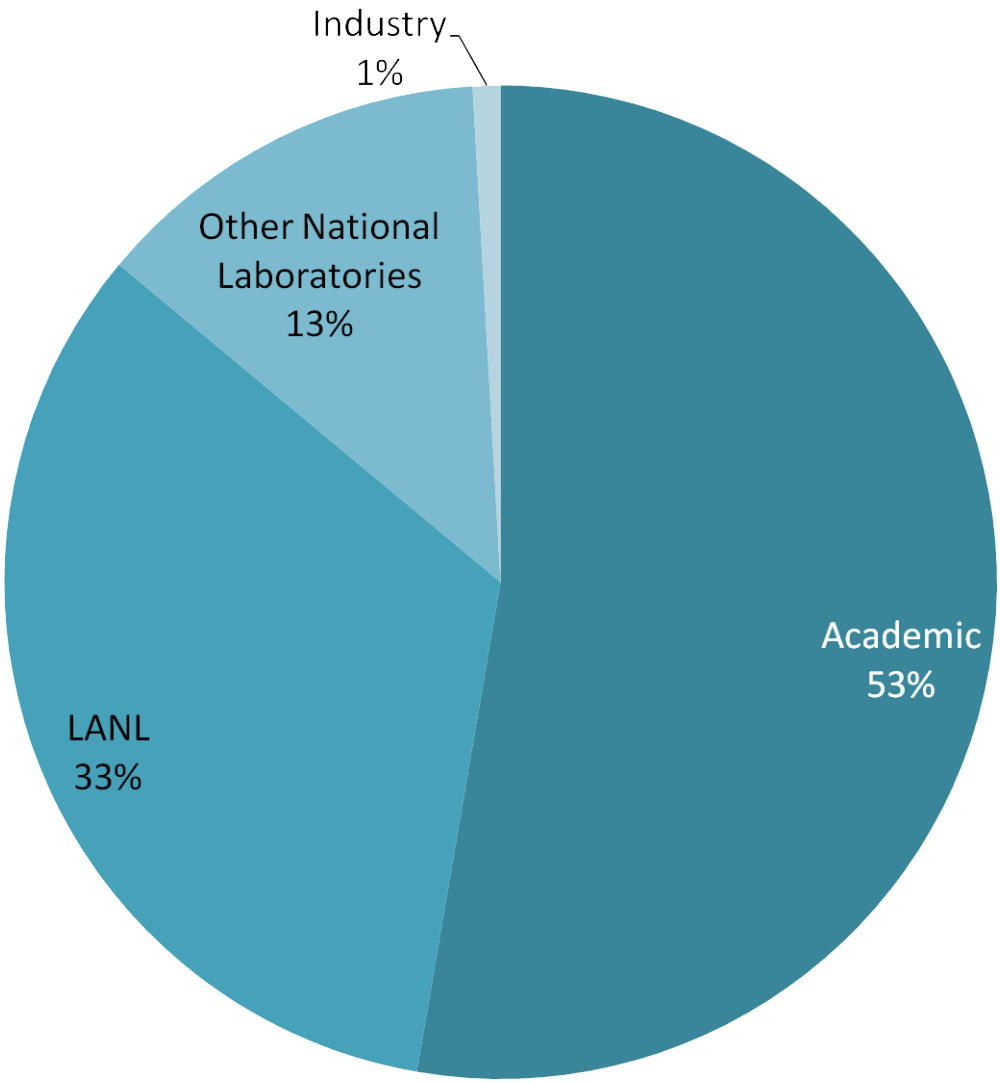


As a National User Facility, the Lujan Center hosts several hundred users from academia, industry, national laboratories, and other research facilities around the world. Beam time on 11 neutron scattering instruments and 3 nuclear physics instruments can be requested by responding to announced calls. Proposals are assessed by an external scientific peer review panel, and beam time is allocated based on scientific merit.

User Demographics



Lujan Center

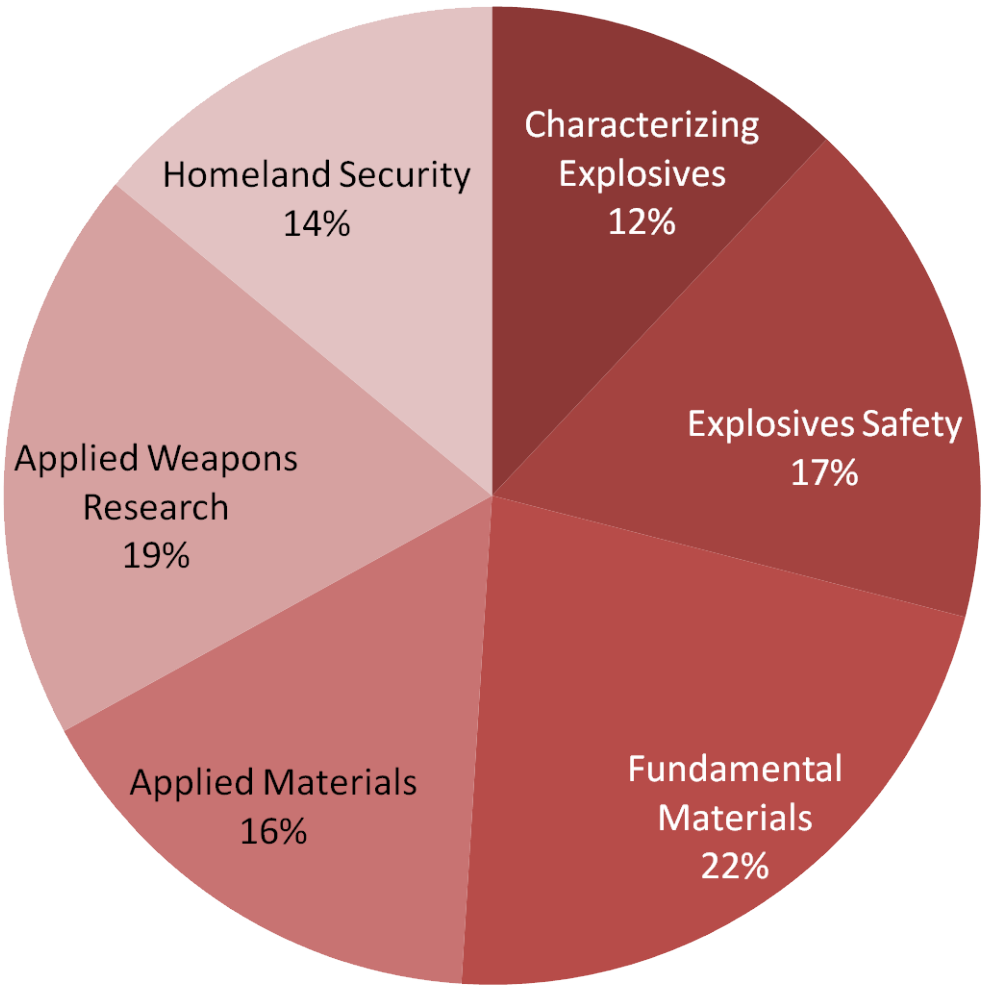


Fast access to Lujan Center instruments and beam time is also available outside of regular proposal calls for cutting-edge science or urgent breakthrough discoveries. A mail-in program also allows users to collaborate with expert scientists at the Lujan Center to perform their experiments remotely. All of these options are available to ensure that users' experiences at the Lujan Center are productive and successful and that they lead to world-class science.

