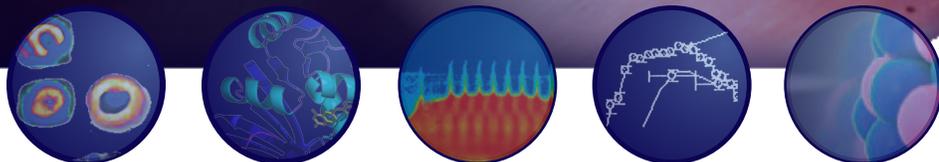
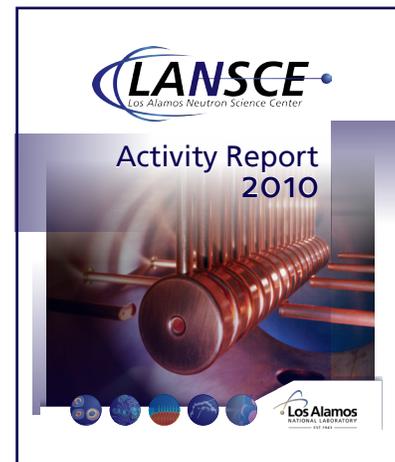


Activity Report 2010



About the Cover

A section of the copper drift tube sits within the LINAC, the core of LANSCE, which uses the RF frequency to accelerate ions. After they leave the injector, the two ion beams are merged, bunched, and matched into a 201.25-MHz drift-tube LINAC for further acceleration to 100 MeV.



LANSCCE Activity Report 2010

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

Abstract

The Los Alamos Neutron Science Center (LANSCCE) Activity Report describes scientific and technological progress and achievements at LANSCE during CY10. This report includes a message from the LANSCE Division Director, a message from the LANSCE Deputy Division Director, LANSCE research highlights, accelerator operations highlights, and user program accomplishments.

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

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Forward

Colleagues,

We are pleased to present to you the 2010 LANSCE Annual Activity Report. This issue will cover major activities and accomplishments during CY2010. As you will be able to see, 2010 was another very successful year for facility-wide improvements and user activities. Among some of our major accomplishments, the completion of the multi-year, multi-million dollar Mark III spallation target was a great success! Due to its innovations, compared to its Mark II predecessor, increased performance has already been observed to several LANSCE-Lujan Center instruments with an overall positive impact to the user community.

NNSA continues to invest in LANSCE's infrastructure. The LANSCE Risk Mitigation project (RLM) began in FY10 and will address a full LINAC modernization. Major beam delivery components of the accelerator will be improved, increasing reliability to all facilities.

During the 2010 run-cycle, the LANSCE-LINAC provided world-class reliability numbers ranging from 85% to 93%. Combined with our unique instrumentation, and technical & scientific talents, LANSCE facilities successfully hosted basic and National Security work.

LANSCE's capabilities continued to deliver a broad science portfolio such as: revealing the first structural details of an HIV-related protein, Nuclear cross-sections, and studies deemed fundamental in modeling nuclear systems in nuclear power reactors. Additionally, we have made a paramount contribution to LANL's hydrodynamic computer codes by investigating high-speed surface dynamics using pulsed proton beams.

2010 was another productive year for LANSCE and its user community. We hope you enjoy reading as much as we did preparing the report.

- *Alex Lacerda and Kurt Schoenberg*



Alex H. Lacerda
Deputy Director, LANSCE



Kurt F. Schoenberg
Director, LANSCE

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Los Alamos Neutron Science Center

Today, five state-of-the-art facilities operate simultaneously at the Los Alamos Neutron Science Center (LANSCCE), contributing to National Security, nuclear medicine, materials science and nanotechnology, biomedical research, electronics testing, fundamental physics, and many other areas. During eight months of the year, while the accelerator is operational, scientists from around the world work at LANSCCE to execute an extraordinarily broad program of defense and civilian research.

LANSCCE is one of the major experimental science facilities at Los Alamos National Laboratory (LANL), underpinning the Laboratory as a world-class scientific institution.

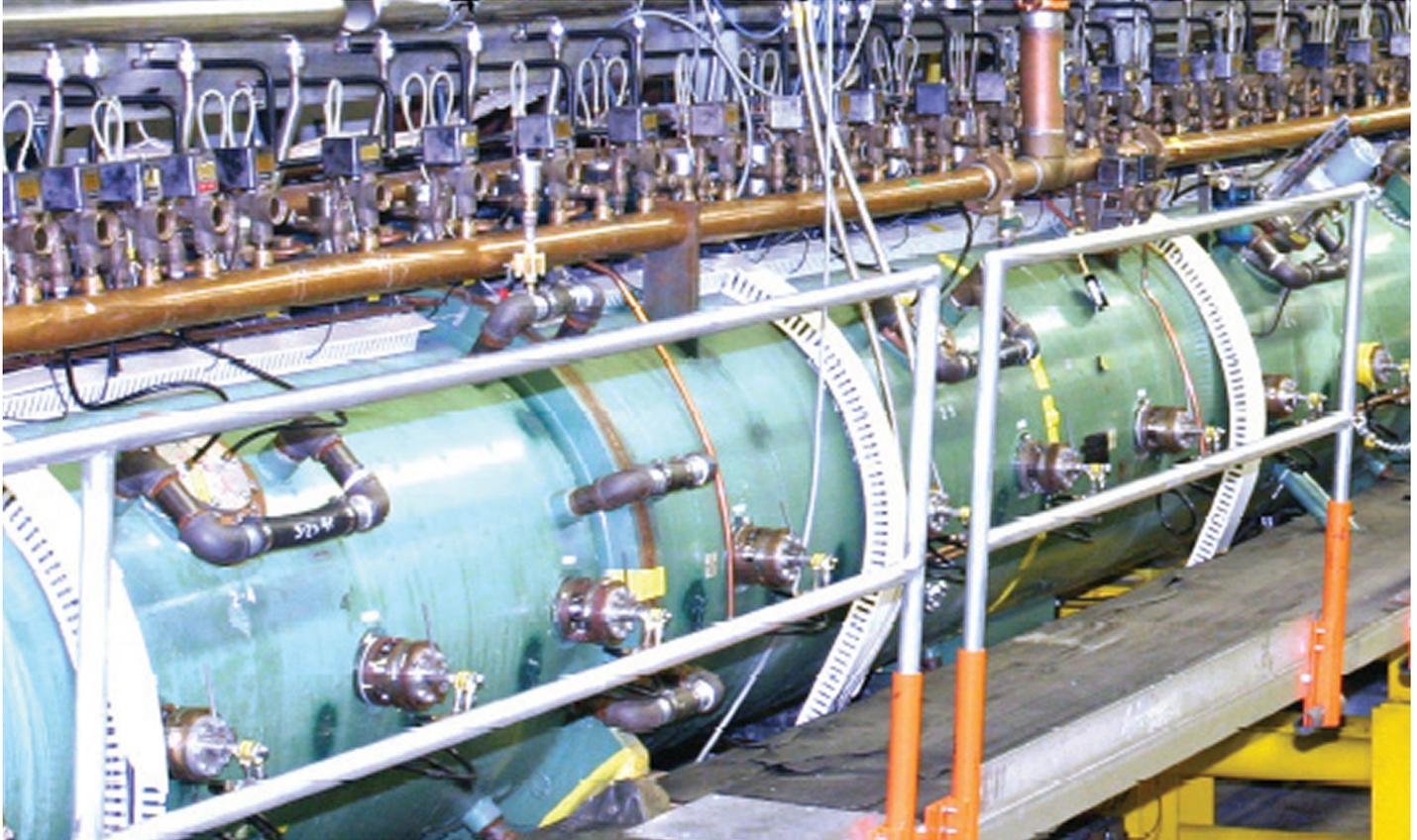
LANSCCE provides the scientific community with intense sources of neutrons with the capability of performing experiments supporting civilian and national security research.

LANSCCE 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 LANSCCE helps to maintain the nation's nuclear deterrent, counter the spread of weapons of mass destruction and lays the foundation for many of the products we use in our daily lives by supporting materials sciences and technology.



 Aerial view of LANSCCE's mesa

The LANSCCE Risk Mitigation Project



The LANSCCE-Linac Risk Mitigation project (LRM) is intended to replace obsolete and end-of-life equipment at LANSCCE and to provide new capability. To date, it has received funding of \$39.3M and our agreement with the National Nuclear Security Administration (NNSA) represents a total investment of \$250M over 10 years, beginning in FY10.

The core elements of the first phase of the LRM project are the RF system upgrade, accelerator system upgrades, and improvements to the integration and control systems. These upgrades emphasize early restoration of 120 Hz operation for the LANSCCE facility. This will be of significant benefit to the Weapons Neutron Research facility, increasing the available beam current to that facility by a factor of 2.5.

 Proton Linear Accelerator (LINAC)
The “heart” of LANSCCE is one of the nation’s most powerful LINAC’s.

The near-term focus is two-fold: establish a new vendor pipeline for the 1.25 MW peak power 805 MHz klystrons and develop and install new 201.25 MHz amplifier systems to replace the present systems that limit facility operation to 60Hz. Installation of a modern high-bandwidth fiber-optic control system network commenced in 2010. This network will form the backbone of an upgrade to the LANSCCE Control System that will begin with replacement of the present Master Timer System with a modern event-based system. The electrical and mechanical design of new 201.25 MHz beam position and phase monitor (BPPM) diagnostics modeled on those developed for recent upgrade projects is complete, and fabrication is being pursued. A prototype device was successfully tested during 2010 turn-on as part of the present Delta-T system that is used to set machine energy.

In 2010 a prototype 201 MHz RF final power amplifier (FPA) has been designed and fabricated. Testing also commenced and we are working towards a schedule that has us complete testing in the third-quarter of 2011. The cavity amplifier is designed to generate a 2.5 MW peak and 250 kW of average power. 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 $\frac{3}{4}\lambda$ from the central electron beam region in the tube and the upper slave tuner $\frac{1}{4}\lambda$ from the same point.

A pair of FPAs of this design will be power-combined for each of the three high-power DTL tanks, resulting in significant headroom for both peak and average power over existing 201.25 MHz systems. In addition, as the existing Burle triode systems are replaced, the anode modulators these systems used for cavity field control will no longer be required. This will reduce the number of vacuum tubes in the 201.25 MHz gallery from 24 to 10, and reducing the types of vacuum tubes in use from five to two unique types of vacuum tubes.

The amplifier development schedule is based on replacing the first 201.25 MHz RF station during the FY13 maintenance outage.

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. In service at LANSCE, typical operation is nominally 1 MW peak at a 120 Hz pulse repetition frequency and a 10% RF duty factor. The klystrons

are directly coupled to the accelerating structure without an intervening circulator.



 Prototype FPA assembly TH628 Diacode® under test.

The lifetime of the existing LANSCE klystrons is unprecedented. The average klystron installed on LANSCE had in excess of 125,000 filament hours at the start of 2010. Based on a Weibull fit of our failure data, there is a 50% probability that we will utilize our five existing spare klystrons within the next 3 years.

In 2010, the prototype for the replacement klystron was ordered. The production order for 45 replacement klystrons is planned for early in 2011. These new klystrons will be almost identical in design to the original LANSCE klystrons manufactured in the 1970s by CPI. All physical interfaces and performance specifications are the same. A handful of modifications to address

safety issues and improve reliability were implemented in the new klystron design including:

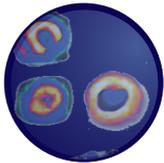
- BeO RF windows are being replaced by Alumina RF windows.
- The X-ray specification for the klystron was reduced to 1 mr/hr for 12 mr/hr, and the radiation shielding is now included as an integral klystron assembly.
- The isolated collector, which had been a source of RF leakage, was eliminated.
- The rubber hoses on the body exterior were changed to copper pipe to minimize water leaks into the modulator tank.

With a successful prototype test in August 2011, Los Alamos will begin receiving approximately two klystrons per month from CPI by December of 2011.

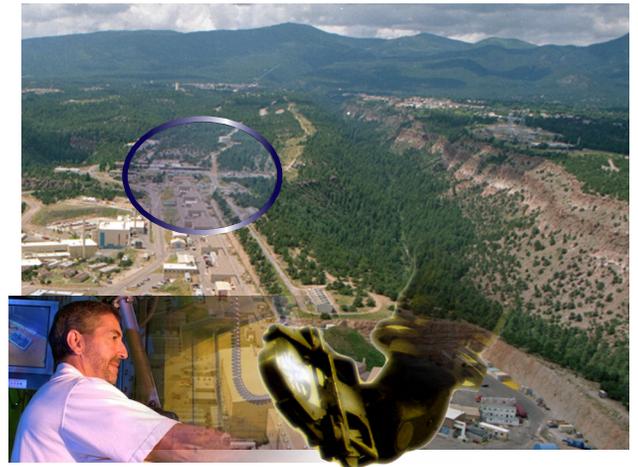
Several new scope elements will be added to the LANSCE Risk Mitigation project. The most important of these is the replacement of the aging Cockcroft-Walton high-voltage injectors with 750-keV radio-frequency quadrupole (RFQ) injectors. Initial conceptual studies indicate that replacement of the H⁺ injector that provides beam for the Isotope Production Facility and the future Material Test Station is straightforward, but that replacement of the H⁻ injector that serves all other experimental facilities may only be accomplished with two RFQs. This is because of the unique micropulse beam structure required by the WNR and proton radiography facilities that is not compatible with the more standard rf structure of the beams for the Lujan Center and the Ultra-Cold Neutron source. A second enhancement under strong consideration is a set of modifications to the Proton Storage Ring (PSR) to enable “pulse-stacking” of WNR-like micropulses on selectable

machine cycles; this capability would significantly enhance the low energy neutron spectra in the 100 keV range at the WNR facility. Required modifications include ring RF bunching, extraction, and kicker systems necessary to direct such pulses “on demand” to the WNR facility rather than the Lujan Center. In FY11, the design effort will start for both the RFQ and pulsed power system that supports the “pulse stacking” concept.

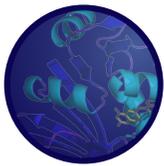
Isotope Production Facility IPF



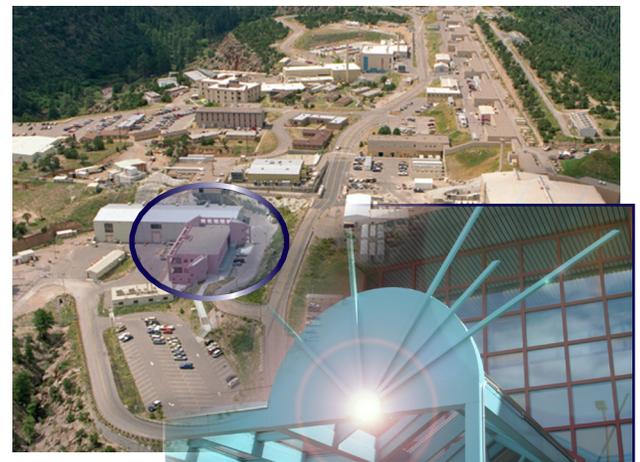
Los Alamos National Laboratory produces radioactive isotopes for medicine and research. The Isotope Production Facility (IPF) at LANSCCE supplies a wide range of radioisotopes to medical researchers all over the world and has been a leader in developing and producing new and unique isotopes for research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



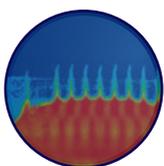
Lujan Neutron Scattering Center Lujan Center



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



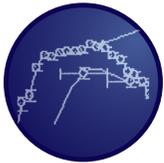
Proton Radiography Facility pRad



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



Ultra-Cold Neutron Facility UCN



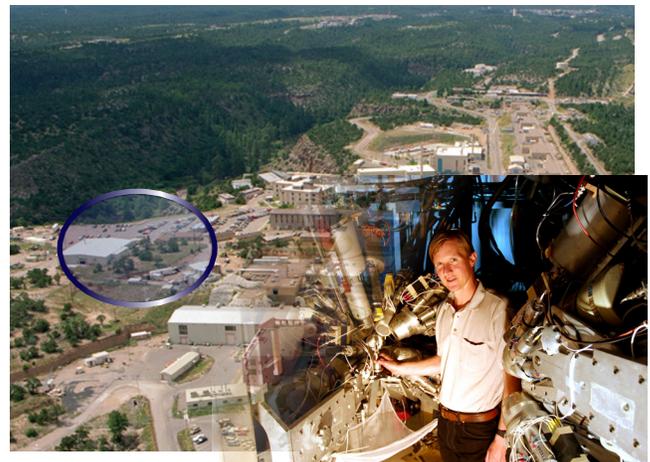
Researchers working at LANSCCE and eight other member institutions of an international collaboration are constructing the most intense source of ultra-cold neutrons in the world, measuring ultra-cold neutron production in their new source for the first time. The ultra-cold neutron extraction port at LANSCCE delivers neutrons from the new ultra-cold neutron source for experiments that could answer questions about the fundamental constants of nature and aid in the quest for new particles.