User Demographics

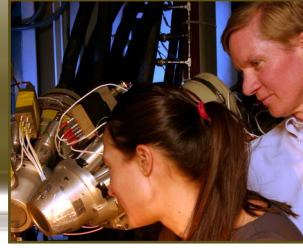
Fundamental Materials 22%

pRad



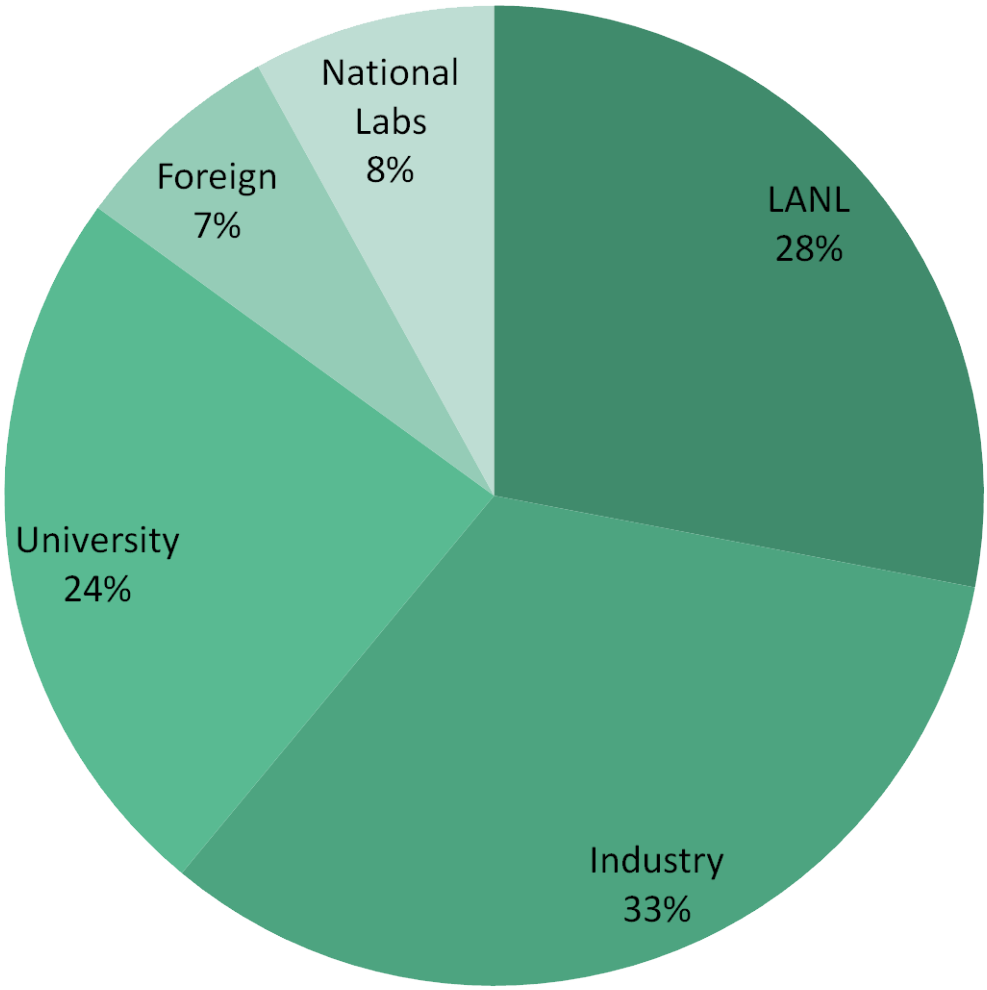
Currently, pRad is a dual-use facility, which allows access for users interested in classified research, as well external users interested in unclassified research. This user program will continue to provide a pool of scientific talent for recruitment into the national weapons program.

Both classified and unclassified experiments are welcome at pRad. Researchers at pRad answer questions crucial to Stockpile Stewardship and also investigate questions in fundamental and applied science. The penetrating power of protons makes it possible to see interior details of various materials (including dense metals) for potential applications in science and industry.

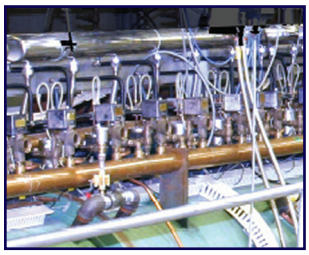


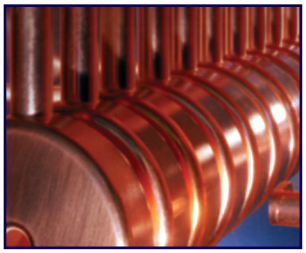
Industry
33%

WNR



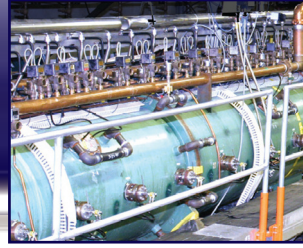
WNR facilities are open to qualified researchers from academia, industry, and laboratories worldwide. State-of-the-art instruments are available to measure properties of nuclear reactions, including fission, neutron capture, inelastic scattering, charged particle production, and total cross sections.





Accelerator Operations Technology 2012

LANSCE
Los Alamos Neutron Science Center



AOT

The Accelerator and Operations Technology (AOT) Division conducts fundamental and applied R&D needed to improve operations and operations support for LANSCE.

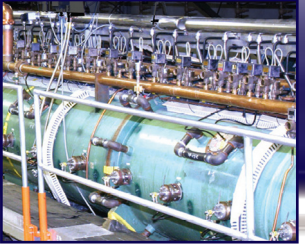
AOT's R&D efforts include

- plasma physics, and ion beam generation;
- accelerator physics, engineering, and design;
- high-space-charge, proton-accumulator/ compressor-ring physics;
- particle-beam-diagnostics physics and engineering;
- high- and low-power radio-frequency (RF) system engineering;
- mechanical engineering and design;
- high-vacuum engineering and technology;

analog and digital control systems engineering and technology based on the experimental physics and industrial control system (EPICS); and

- specialized H-furnace brazing.

Image (right): At the core of the LANSCE's international user facility is a highly flexible LINAC system, which is overseen by the Beam Delivery team.



LANSCE Risk Mitigation

The LANSCE-LINAC Risk Mitigation (LRM) project will replace obsolete and end-of-life equipment at LANSCE and will provide new capabilities.

The core elements of the first phase of the LRM project are the RF system upgrade; instrumentation, control, and diagnostic systems improvements; and accelerator system upgrades. These upgrades emphasize early restoration of 120-Hz operation for LANSCE, 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 twofold: 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 current systems that limit LANSCE's operation to 60 Hz. The goal is to restore 120-Hz operation coming out of the fiscal-year (FY)14 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. By the end of CY12, LANL had taken delivery of 25 new 805-MHz klystrons from Communication and Power Industries (CPI); the first of these klystrons has been installed and is operating in support of the user programs.

A prototype 201-MHz RF final power amplifier (FPA) has been designed and fabricated. This prototype demonstrated the design requirements to generate 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 ¾ λ from the central electron beam region in the tube and the upper-slave tuner ¼ λ 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 DTL.

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. 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 of 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).

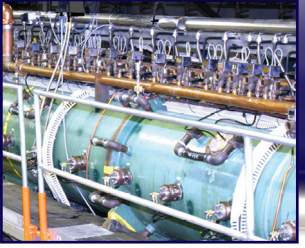
Low-Level RF (LLRF) Feedback Controls, High-Voltage Systems, and Modulators

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. In FY12 prototype designs were completed of 15 of the 19 required modules. Of the prototypes, 11 were tested and 4 are still in progress.

The LANSCE klystron modulators are based around a modulator tube that is no longer available. LANSCE LRM project is funding the design of a new modulator topology around a modern modulator tube. The prototype of this modulator was completed in FY11 and was tested extensively in FY12.

Also in FY12, the first high-voltage (HV) systems were sent out for refurbishment. Degradation of oil-filled HV equipment can be measured through an analysis of the dissolved gasses in the HV insulating oil. The LANSCE RF system's HV equipment was screened using this tool and compared against the Institute of Electrical and Electronics Engineers standard. Five transformer rectifiers (TRs) and eight Inductrol Voltage Regulators (IVRs) were selected for refurbishment. In FY12, both an IVR and TR set were sent to vendors. The TR set was returned and installed and is currently supporting beam operations. The IVR set is due back to LANL early in FY13.

First article replacement: LANSCE klystron.



LANSCE Beam Facts

At IPF, 100-MeV protons are used to produce radioisotopes for both research and nuclear medicine.

Pulses of 800-MeV negative H-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 H-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.

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 these neutrons 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.

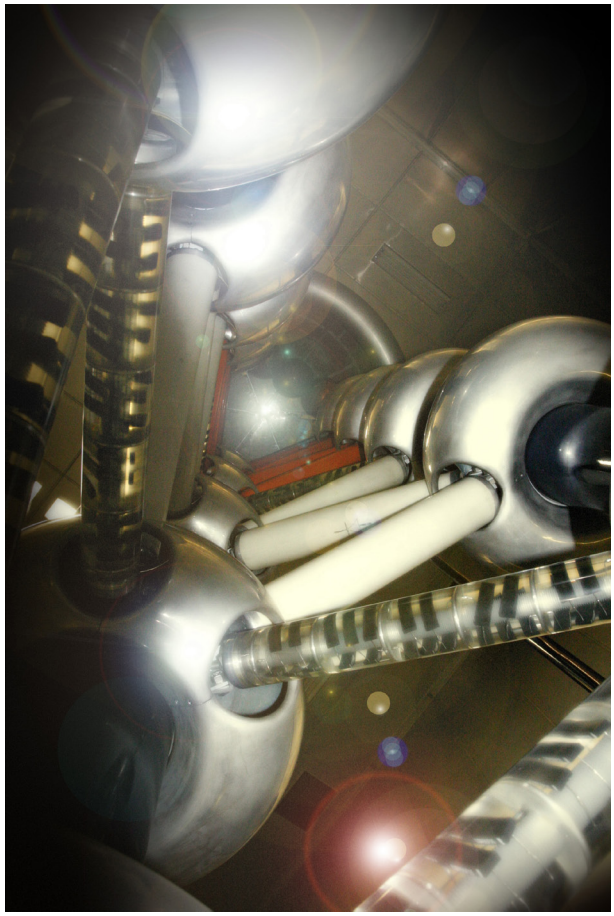
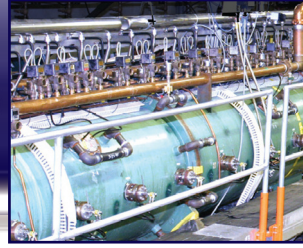


Image: Cockcroft-Walton Generator
After pre-acceleration out of an ion source, H- ions are furtheraccelerated by the 670,000-volt electric field created by the generator.