Weapons Neutron Research Facility WNR



The Weapons Neutron Research Facility (WNR) provides neutron and proton beams for basic, applied, and defense-related research. Neutron beams with energies ranging from 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 the LANSCCE linac. In the Target-2 area (Blue Room) samples can be exposed to the direct 800 MeV proton beam.



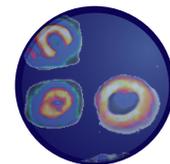
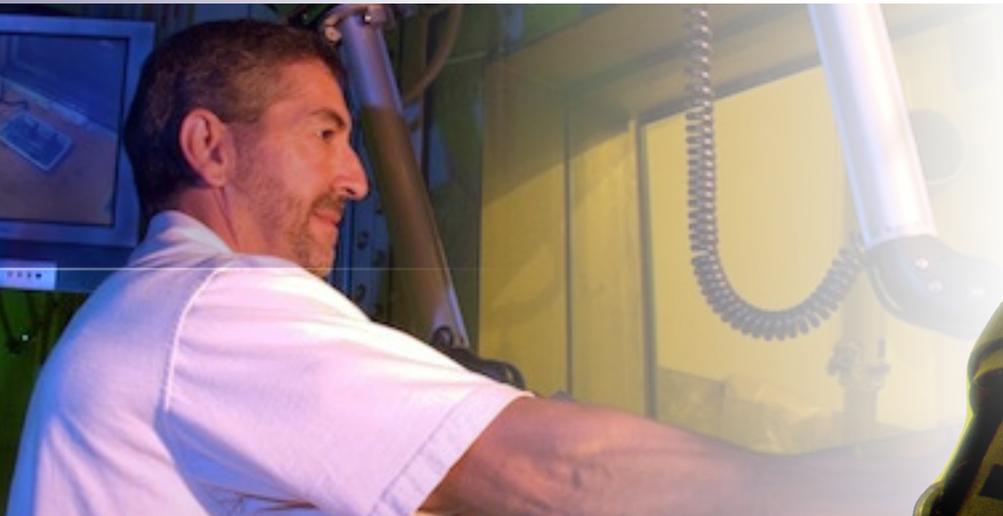
User Program



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

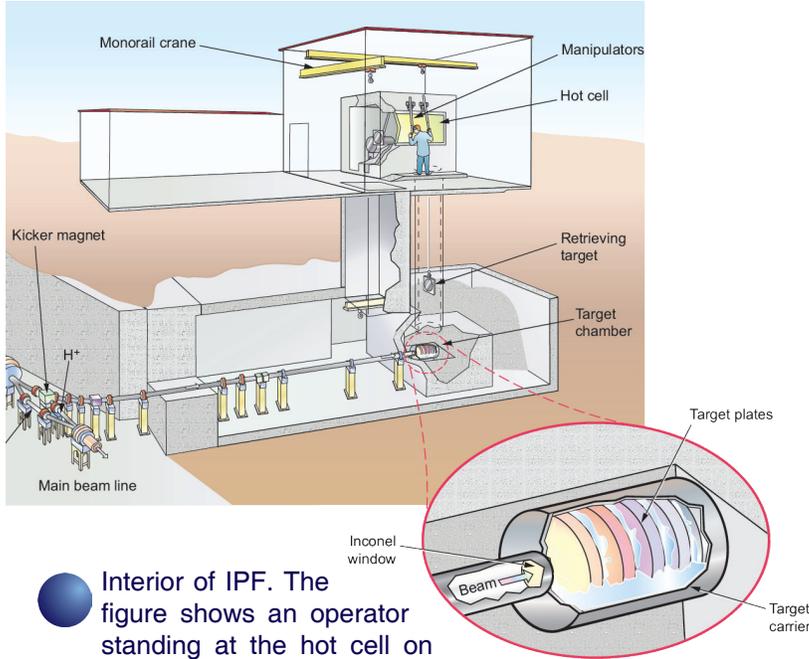


Isotope Production Facility 2010



IPF

Isotope Production and Applications



Interior of IPF. The figure shows an operator standing at the hot cell on the upper level of the IPF, remotely manipulating targets and equipment. The remote-controlled chain-drive shuttle system is visible, and a stack of targets is in the cave on the lower level, being irradiated with protons. The blowup shows the proton beam entering the target chamber through an inconel window and cooling water flowing through the spaces between the stacked targets.



A target stack for strontium-82 and germanium-68 production.

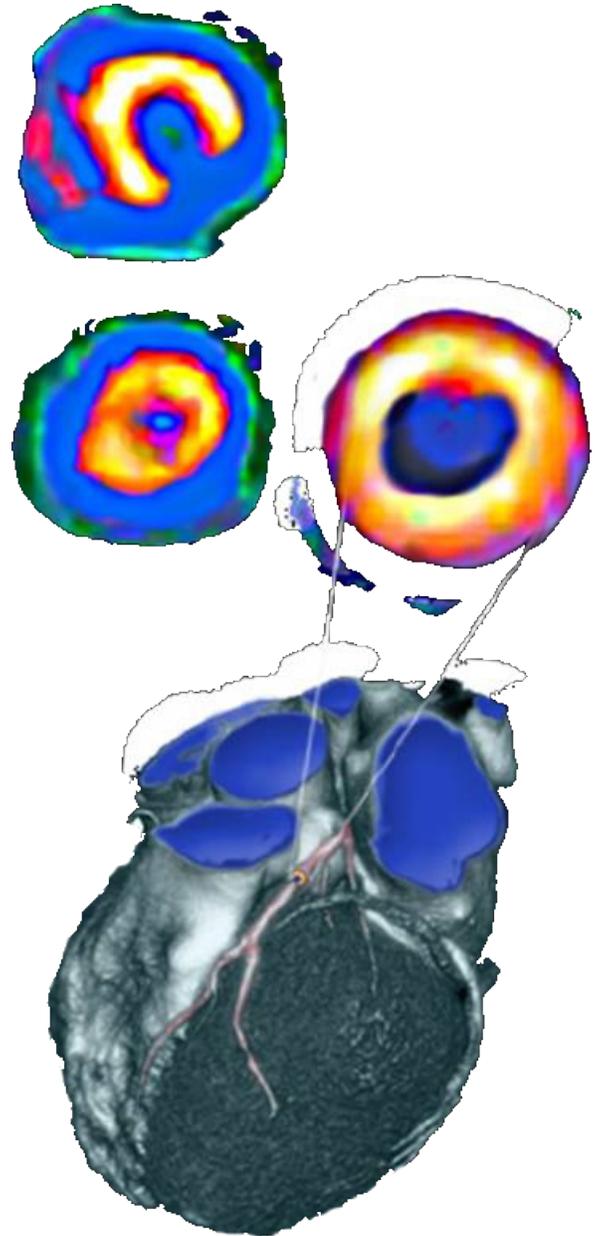
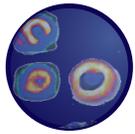


Image of a heart during a normal rest stress myocardial perfusion positron emission tomography (PET) study. Isotopes produced at IPF are critical for medical diagnosis and disease treatment. These PET images were made possible using Sr-82. Production of this critical isotope impacts approximately 23,000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



Nuclear Cross-Sections for Accelerator Production Therapy Isotope

Actinium-225 (^{225}Ac) has extraordinary potential for the treatment of metastatic cancer, and it is one of a few alpha emitters being considered for clinical trials. The isotope decays via four daughter isotopes, each yielding an alpha particle useful for local destruction of tumor sites. The alpha particles could destroy cancer cells while causing little damage to surrounding healthy tissue (e.g., alpha-immunotherapy). However, if brought into use, the demand for this isotope would greatly exceed the current national supply, which is from a single 150 mCi thorium-229 source harvested from uranium-233 by Oak Ridge National Laboratory many years ago. The National Institutes of Health and the Nuclear Science Advisory Committee have identified ^{225}Ac as a critical isotope that requires additional production to address potential use in cancer therapy. Therefore, the DOE Office of Science is funding work at LANL to develop a proof of concept accelerator production process for this important isotope, using proton beams available at LANSCE at IPF and WNR Blue Room.

^{225}Ac can be produced via proton-induced nuclear reactions on thorium-232 (^{232}Th). Other nuclear reactions can also occur; therefore detailed knowledge of the proton energy-dependent cross-sections of all relevant nuclear reactions is needed to develop an accelerator based process to maximize the production of ^{225}Ac and minimize the production of long-lived impurities.

Scientists from Chemistry (C-IIAC and C-NR) and LANSCE (LANSCE-NS) divisions completed the first phase of measuring the nuclear cross sections for the accelerator production of ^{225}Ac . The researchers irradiated ^{232}Th foils with 800 MeV protons at LANSCE in the WNR facility, and then transported the foils to TA-48 for gamma counting and alpha assay. They dissolved one of the thorium foils and separated the fractions by

ion exchange for the alpha assay. This complex and time-critical portion of the experiment was executed in early December 2009. Since then,



 Prototype FPA assembly TH628 Diacrode® under test.

the foils and separated fractions have been subjected to continuous gamma and alpha assay to follow the decay of the actinide isotopes of interest as well as as their coproduced fission products. Despite the complexity of the spectra, it is clear that ^{225}Ac is present among the nuclear on deconvolving the spectra to quantify all of the contributing isotopes that were created in the 800 MeV beam and subsequent decay chains.

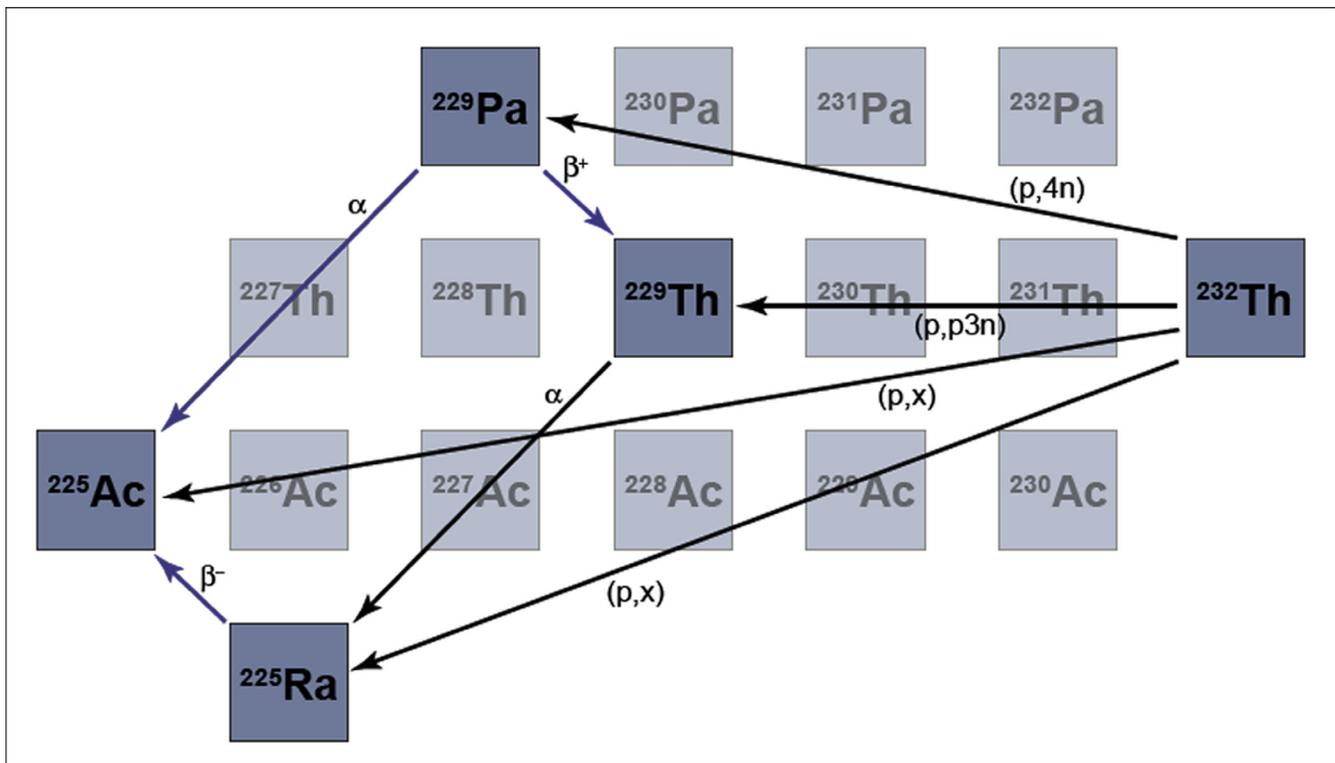
Similar irradiations using the 100 MeV beam at IPF and a specially generated 200 MeV beam at WNR are planned for later in 2010.

Complete data analysis will provide the first set of energy dependent cross-section measurements for this important set of nuclear reactions.

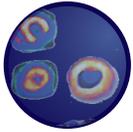
Hong Bach, Mike Fassbender, John Weidner (XTD-5), George Goff, Meiring Nortier (lead), Wayne Taylor, Frank Valdez, and Laura Wolfsberg (C-IIAC); Mike Cisneros, Don Dry, Mike Gallegos, and Russ Gritzo (C-NR); Leo Bitteker, Aaron Couture, John Ullmann, and Steve Wender (LANSCE-NS) are involved in this work.

The DOE Office of Science, National Isotope Program (Kevin John, LANL Program Manager; Wolfgang Runde, National Isotope Program Manager) supports the work. American Recovery and Reinvestment Act stimulus funding through DOE was provided to the LANL Isotope Program to investigate and enhance the isotope production capabilities for ^{225}Ac .

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 Schematic of nuclear reactions of interest (follow arrows) for the production of ^{225}Ac in a thorium target. The blue arrows indicate decay from parent isotopes.



Production Levels:

- Production levels are at an all-time high and anticipated to grow
- Sr-82 shipments expected to exceed 100 Ci in FY11 to meet increasing cardiac demand
- IPF Target R&D will be required to exceed current production capacities in anticipation of future demand In addition to production demands, we have developed a robust R&D portfolio

R&D Portfolio:

- In addition to production demands, we have developed a robust R&D portfolio
- Strong collaborative interactions with Missouri Research Reactor (MURR) staff and students focused on new medical imaging isotopes
- Proof-of-concept Ac-225 production effort for cancer therapy could lead to new university, national lab, and customer interactions
- Anticipate future efforts focused on strengthening university collaborations and leveraging unique capabilities (40 MeV operation of IPF)