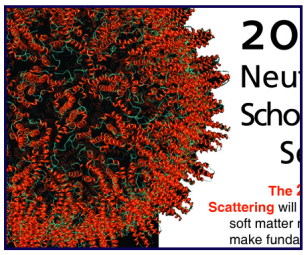
In the image here, a voltage-rectifier and multiplier ladder steps up an initial 56,000 volts to 670,000 volts, completing the first acceleration stage of the H- ionsacceleration stage of the H- ions

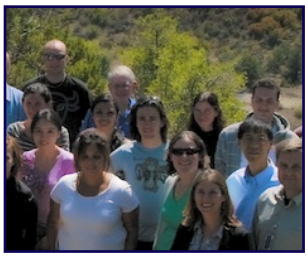


Reliability
89.6%

2012 Production Delivery Summary

Area	Scheduled Hours	Delivered Hours	Reliability
IPF	3237.5	2996.8	92.6%
Lujan	996.0	877.8	88.1%
pRad	625.4	555.9	88.9%
UCN	1965.6	1838.0	93.5%
WNR	3165.2	2844.8	84.8%
Total	**9989.7**	**9113.3**	**89.6%**





Conferences, Workshops, and Tours 2012

LANSCE
Los Alamos Neutron Science Center

Conferences, Workshops, and Tours

Attendees from government, academia, and industry come to LANSCE for topical conferences and workshops. In conjunction with NMSU, LANSCE also annually runs the LANSCE School on Neutron Scattering, now in its ninth year. The Stewardship Science Academic Alliance Center of Excellence also meets at LANSCE once a year.

In addition to our conferences and workshops, throughout the year LANSCE hosts a variety of visitors, many of whom request tours of the accelerator, instruments, and laboratories. 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 and fully supports educational outreach tours to higher education, K-12 schools, and youth organizations.

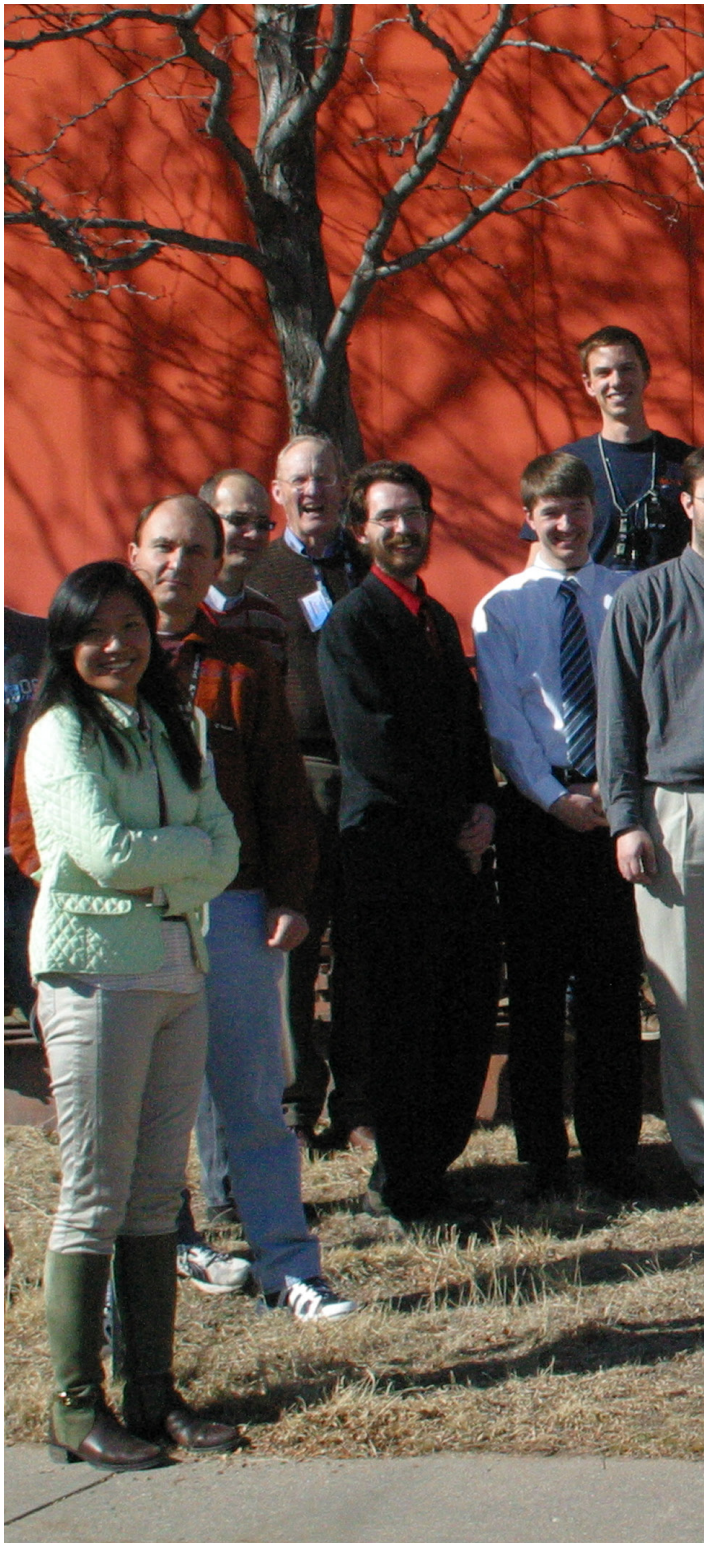


Image: Participants from the Stewarship Science Academic Alliance Center of Excelllence.

Stewardship Science Academic Alliance Center of Excellence Meets

Scientists from the Stewardship Science Academic Alliance (SSAA) Center of Excellence for Radioactive Ion Beam Studies for Stewardship Science visited LANSCE on March 12–13. This center is the only nuclear physics research center in the NNSA-sponsored SSAA. Professor Jolie Cizewski (Rutgers University) heads the Center, which includes participants from Rutgers, University Radioactive Ion Beam/Oak Ridge Associated Universities, Tennessee Technological University, the Colorado School of Mines, the University of North Carolina, Michigan State University, LANL, and LLNL. The SSAA's goal is to create opportunities for scientists in physics disciplines that are important to NNSA missions. An important focus of the program is the training of students and postdocs who can contribute to scientific discovery in nuclear physics and potentially be employed at one of the national laboratories.

The Center brought 15 participants, including 4 postdocs, 9 graduate students, and 1 undergraduate student to the meeting. The Center described many of its nuclear physics projects in 14 presentations. To acquaint these visitors with LANL programs, LANL researchers gave talks regarding LANSCE and gave one talk each from the DARHT on flash radiography; Safeguards Science and Technology (NEN-1) on safeguards; Space Science and Applications (ISR-1) on space science; and Nuclear and Particle Physics, Astrophysics, and Cosmology (T-2) on modeling basic nuclear physics reactions. The group toured the WNR and Lujan Center facilities. The work supports LANL's Nuclear Deterrence and Global Security mission areas and the Materials for the Future science pillar.

Image: Participants from the SSAA Center and some LANL researchers.

Advanced Simulation Techniques for Total Scattering Data Workshop

The LANL Center for Nonlinear Studies (CNLS), LANSCE, and ORNL are organizing a workshop to take place October 16–19 in Santa Fe, New Mexico. The workshop will bring together leading scientists in the areas of total scattering, local structure, and advanced atomic simulations. The workshop will provide an opportunity to discuss current limitations in methods for modeling total scattering data, potential directions forward, complementary simulations and experiments, and how total scattering can be used to validate atomistic simulation results.