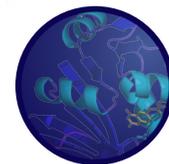
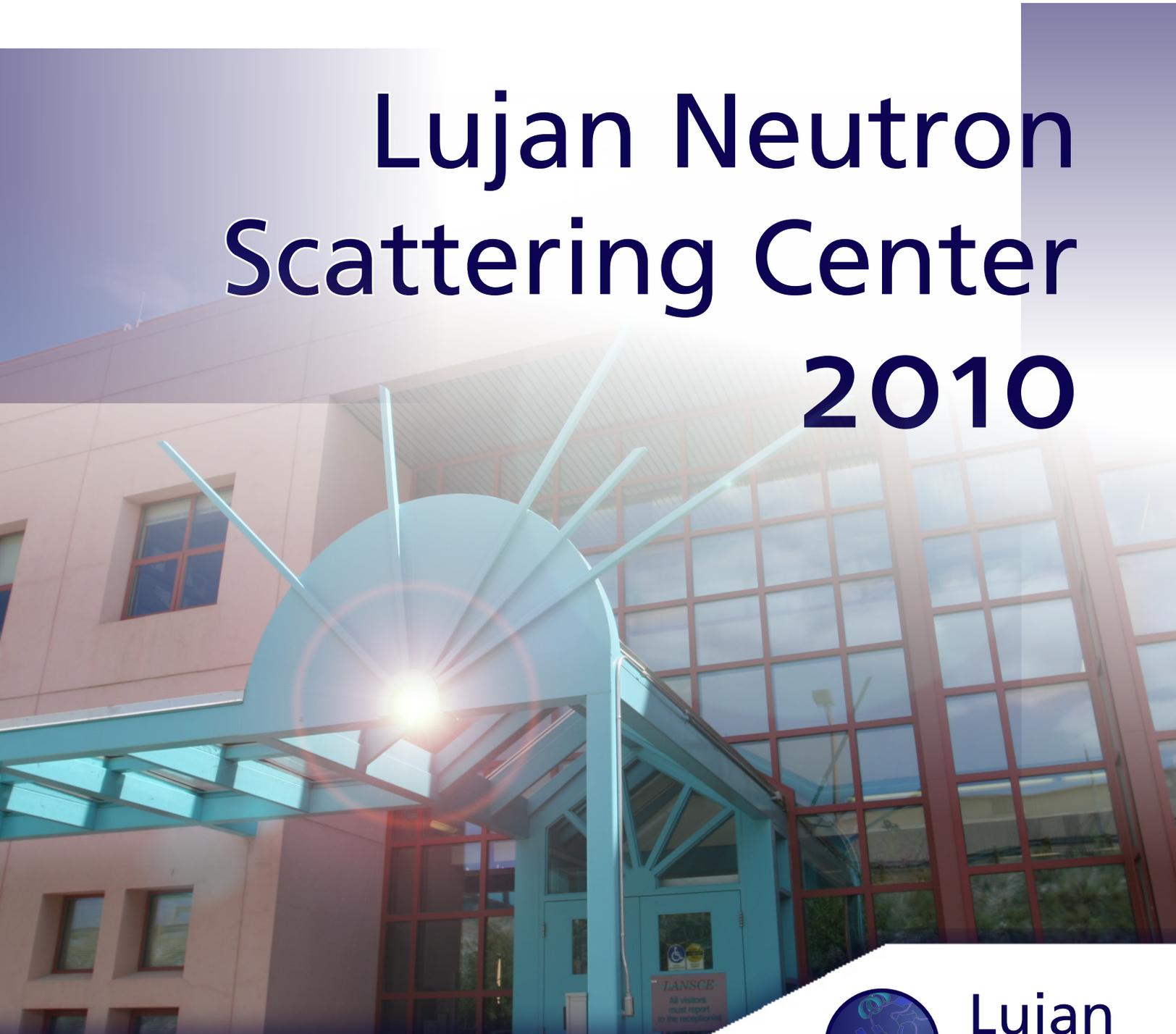
Stewardship of Resources:

- LANL continues to steward resources to insure the reliability and availability of IPF
- FY10 key investments in replacement of IPF beam window and initialization of project to replace the IPF control system [replacement with a standardized Experimental Physics and Industrial Control System (EPICS-based) platform]
- The LANSCE Risk Mitigation project will further steward these resources; careful outage scheduling will minimize programmatic impact

Isotope	Use	# of Shipments	Units Shipped (mCi)
As-73	Environmental Tracer	5	7.19
Gd-148	R&D	1	0.002
Cd-109	X-ray Fluorescence	3	4.20
Ge-68	PET Calibration	58 (26)	11,088 (10,037)
Na-22	Positron Source	1	100
Sr-82	Cardiac Imaging	104 (99)	67,704 (60,912)
Total		172 (140)	78,903.6 (71087.1)

- Sr-82 impacts approximately 20-25,000 domestic cardiac patients each month while LANSCE is in production
- Ge-68 impacts roughly 1M patients annually through PET calibration sources worldwide
- Shipped 172 isotope items; 0 late
- FY 2009 values in *red*

Lujan Neutron Scattering Center 2010



Lujan
Center

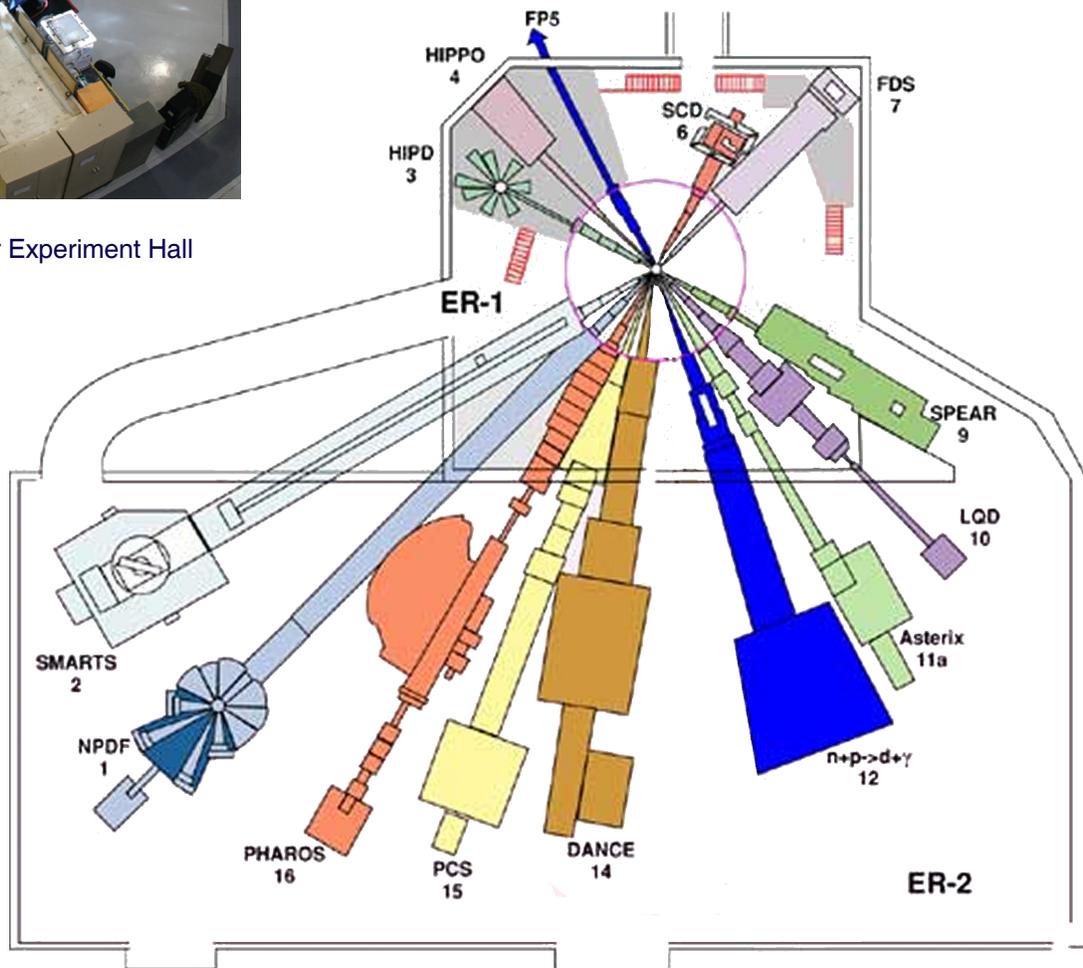
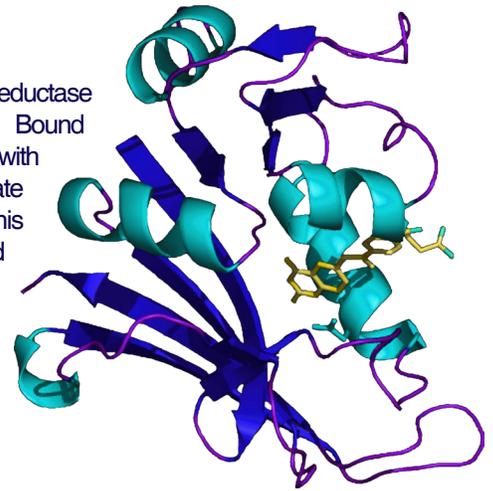


Instrumentation and Applications

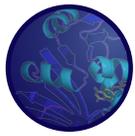


 Lujan Center Experiment Hall

 Figure: Dihydrofolate Reductase with Methotrexate Bound (DHFR). DHFR structure with the anticancer drug methotrexate bound to the active site. This structure was determined using neutron scattering and provides information to improve antitumor therapies.



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



A Nano Look at Ammonia Borane and Hydrogen Storage

Molecular hydrogen is a potential clean energy source for fuel cells if the reactions to store and release hydrogen can be controlled. Scientists investigating ammonia borane (AB) as a high-capacity hydrogen storage agent found that size reduction to the nanometer scale leads to enhanced hydrogen storage properties. When AB is packed into mesoporous silica, it releases higher quality hydrogen at more favorable temperatures than from its bulk form (see figure). Understanding the mechanism for this phenomenon is challenging because the light molecular ammonia borane (NH_3BH_3) nano-crystals must be identified inside the relatively heavy nano-containers of silica (SiO_2).

Hyunjeong Kim, Thomas Proffen (LANSCE-LC) and collaborators from Pacific Northwest National Laboratory and Argonne National Laboratory examined how the nano-size packaging influences the structure and phase transition of AB. The team conducted synchrotron X-ray powder diffraction experiments on AB embedded within mesoporous silica, which contains approximately 4 nm-sized pores. The researchers collected data over the temperature range of 80 K to 300 K at Argonne National Laboratory's Advanced Photon Source. They used a local structural probing technique, called the atomic pair distribution function (PDF), to unravel the X-ray data (see figure).

The scientists found that AB molecules in silica are arranged in a same similar way as in the tetragonal phase of bulk form. However, nano-confined AB loses its well-ordered crystalline character and becomes amorphous above 270 K. Such amorphization occurs at 343 K in bulk form. Confined AB does not undergo the structural phase transition at 225 K that the bulk form experiences. Instead, the molecular crystals retain their tetragonal phase over a temperature range from 110 K to 270 K.

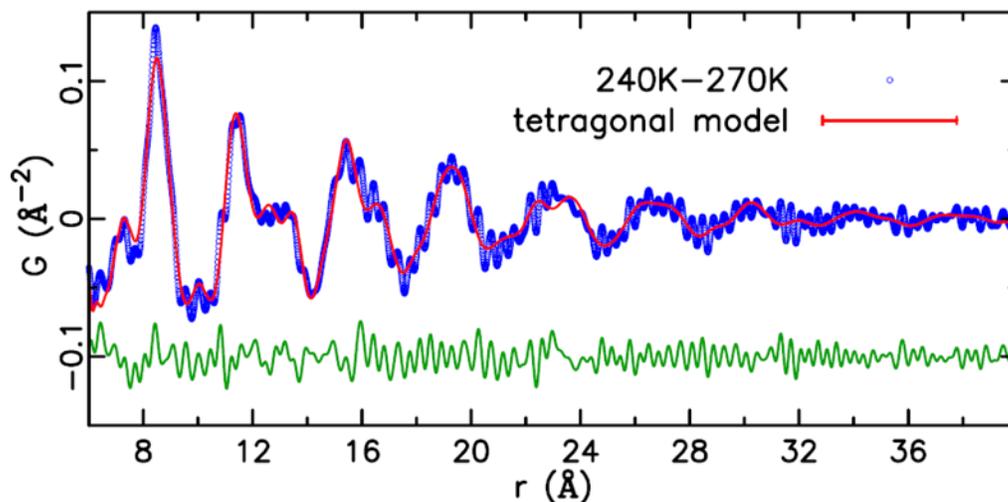
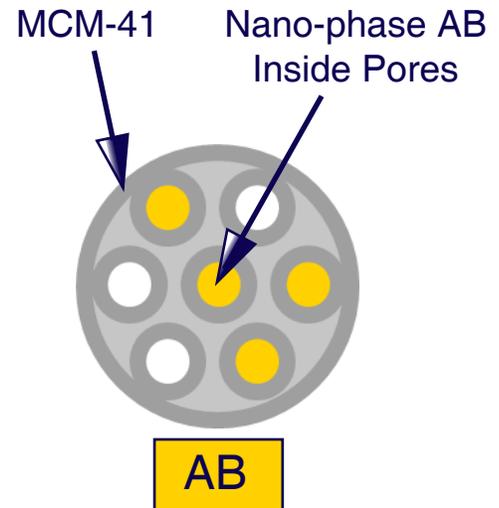
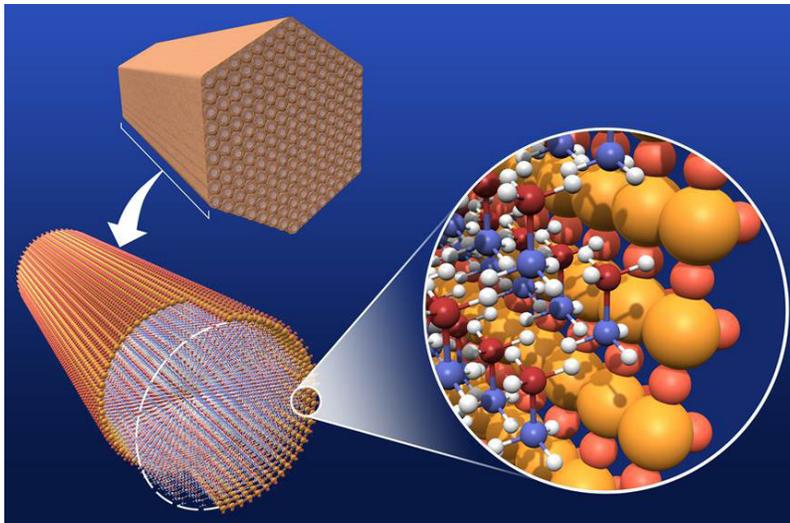
Therefore, less heat is needed to free the hydrogen when AB is confined in the mesoporous silica.

The results of the atomic pair distribution function analysis, combined with their earlier studies, suggest a possible means to control the hydrogen release reaction of hydrogen-rich molecules by the mesoporous silica packaging. The study also demonstrates how the atomic pair distribution function analysis could be applicable to investigate confined species, which cannot be analyzed by conventional structural probing techniques. A broad application of the technique to analyze encapsulated materials is possible.

Reference: "Determination of Structure and Phase Transition of Light Element Nanocomposites in Mesoporous Silica: Case Study of NH_3BH_3 in MCM-4," *Journal of the American Chemical Society* 131, 13749 (2009); doi:10.1021/ja904901d.

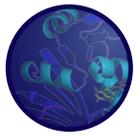
The Lujan Neutron Scattering Center, funded by the DOE Office of Basic Energy Sciences, supported the LANL research.

AOT and LANSCE - The Pulse, May 2010.
LALP-10-020



● Figure: (Top) Schematic of the molecular configuration of the packed ammonia borane. AB is ammonia borane and MCM-41 is mesoporous silica.

(Bottom) Changes in atomic pair distribution functions at 240 K and 270 K (blue open circle) are explained by the tetragonal structural model of bulk ammonia borane (red solid line). This indicates that ammonia borane inside MCM-41 has a tetragonal structure at 240 K. The structural order is lost at 270 K, and it becomes amorphous. The green line is the difference between observed and measured PDF.