Total scattering from neutron and x-ray diffraction investigates the structure of amorphous, disordered, and nano-sized materials. This method provides both Bragg and diffuse scattering components, revealing information about the local atomic to long-range structure of materials. The use of total energy calculations (such as ab-initio and force-field-based methods) in conjunction with these experimental tools reveals the atomistic nature of increasingly complex materials. These methods can replicate total scattering data while remaining energetically feasible. The workshop will explore the synergy between total scattering and various forms of total energy calculations used to simulate complex materials.

Local organizing committee: C. White and K. Page (Lujan Center) and N. Henson (Physics and Chemistry of Materials, T-1).

Sponsored by the CNLS at LANL, the event is free and open to the public.

http://cnls.lanl.gov/totalscattering/

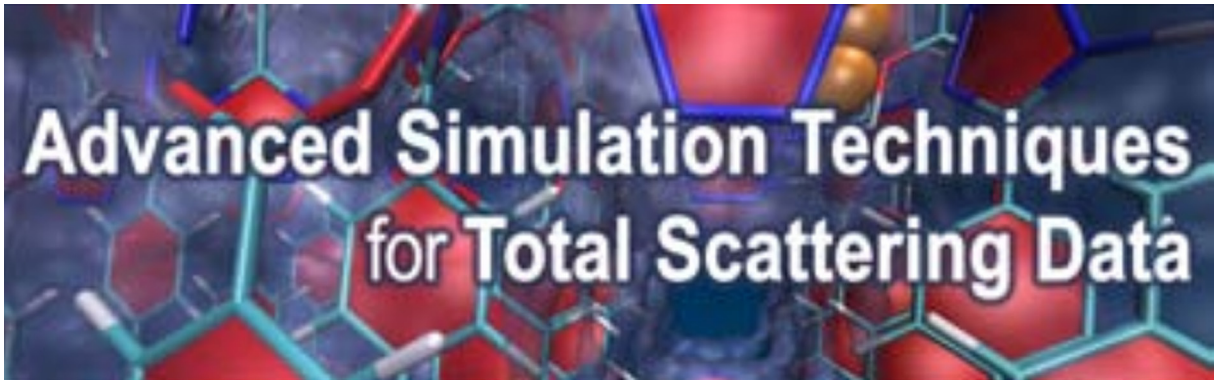
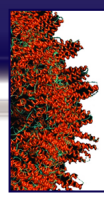


Image: Workshop logo



2012 LANSCE School on Neutron Scattering

The 2012 LANSCE School on Neutron Scattering was held September 12–21. The 2012 school featured applications of neutron scattering techniques in basic and applied soft matter research, with a focus on applications to energy, medical, and materials science. A special track on neutron crystallography for structural enzymology was included. The school is intended primarily for doctoral graduate students in the physical, chemical, or biological sciences or postdoctoral researchers desiring an introduction to neutron scattering techniques in soft condensed matter or structural enzymology.

The school focuses on specific science topics to which neutron scattering makes a critical impact. The focus-driven agenda makes it distinct from other neutron schools in the nation. The LANSCE School on Neutron Scattering began in 2004 and has operated annually since. The general format of the school typically consists of three to four lectures each day, followed by intense afternoons of conducting experiments. The hands-on studies involve neutron-scattering instruments and research topics appropriate for the school's focus. The instructors place emphasis on the physical meaning of the experiments and how neutron techniques provide complementary information to other types of experiments. Lectures are given by experts relevant to that school's focus. Small groups of students are involved in five or six different experiments and learn how to analyze data taken on different instruments under the guidance of the instrument scientist.

The 2012 School, held at the Lujan Center, covered:

- Basic concepts of neutron production, scattering methods and instrumentation.
- An introduction to soft matter, with an emphasis on areas of basic and applied research in energy, medical, and materials topics where neutrons can and do make fundamental contributions.
- Concepts behind neutron instrumentation and experimental approaches for soft matter.
- Use of deuteration in soft matter neutron scattering.
- Detailed case studies in soft matter research using small-angle neutron scattering; NR; and chemical neutron spectroscopy, diffraction, and radiography.
- Technical aspects of measurement techniques and data analysis.
- Computational techniques that complement and aid in the planning, analysis, and interpretation of neutron measurements.
- An open session for discussion and/or a lecture of an additional topic selected by the students.
- Additional topics in protein crystallography techniques in the special track on structural enzymology

Lectures will be complemented by hands-on exercises, applying concepts to specific problems using Lujan Center instrumentation. Students will make presentations of their findings on the final day of the school.

Students chose among exercises using the small-angle neutron scattering Low-Q Diffractometer (LQD), NR (SPEAR), chemical neutron spectroscopy (FDS), diffraction using the Spectrometer for Materials Research at Temperature and Stress (SMARTS), radiographic imaging, and local structure and pair distribution functions (NPDF and HIPD). The special track for protein crystallography using joint neutron and x-ray diffraction for structural enzymology will address the use of neutrons to better understand enzyme structure and mechanism.

Conferences and Workshops

School directors: J. Rhyne (Lujan Center) and H. Nakotte (NMSU).

Local organizing committee: S.Z. Fisher (Bioenergy and Environmental Science, B-8), R. Hjelm, and J. Majewski (Lujan Center).

LANSCE, DOE's Office of Science, NMSU, and the NSF cosponsor the school.

Image: 2012 school poster.

Image: School participants, lecturers, and organizers.

LANL Co-Organizes Symposium at the International Materials Research Congress

Los Alamos researchers and collaborators presented high-impact scientific findings during a 2-day symposium on "Novel Characterization Methods for Biological Systems." Jarek Majewski (Lujan Center), Alan Hurd (LANL), and partners from Universidad Nacional Autonóma de Mexico and the USF organized the symposium, which focused on physical, chemical, and theoretical techniques that transcend traditional inference to establish concrete models of structure, function, and dynamics in biosystems.

The symposium featured eight speakers citing LANL key results. Zoë Fisher (Bioenergy and Environmental Science, B-8) gave an invited talk, "Mechanistic Studies of Carbonic Anhydrase Using Joint X-Ray/Neutron Crystallography." Research accepted for publication in the *Proceedings of the National Academy of Sciences* on the day of presentation represents the first neutron diffraction protein structure with better than 1-Å resolution, taken on LANSCE's PCS instrument. Another researcher discussed high-resolution x-ray and neutron scattering data leading to an increased understanding of the interactions of biotoxins with cell membranes. The findings, published in *Proceedings of the National Academy of Sciences*, were the result of collaboration with LANSCE scientists using SPEAR.

The Novel Characterization symposium was one of 27 symposia in a large international meeting. Over 1400 scientists from 46 countries converged on Cancun, Mexico, on August 13–17, for the 21st annual International Materials Research Congress (IMRC).

The Sociedad Mexicana de Materiales (SMM) and the Materials Research Society (MRS) sponsored the IMRC. The Office of Naval Research-Global, NSF, and the USF funded the Novel Characterization symposium.

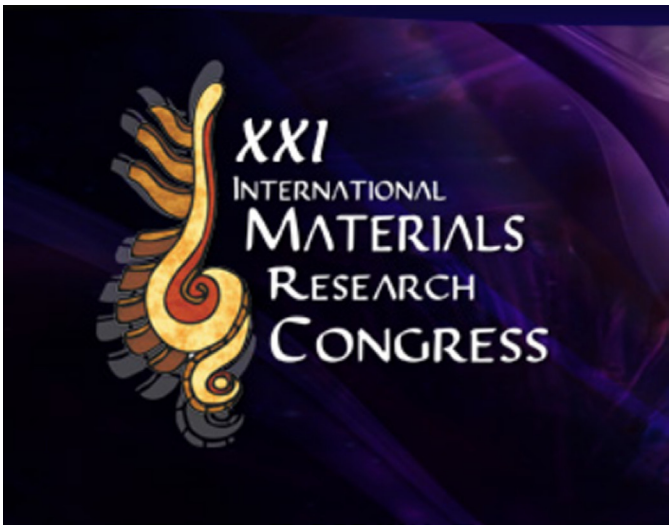


Image: Conference logo.

Image: Excerpt from conference poster.

2012 National User Facility Organization Annual Meeting

The 2012 National User Facility Organization (NUFO) Annual Meeting was held in Santa Fe, New Mexico. The topic of the 2012 meeting was to discuss what "NUFO can and will do for you [National User Facilities]!" LANSCE and LANL were the technical hosts for this meeting, with LANSCE providing logistical support.

Several breakout sessions focused on university relations; industrial access and interactions; user data management, computing, and cyber security; nanotechnology security; financial best practices; user administration benchmarking and best practices; and social media outreach.

User representatives, user administrators, NUFO general members, and others interested in user facilities attended this meeting.