Structural Materials for Nuclear Applications & Highly Irradiated Steels

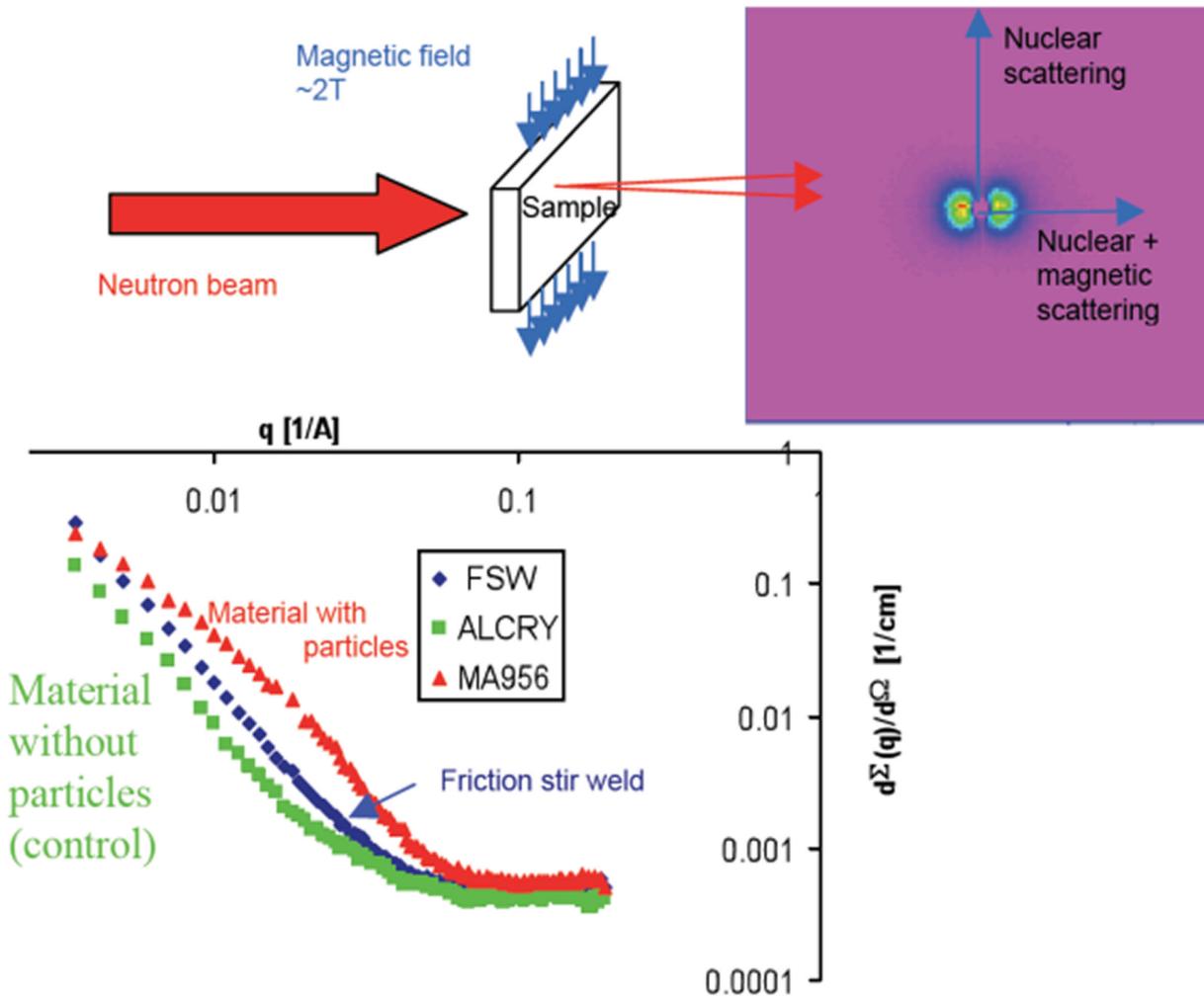
Peter Hosemann, Joris Van den Bosch, and Stuart A. Maloy (MST-8); Amy Clarke (MST-6); Rex Hjelm (LANSCE-LC); and collaborator G.R. Odette (University of California – Santa Barbara) conducted small angle neutron scattering (SANS) measurements on structural materials for nuclear applications. The purpose of this research was to measure particle density and particle size in oxide dispersion strengthened steels and carbide hardened materials, as well as radiation defect clusters and irradiation enhanced precipitation on samples irradiated at the Fast Flux Test Facility.

SANS is currently used to characterize these types of structures at the National Institute of Standards and Technology (NIST), Paul Scherrer Institute in Switzerland, the GKSS Research Centre in Germany, and other research facilities. However, the low Q diffractometer at the Lujan Center is the only SANS instrument using time of flight, which allows scientists to gain additional data without moving the detector. Since the Lujan Center is a radiological controlled facility with well-organized radiological support, researchers are also able to investigate radioactive materials from reactor irradiations. The research using ferritic alloys requires the use of a high magnetic field (approximately 2T) to separate the neutron scattering signal from the magnetic scattering signal. This separation enables good contrast between the matrix material and the features of interest.

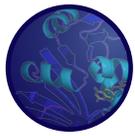
Performing measurements on more than 50 samples at the Lujan Center has established SANS at LANL for this type of purpose.

The DOE Nuclear Energy–Fuel Cycle Research and Development Program (Stuart Maloy, LANL Program Manager) funded the work.

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 Schematic of the experiment and SANS results on a friction stir welded oxide dispersion strengthened alloy (MA956). The reduction in the scattering signal on the welded material leads the scientists to the conclusion that no oxide particles remain after welding.



LANSCCE Helps to Reveal the First Structural Details of an HIV-Related Protein

Jarek Majewski (LANSCCE-LC) and collaborators have used neutron scattering to reveal the first structural details of a key protein found in the human immunodeficiency virus (HIV-1). Their work may have important ramifications for the study of the causes and treatment of HIV.

HIV-1 encodes six accessory proteins, including the Nef protein. Nef is expressed in high concentrations shortly after viral infection, is required for achieving and maintaining high viral loads, and plays a role in AIDS progression. Clinical studies of long-term HIV-infected humans with apparent deletions and/or alterations within the Nef gene showed impaired progression to AIDS. Because the Nef protein is an important factor for the progression of AIDS, obtaining details about its function is extremely desirable. Many of the functions of Nef appear to be structurally driven or intimately tied to conformation and conformational changes. In addition, cell membrane association plays an important role in many of the functions of Nef.

In spite of the wealth of knowledge about what Nef does, there is much less information about how it accomplishes its functions. Knowledge of Nef structure-function relationships both in solution and in association with lipid membranes is important for understanding and combating the actions of Nef in vivo. Such an endeavor requires conformational details about Nef. It has been hypothesized that a transition from a “closed” conformational form to an “open” form enables interaction of Nef with cellular proteins. However, obtaining structural information about Nef, particularly when associated with membranes, is difficult. The full-length Nef protein is partially disordered and contains intrinsically flexible regions.

Neutron reflectometry is one of a few methods that can resolve structural details of membrane associated proteins in physiological conditions. It may be unique in its ability to directly resolve details of the full membrane-bound protein structure. Majewski and collaborators [M. S. Kent and J. K. Murton (Sandia National Laboratories), S. Satija, B. Akgun, H. Nanda, and J. E. Curtis (National Institute of Standards and Technology); C. R. Morgan and J. R. Engen (Northeastern University)] have performed the first in-situ “visualization” of the Nef protein structure interacting with model lipid membrane. The scientists found that the Nef core domain is located within a few Angstroms of the lipid headgroups of the membrane. This result indicates that the Nef protein structure is compact. Analysis involving a simulated ensemble of conformations suggests that the disordered loop extends from the core domain. The researchers conclude that a small portion of Nef’s N-terminal arm inserts into the membrane.

Reference: “A Study of the Conformation of HIV Nef Bound to Lipid Membranes by Neutron Reflectometry,” *Biophysical Journal* in press.

The DOE Office of Basic Energy Sciences supported the Los Alamos portion of the research.