"Founded in 1990, NUFO represents the interests of all users who conduct research at U.S. national scientific user facilities, as well as scientists from U.S. universities, laboratories, and industry who use similar facilities outside the United States.

Our primary mission is to facilitate communication among users, user organizations, facility administrators, and other stakeholders on topics of importance to the facilities.

These topics include publicizing the benefits and significance of research conducted at user facilities, as well as conveying their operational needs.

Fundamentally, we strive to provide a unified message at the national level on issues of resources for scientific work, economic competitiveness enabled by advances in science and technology, and education of the next-generation scientific workforce."

- Katherine Kantardjieff, Chair of the NUFO Steering Committee

Image: NUFO logo.

Image: NUFO participants.

Biennial National Neutron Scattering Conference Features Strong Lujan Center Presence

The 2012 American Conference on Neutron Scattering was held recently in Washington, DC, and featured a number of presentations by LANL researchers.

A highlight of the meeting included Claire White receiving the inaugural Prize for Outstanding Student Research from the Neutron Scattering Society of America. White is a Director's Postdoctoral Fellow at the Lujan Center and Theoretical (T) Division.

At the conference, she also presented a talk in a plenary session on "Recent Progress in Elucidating Accurate Structural Representations of Disordered Complex Materials," which described her work on geopolymeric concrete. This material holds great potential in reducing greenhouse gas emissions implicit in the ubiquitous construction material. The work integrates neutron measurements of short-range atomic order measured at the Lujan Center with first-principles calculations using density functional theory calculations that were performed in conjunction with T Division.

Other Lujan Center researchers presenting invited talks included Thomas Huegle discussing "Triphenylmethane and Its Potential Applications in Moderator Design," Monika Hartl, "Small Angle Scattering of Methane Dissolved in Water," and Saurabh Singh, "Influence of Capping Layer Rigidity on Properties of Supporting Temperature Sensitive Hydrogel Polymers Using Neutron Reflectivity."

Image: Claire White receiving the Prize for Outstanding Neutron Scattering Student Research from Bruce Gaulin, president of the Neutron Scattering Society of America.

Tour Stats

Institutions (A - Ka)	Number of Visits	Number of Attendees
Adlink Technologies	1	3
Agilent Technologies	1	2
Apple Distinguished Educators Programme, United Kingdom	1	5
Argonne National Laboratory	3	4
Associate Director of Nuclear and High-Hazard Operations	1	1
ATC	1	1
BCD. inc.	1	1
Bechtel Corporation	1	2
Bechtel National Inc.	1	1
Boy Scouts of America	1	23
Brown University	1	1
Carnegie Mellon University	1	2
Ch2M Hill	1	1
Colorado School of Mines	1	1
Colorado State University	1	14
Defense Threat Reduction Agency	3	4
Defense Nuclear Security Facilities Safety Board	1	4
Department of Energy	7	17
Department of Energy—Headquarters	3	7
Domestic Nuclear Detection Office	1	2
Emory University	1	1
Engineered Resource, LLC	1	1
Facility for Antiproton and Ion Research	1	1
Fox Chase Cancer Center	1	1
Harvard University	1	1
Harvey Mudd College	1	5
Idaho National Laboratory	1	5
Imperial College—London	1	1
Institute of Defense Analyses	1	1
Iowa State University	1	1
Jefferson Lab	2	2
Kadir Has University, Turkey	1	1

Tour Stats

Institutions (Ky - S)	Number of Visits	Number of Attendees
Kyocera	1	3
Laboratori Nazionali di Franscati—Italy	1	1
Lawrence Livermore National Laboratory	2	3
Los Alamos National Security	1	1
Los Alamos Site Office	2	3
Louisiana State University	1	1
MacMaster University	1	2
Massachusetts Institution of Technology	4	5
Morgridge Institute for Research	2	6
National Geospatial—Intelligence Agency	1	1
National Institute of Standards and Technologies	2	2
National Intelligence Estimates	1	1
National Nuclear Security Administration	5	9
National Security Technologies	9	22
Naval Research Laboratory	1	1
North Carolina State University	3	3
Nuclear Regulation Commission	1	1
Oak Ridge Associated Universities	1	1
Oak Ridge National Laboratory	5	6
Office of Governmental Accountability	1	1
Office of Secretary of Defense	1	5
Pacific Northwest National Laboratory	4	3
Raytheon	1	3
Rensselaer Security Institution	1	1
Reserved Case Western University	1	1
RMD, Inc.	1	1
Rutgers University	1	6
Sandia National Laboratories	4	11
SHINE Medical Technologies	2	4
Snow College, Utah	1	7
STAR Cryoelectronics	1	1
Stony Brook University	1	2

Tours

Tour Stats

Institutions (T - Z)	Number of Visits	Number of Attendees
Tech-X Corporation	1	1
Toshiba	2	2
Transportation Safety Institute	1	4
United States Air Force	1	1
University of California—San Diego	2	4
University of California—Santa Barbara	1	3
University of Cambridge	1	2
University of Chicago	1	1
University of Florida	1	1
University of Illinois	1	2
University of Kansas	1	1
University of Kentucky	2	2
University of Manchester	1	1
University of Notre Dame	1	1
University of Pennsylvania	1	1
University of Rochester	1	1
University of Sussex	1	1
University of Tennessee	1	1
University of Tennessee—Knoxville	1	4
University of Vienna	1	2
University of Washington	1	1
University of West Scotland—Paisley UK	1	1
Vanderbilt University	2	2
Washington Post	1	1
Wisconsin Alumni Research Foundation	1	1
WMC Corporation	1	1
Worcester Polytechnic Institute	1	1
Yale University	2	2
Ztec	3	4

News and Celebrations 2012

LANSCE
Los Alamos Neutron Science Center

News and Celebrations

News
The remarkable men and women of LANSCE go above and beyond in their service to our facility—the stories featured here are some of the newsmakers for 2012.

- M. Bourke
- R. Casten
- G. Holladay
- S. Nath
- M. Roth
- M. Zumbro

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

- N. Brennan
- E. Fernandez
- S. Singh
- C. White

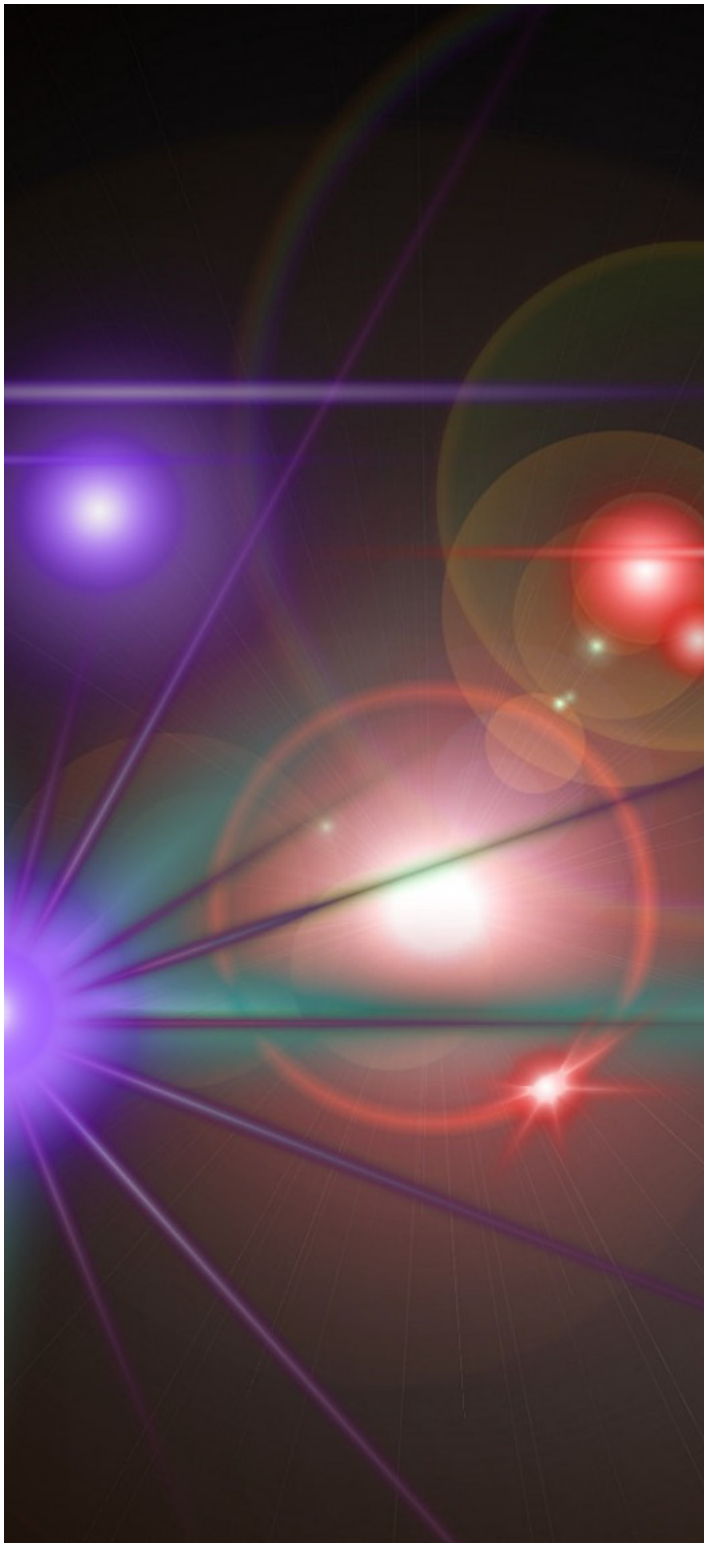


Image (right): Artist's rendering of excited beam and spectra in celebration of the oustanding newsmakers at LANSCE.

Mark Bourke: Queuing up New Research Possibilities at the Lujan Center

As Mark Bourke takes the reins as director of the Lujan Center, users can expect the same stellar service—and a commitment to new sample environments. In addition, senior staff scientists can expect more time for their own research, as well as encouragement to assume prominent roles in the neutron scattering community.

The combination, Bourke believes, will elevate the Lujan Center's presence at LANL and around the globe, resulting in new research opportunities.

In June, Bourke returned to the turquoise-and-pink-painted center where, in 1990, he began his LANL career as an instrument scientist. In the US, scientists can choose from 13 user facilities for their neutron scattering experiments. The Lujan Center, a vital part of the LANSCE since 1985, was one of the first. Bourke's ambition is to make it even more competitive than it already is.

"There is a set of research and development that we do as well as anyone, given our talented instrument scientists and exclusive sample environments," Bourke said.

To assist him with that goal, he enlisted staff scientists Anna Llobet and Guenter Muhrer as acting science deputy center directors and Experimental Area Manager Charles Kelsey to oversee technical support.

Though relatively small compared with other national user facilities, the Lujan Center is highly productive, attracting more than 300 unique users and generating up to 150 scientific papers a year, including many by the center's 15 PhD instrument scientists.

"We have a very happy group of users," said outgoing Lujan Center Interim Director Jim Rhyne, citing recent survey results and positive reviews from the Office of Science.

The US DOE's Office of Science, BES sponsors the lion's share of the Lujan Center's research and judges the center's success by the strength of its user program. The weapons program, industry, and DOE's Office of Nuclear Energy are important customers, as well.

Key to Bourke's vision is a commitment to safety and security. He also wants the Lujan Center to pursue research projects that fulfill the missions of both the Office of Science and the Laboratory, citing, as an example, plutonium measurements. Additionally, research in forensics, nuclear energy, energy security, and advanced materials would expand the Lujan Center's ties with both industry and the Laboratory community, he said.

The Lujan Center offers a variety of instruments that probe the structure of materials using different neutron scattering techniques and a pulsed spallation neutron source. The interactions of neutrons with matter at the Lujan Center offer unique insights that are, in many cases, complementary to the insights available from Imagen-based scattering capabilities at light sources elsewhere in the nation.

Bourke said he believes the Lujan Center should distinguish itself in two ways: by retaining and attracting world-class scientists and by creating "a unique set of sample environments that span a spectrum of extreme conditions." The latter could help forge the way for MaRIE, LANL's proposed signature experimental facility for the discovery and design of advanced materials, and for which Bourke serves on its core planning team.

To attract and retain standout scientists, Bourke believes that succession planning is important to allow senior scientists more time to devote to project development and to be ambassadors for the Lujan Center and the neutron scattering community as a whole. Conversely, he believes there is a need to provide opportunities for junior staff to operate instruments. Such changes could give the Lujan Center greater visibility, he said, which is crucial both for recognition within the Office of Science and for communicating the opportunities that neutron scattering affords the larger scientific community.

Bourke has a reputation for being a good listener and a calm problem solver, with "British-style diplomacy," according to Materials Science in Radiation and Dynamics Extremes (MST-8) Group Leader Anna Zurek, his former boss. Not one to make hasty decisions, "he definitely likes to get consensus from all parties involved," she said.

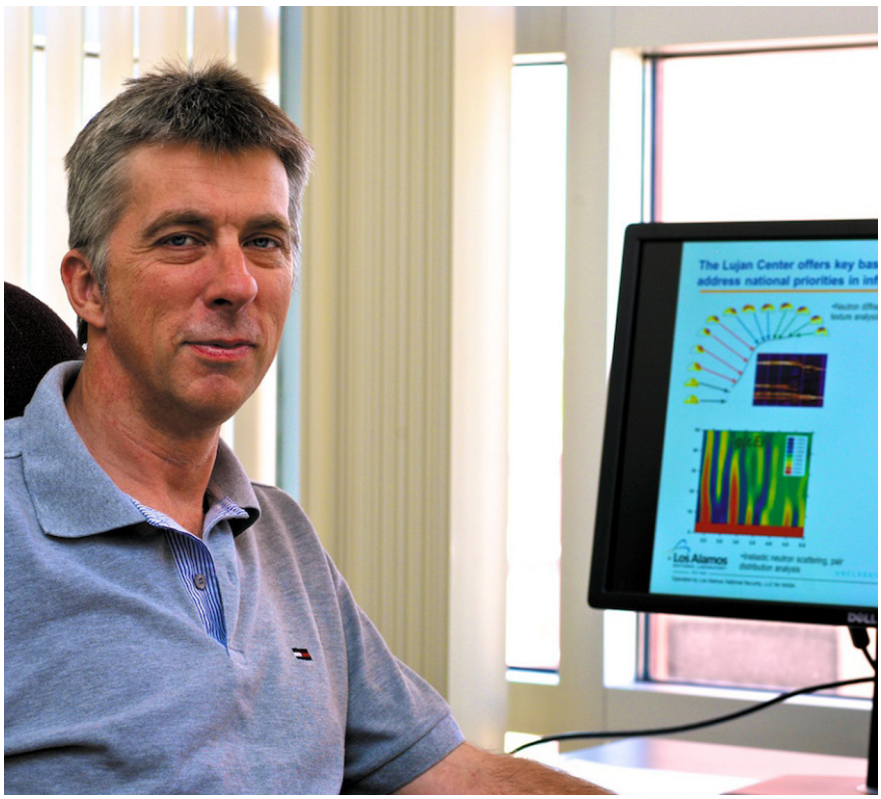


Image: Mark Bourke

Martha Zumbro and Subrata Nath: Accelerating the Pace of Scientific Research

As joint AOT deputy division leaders, Subrata Nath and Martha Zumbro are doing double duty.

Together, they're keeping LANSCE humming while prepping for the creation of MaRIE, which will bring transformational materials solutions to national security challenges.

Both started their careers at LANSCE and have paired up before on high-visibility projects, including the DARHT facility.

Last summer, Zumbro began overseeing the operations of the linear accelerator as Nath, in a newly created position, honed in on the technology driving the national user facility's five experimental areas.

Both are looking toward the future. For Zumbro, that means facing plenty of challenges as the 40-year-old accelerator undergoes renovation. For Nath, that means advancing accelerator science and technology through R&D projects and program development. Both roles are critical as plans for MaRIE move forward.

Tried and True Leadership

Imagine remodeling a mansion while tour groups tramp in and out. Similarly, old parts must be swapped for new ones, even as LANSCE continues to provide beam time to scientists from around the world. In the LANSCE "remodeling project," known as the LRM Project, everything must be "carefully staged and planned," said Zumbro.

Zumbro is also responsible for the safe and effective day-to-day operation of the accelerator. She starts each day reviewing beam status and call-in logs from from the night before to assess equipment operation.

She and Nath meet every day to discuss concerns. "I worked in a user role at DARHT for awhile, reminding me of how it feels to be a user and the frustrations that can accompany being dependent on an accelerator for a successful experiment," she said.

For 7 years Zumbro ran the Los Alamos Meson Physics Facility (LAMPF) operations group (now known as LANSCE). Most recently the deputy division leader for Weapons Experiments, she returned to LANSCE in June.

"Martha brings a wealth of experience in working to improve efficiency," said Accelerator and Operations Technology Division Leader John Erickson.

In Nath's deputy division leader role, which he began in July, he uses his more than 30 years of accelerator operations and construction experience to create an R&D program for the future and strengthen partnerships with other LANL programs and divisions. Previously group leader for DARHT Physics and Pulsed Power and Deputy project director at DARHT, Nath is now busy fleshing out technical realities for MaRIE.

"Subrata brings a tremendous breadth of knowledge from several accelerator facilities and a wealth of experience in working to develop technology," Erickson said.

Returning to LANSCE

Upon their return to LANSCE to face new challenges, Zumbro and Nath said they drew confidence from their triumphs at DARHT. Consisting of two linear-induction accelerators, DARHT was built to predict weapons performance after the US declared a moratorium on underground nuclear testing. Now it is the world's most powerful and unique x-ray machine for capturing the dynamic events that trigger a nuclear detonation.

"When the head of Defense Programs went to France and was given a tour of AIRIX [the French version of DARHT], the personnel there flat out told him that what we were proposing to do on the second axis of DARHT was physically impossible," said Deputy Associate Director Weapons Physics Mary Hockaday.

But LANL refused to put a lock on the door and throw away the key. "[DARHT Project Director] Ray Scarpetti and AOT's Subrata Nath and Martha Zumbro led the team that not only proved them wrong," Hockaday said, "but has given the United States an absolutely exquisite tool for Stockpile Stewardship."

Image: Martha Zumbro and Subrata Nath

2012 LANSCE Rosen Scholar

The Rosen Scholar fellowship was created to honor the memory of Louis Rosen, his accomplishments, hard work, and affection for the broad range of science performed at LANSCE. Louis Rosen's outstanding leadership and scientific career at LANL covered six-and-a-half decades and included the conception of LAMPF in 1960, which culminated with its commissioning in 1972. LAMPF was a unique nuclear science research tool through the 1990s. Now called LANSCE, the facility continues to play a paramount role in basic sciences and national security needs for the country. From his scientific vision to his kind and effective mentoring, Rosen's tenure, from the Manhattan Project in 1943 till his passing in 2009, exemplified the best in leadership at all levels.

The Rosen Scholar fellowship is intended to attract visiting scholars to LANSCE in the fields of nuclear science, materials science, defense science, and accelerator technology. The Rosen Scholar fellowship is reserved for individuals whose career accomplishments in 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. The position will support Rosen scholars at their current salaries, including relocation expenses for up to 1 year.

The Rosen scholars for CY12 brought together the disciplines of nuclear physics, accelerator technology, material science, and electrodynamics. This range of activities is the foundation of the LANSCE complex and fits well with the vision of a multi-disciplinary facility developed by Louis Rosen.

Nominees for Rosen Scholar candidates are to be sponsored by at least one of LANSCE's Facilities: IPF, UCN, pRad, Lujan Center, and WNR.

The nomination package should include a two-page research statement, a one-page letter of support from one of the sponsoring facilities, and a recent curriculum vitae. The research proposal should address at least one of the following two points: (1) advancement of LANSCE's research portfolio or mission and (2) future capabilities that advance LANSCE-based scientific research.

Image: Louis Rosen

2012 LANSCE Rosen Scholars

Richard Casten

Professor Casten has had many accomplishments and received many awards, including Fellowships in the American Physical Society and the American Association for the Advancement of Science. He was recently awarded the prestigious Tom W. Bonner prize in nuclear physics and received the APS Division of Nuclear Physics Mentoring Award. Professor Casten is very active in the nuclear physics community. He is the current Chair of the Facility for Rare Isotope Beams (FRIB) Science Advisory Committee and the past Chair of the Nuclear Science Advisory Committee (NSAC). He has served on all four long-range-plan panels since 1989 (1989, 1995, 2001, and 2007) and was Director of the Wright Nuclear Structure Laboratory form 1995–2008. Dr. Casten will work at LANSCE to develop new research ideas and possible directions for basic research in nuclear structure. Specific areas of interest include exotic nuclei, the mechanisms for the emergence of collectivity in nuclei, the evolution of shell structure, the stability of the heaviest nuclei, recognition and interpretation of the simple and regular patterns that complex nuclei exhibit, the order and chaos in nuclei, the relationship between mass (binding) and structure, and new signatures of structure and its changes with N and Z.

Image: Richard Casten

Markus Roth

Professor Markus Roth is a distinguished professor of physics at the Institut für Kernphysik, TU-Darmstadt. His current research is in the area of neutron production following high-power laser interactions with materials. This emerging field brings together the disciplines of nuclear physics, materials science, plasma physics, and high-power lasers. His research goal is to ultimately produce neutrons over a broad energy range using pulsed lasers. Such a source promises to be very compact and cost effective compared with existing neutron sources. If successful, such laser-based neutron sources could be used in a wide range of applications, from basic nuclear physics research to industrial applications. Dr. Roth worked with LANSCE and Physics Division to research novel, compact, high-brightness sources of neutrons using ultra-intense lasers.

Image: Markus Roth

Gary Hollady Taking Action in Working Safely

Gary Holladay of AOT had just started the Friday night shift when the letters "DPW" turned red on a status screen in the Central Control Room of LANSCE, indicating an equipment problem.

Two neutron detectors had faulted electronically. Holladay, the operations shift supervisor who runs the beam for the half-mile-long linear accelerator, jumped up to fix the problem. He drove across La Mesita Road and descended the steps to Lujan Center Experimental Room 1 (ER-1).

While plugging in a surge protector and checking connections, Holladay was unaware that his right knee, his right elbow, and his feet were brushing against a thin film of powder. On his way out, he ran his hands along the stair railings.

At that point, Holladay's task in ER-1 was complete. He could have headed straight back to his workstation; however, Holladay's sound work practices are deeply ingrained.

On August 24, he stepped into the Blue Room's radiation portal monitor, adjacent to ER-1, and the beeps rang out. Over the years, Holladay had never triggered a positive reading. Promptly and properly he reported the issue. He also instructed the other accelerator operators to stay out of ER-1. "I was more concerned about my crew than the beam at that point," he said.

Before routine radiation surveys in ER-1 were scheduled to take place, Holladay's diligence and sound safety practices alerted LANL to the inadvertent spread of ^{99}Tc. The substance is a source of beta radiation—low-power, fast-moving electrons that can travel through several feet of air but that are generally stopped by clothing and skin. The on-site and off-site contamination posed no danger to the public, but the event shut down the Lujan Center for a considerable amount of time as the contaminatoin was cleaned up.

In recognition of his conscientiousness, he received a handwritten note from NNSA Administrator Thomas D'Agostino thanking him for his "excellent work and safety practices," plaudits from Laboratory Director Charlie McMillan during a meeting in his office, and a Laboratory Spot Award.

"I felt it was very important, especially in the immediate aftermath of the event, to 'catch someone in the act of doing something right,' " said McMillan. "Had Gary not done what he did—in fact, what he always does—the contamination would have spread even further."

The Laboratory addressed the root causes of the event. Additionally, as part of the resumption process, several radiological foot and hand monitors are now installed in ER-2 to be shared by both experimental halls.

So, why did Holladay use the whole body monitor when he was in the middle of solving a problem?

It was simply part of his routine and his tendency to err on the side of caution. Flip through the log book and you'll see Holladay is one of only a few people who continued to "portal out" of ER-1 when exiting through the Blue Room, even though the requirement was lifted years ago. This sense of caution was instilled in Holladay in part by (now retired) crew chief Chuck Burns, who encouraged Holladay to self-monitor before heading back to his workstation.

"I'm religious about it," Holladay said. "I look forward to the future, and I don't want to make a mess anywhere." Besides, he noted, the time it takes to prevent a mess is less than the time it takes to clean up one.

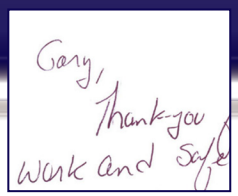
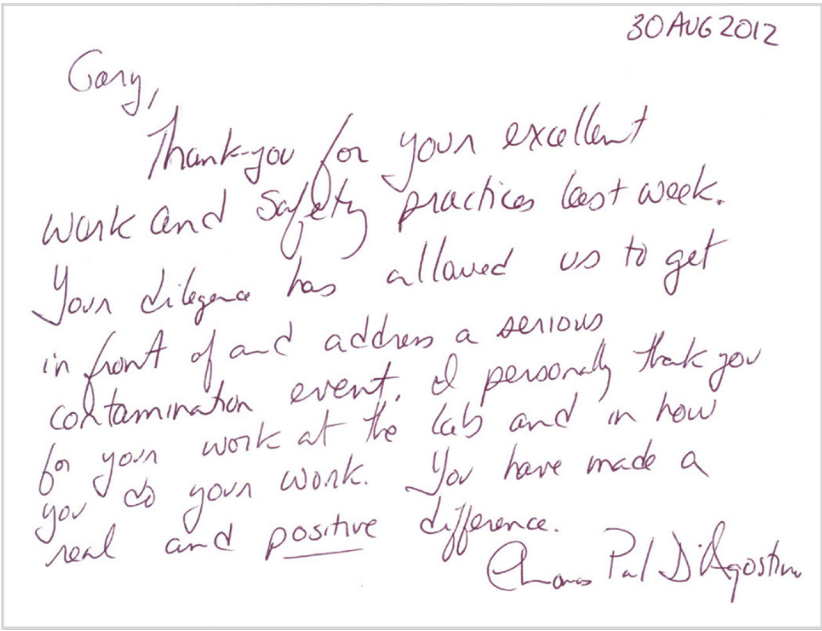


Image: Gary Holladay monitors the beam status in the Central Control Room at LANSCE. (Images by Ethan Frogett)



30 AUG 2012

Gary,

Thank-you for your excellent work and safety practices last week. Your diligence has allowed us to get in front of and address a serious contamination event. I personally thank you for your work at the lab and in how you do your work. You have made a real and positive difference.

Thomas Paul D'Agostino

Image: Holladay's note from NNSA Administrator Thomas D'Agostino.

Claire White Selected for Outstanding Student Research Prize

Claire White (Lujan Center) received the first-ever-awarded Prize for Outstanding Student Research from the Neutron Scattering Society of America. The Society created the award to recognize graduate and undergraduate students performing exceptional research in North American neutron facilities. A committee of experts in the field of neutron science reviewed the nominations. White will also receive a $1,000 honorarium during the American Conference on Neutron Scattering in Washington, DC.

White is a former Lujan Neutron Scattering Center user and a current Director's Postdoctoral Fellow at the Lujan Center and T Division. The Neutron Scattering Society cited her for "pioneering a new methodology to elucidate accurate structural representations of complex materials by combining neutron diffraction and computational chemistry."

The award is based on research she performed as a graduate student at the University of Melbourne, Australia, in the Geopolymer and Minerals Processing group. She helped develop "geopolymers," a greener class of concrete capable of replacing conventional cement-based concrete, which accounts for 5%–8% of all human-produced CO_2 emissions. White combined neutron diffraction and computational chemistry to analyze metakaolin, a cement additive and geopolymer precursor. With this new methodology, she showed for the first time that metakaolin contains Institut Laue-Langevin (ILL)-coordinated Al, an uncommon and highly strained local environment. A more accurate understanding of the nanostructural behavior of geopolymer precursors and concrete enables White and her collaborators to begin to answer key questions regarding the long-term performance of this important alternative concrete.

In 2009, she used the Lujan Center's NPDF and HIPD to help generate new tools that can produce higher-quality total scattering data. The tools remove the incoherent scattering contribution from elements such as H. White, who has a doctorate in chemical engineering, continues to study the nanostructure of geopolymers. She uses computational methods and a variety of experimental techniques, many of which are based at the Lujan Center.

Image: Claire White

Saurabh Singh Chairs Session during the American Conference on Neutron Scattering

Saurabh Singh, a postdoctoral fellow at the Lujan Center, chaired a session on "Lipids and Membranes" at the American Conference on Neutron Scattering (ACNS 2012). The Neutron Scattering Society of America sponsors the ACNS to promote and broaden the use of neutrons in science and technology and to integrate neutron scattering scientists in a wide spectrum of disciplines. The National Institute of Standards and Technology hosted the conference in Washington, DC, this year. The ACNS attracts scientists from around the globe.

Singh received his PhD in biomedical engineering from Texas A&M University. Since beginning his research on neutron reflectometry in December 2011 at the Lujan Center, he has contributed to neutron scattering investigations of soft condensed materials, including biointerfaces. During his short tenure at LANL, he has coauthored three journal articles and steered (with Ann Junghans) the use of poly-electrolyte films in biostructures. His research focuses on the fabrication of multifunctional nano-films using self-assembly techniques.

Image: Saurabh Singh

AOT Student Wins Award for Engineering Research

Nicholas Brennan (Radio Frequency Engineering, AOT RFE) is the recipient of a 2012 Student Symposium outstanding presentation award for work that could lead to improved performance and reliability of the LINAC at LANSCE. His mentor is John Lyles (AOT-RFE).

In his technical talk, "Optimizing the Performance of a 3-Megawatt VHF Amplifier," Brennan described a method for validating a replacement 201-MHz amplifier system for the DTL, an essential part of the LANSCE accelerator restoration project.

A 3-MW prototype of the diacrode amplifier system currently is undergoing testing at LANSCE.

A visiting graduate research assistant, Brennan built upon a 3D electromagnetic model that he developed last summer. He extended the model to include the entire amplifier. The amplifier now has higher efficiency and power gain because he refined design features of the input cavity using simulation software. In the past, design features were adjusted solely by empirical testing.

Brennan studies electrical engineering at Texas A&M University.

Image: Nicholas Brennan and John Lyles.

Elena Fernandez Receives 2012 APEX Award of Excellence

Elena Fernandez, Senior Public Information Specialist (LANSCE DO), received the 2012 APEX Award of Excellence for the 2010 LANSCE Activity Report. The report was entered in the Annual Reports—Electronic category.

The APEX Awards is an annual competition for communications professionals, such as publishers, writers, and designers who create print, Web, electronic, and social media. "The twenty-fourth annual awards program recognized excellence in publications work by professional communicators. APEX Awards are based on excellence in graphic design, editorial content and the ability to achieve overall communications excellence. With close to 3,400 entries, competition was exceptionally intense." - John De Lellis Editor and Publisher

Fernandez is deployed from NMSU on a special contract with LANSCE and has worked with LANSCE since December 2010. Her work with LANSCE has already resulted in a 2011 APEX Award of Excellence for the 2011 LANSCE School on Neutron Scattering.

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

This is Fernandez's sixth APEX Award of Excellence.

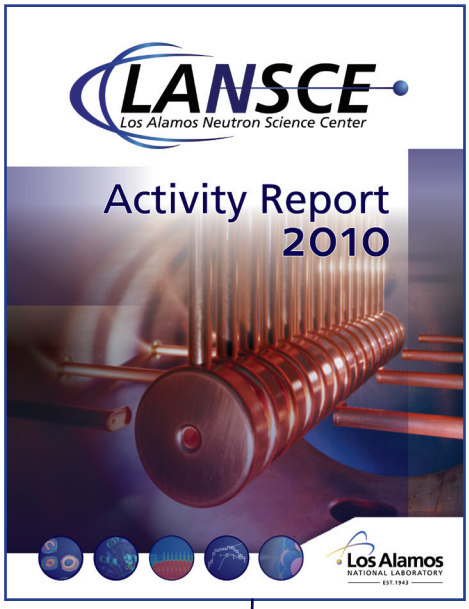


Image: Cover of LANSCE Activity Report 2010

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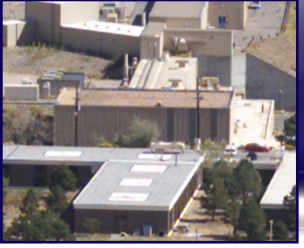

Acknowledgments

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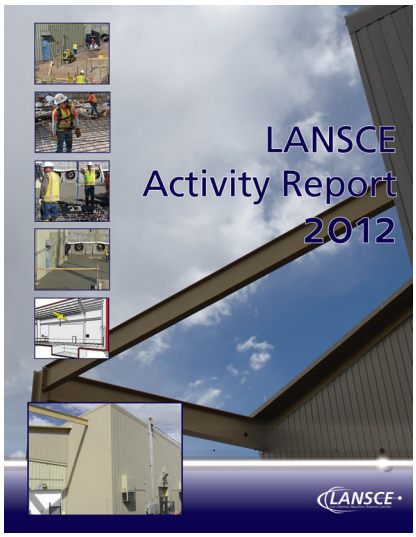
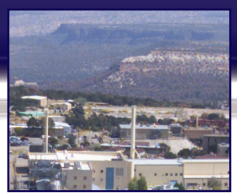
This is the twelfth report in this series.

About the Back Cover

From excavation to completion—the new WNR building provides a special flight path essential to the success of the Chi-Nu experiment. The new 30-Degree Flight Path doubles the capacity to accommodate industrial users.





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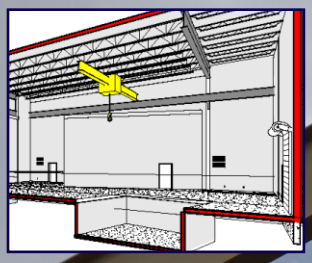

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