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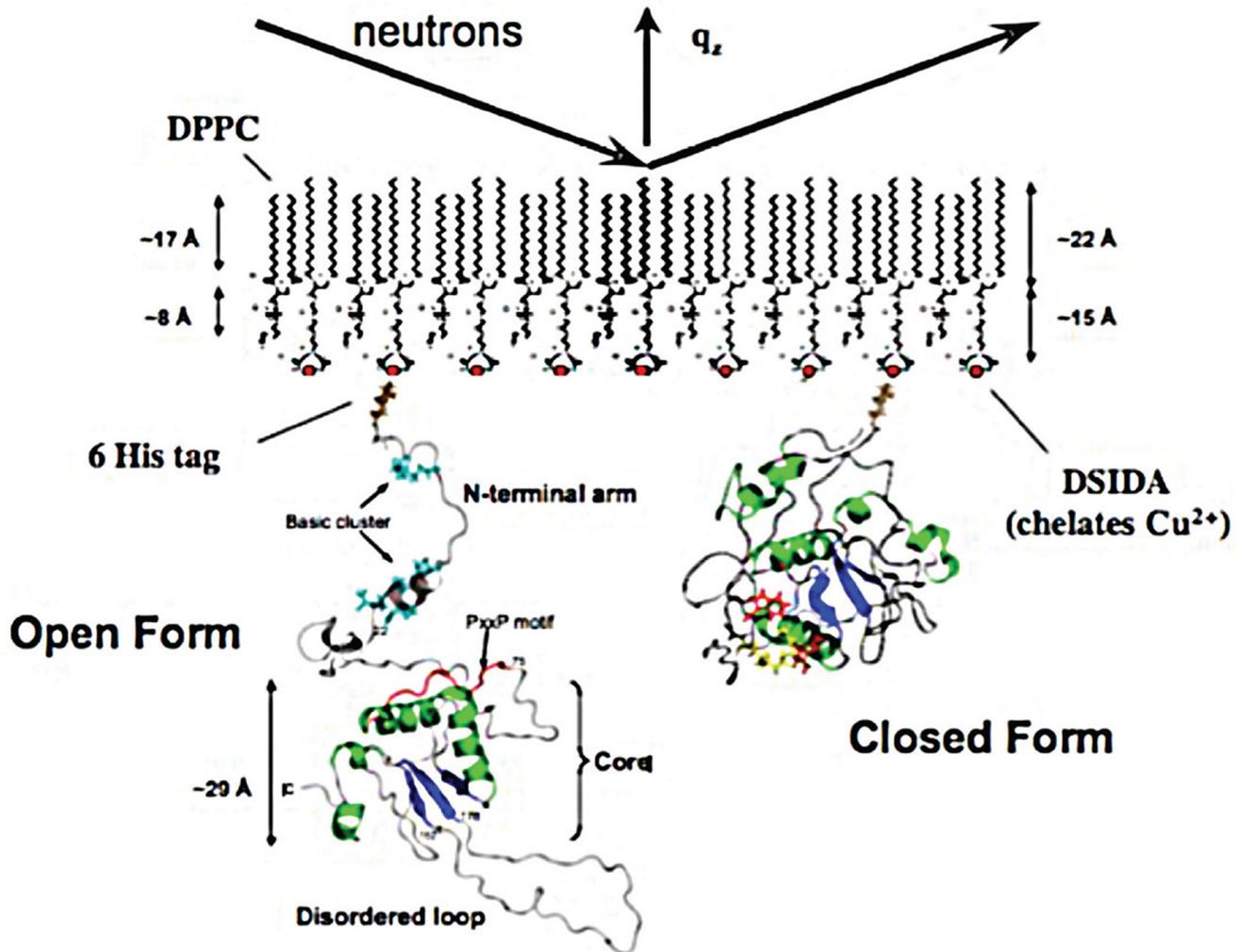
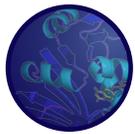


Figure: The model lipid membrane composed of DPPC {1,2-dipalmitoyl-sn-glycero-3-[phosphocholine]} and charged DSIDA (1,2-distearylglycero-3-triethyleneoxideiminodiacetic acid) molecules is created at the air-liquid interface. Molecules of Nef proteins are injected into the liquid subphase, and their structural conformations (here shown in the “open” and “closed” forms) are studied using neutronreflectometry.



Studies of the Mechanism of Mercury Neurotoxicity

Mercury (Hg) is one of the most serious environmental pollutants. Although the acute and chronic effects of mercury toxicity are well known, the mechanism of mercury toxicity at the cellular level is less clear. Because of its significant affinity to thiol (-SH) groups, mercury binds non-specifically to proteins, changing and disabling their functions, which, in consequence, can lead to dysfunctions of the cells, and, at a larger scale, to pathological changes in the target organs. Mercury also interacts with other functional groups. When it reaches different target cells, mercury first must penetrate the cellular membrane barrier to gain entry into the cell. Therefore, the interactions with cellular membrane components are of great importance regarding the molecular mechanism of mercury toxicity.

Jarek Majewski (LANSCE-LC) and collaborators of Jagiellonian University, Poland, report research that sheds new light on the neurotoxic effects of mercury in living organisms. The scientists, with professional advice from the Lujan Center safety officer, Frances Aull (Industrial Safety and Deployed Services, IHS-IS), performed systematic studies applying synchrotron X-ray scattering methods to model membranes containing phospholipid monolayers. They examined the interactions of inorganic mercury salts dissolved in the aqueous subphase with selected membrane phospholipids: dipalmitoylphosphatidylglycerol (DPPG), dipalmitoyl-phosphatidylcholine (DPPC), 1-octadecyl 2-sn-phosphatidylcholine (lyso-PC), and sphingomyelin (SM).

The results show that the elastic properties of phospholipid monolayers are a key factor regarding the interactions with mercury ions. DPPG and DPPC form well-organized, solid-like monolayers in which dense packing of the headgroups limits the possible contact of the donor atoms with mercury ions and reduces the possibility of complex formation. Significant differences occur for phospholipids

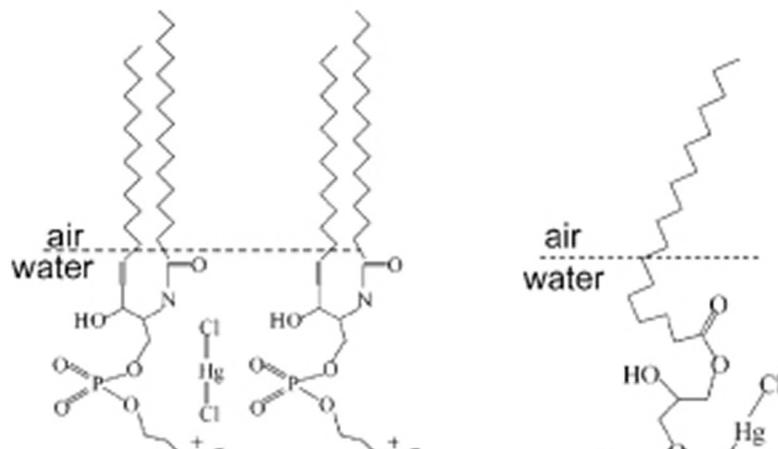
that form more compressible films (SM and lyso-PC), which can complex permanently and accumulate mercury ions at the water/air interface.

The scientists propose a limiting case model for SM in which two SM molecules complex one $\text{Hg}(\text{Cl})_2$. This is an important finding because mercury accumulates in the central nervous system and causes neurotoxic effects. Given that SM is one of the most abundant lipids in the neuron sheath, and it is the main lipid component of the myeline shell, SM can be considered as a target lipid to complex mercury ions.

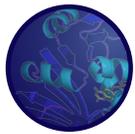
Reference: "Grazing Incidence Diffraction and X-Ray Reflectivity Studies of the Interactions of Inorganic Mercury Salts with Membrane Lipids in Langmuir Monolayers at the Air/Water Interface," M. Broniatowski, M. Flasiński, P. Dynarowicz-Latka, J. Majewski), *The Journal of Physical Chemistry*, in press; doi: 10.1021/jp101668n.

The DOE Office of Basic Energy Sciences funded the LANL work.

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● Complexation of inorganic mercury to (left) SM, and (right) lyso-PC.



Neutron Scattering Reveals Removal of Cholesterol Molecules From Membranes

Cellular membranes contain ordered microstructures, called “lipid rafts,” which display different physicochemical properties from their disordered fluid surroundings. The rafts are vital for a cell’s functionality. These small, closely packed domains of 100-2000 Å contain cholesterol (Chol) and sphingolipids in a molar ratio of 2:1. At this composition, they form a stable complex, which is resistant to many disruptor substances that can disturb the less organized, surrounding domains of biomembranes. β -cyclodextrin (β -CD) is a disruptor that modifies the structure and function of cellular membranes. The external surface of the β -CD is hydrophilic, while its nonpolar cavity can form inclusion complexes. β -CD has applications in many scientific and industrial fields, such as pharmaceuticals, food processing, cosmetics, environmental protection, and biochemical production. Because β -CD has been shown to bind to cholesterol molecules, it has been used to probe the stability of lipid rafts. However, the complexity of the previously investigated experimental systems has made it difficult to assess the effect of β -CD on the structure of the membrane.

Jarek Majewski, student Michael Jablin, and postdoc Manish Dubey (LANSCE-LC); and collaborators from the Jagellonian University (Poland) and Clemson University examined the influence of β -CD on the structure, composition, and reorganization of model membranes composed of mixed sphingomyelin (SM)/Chol bilayers. The scientists created and structurally characterized model bilayer membranes at a solid-liquid interface and subjected them to interaction with β -CD. The model membranes consist of controlled molar ratios of SM and Chol above and below the stable complexation ratio (2:1). The researchers used neutron reflectivity at the Lujan Center’s Surface Profile Analysis Reflectometer (SPEAR) to assess

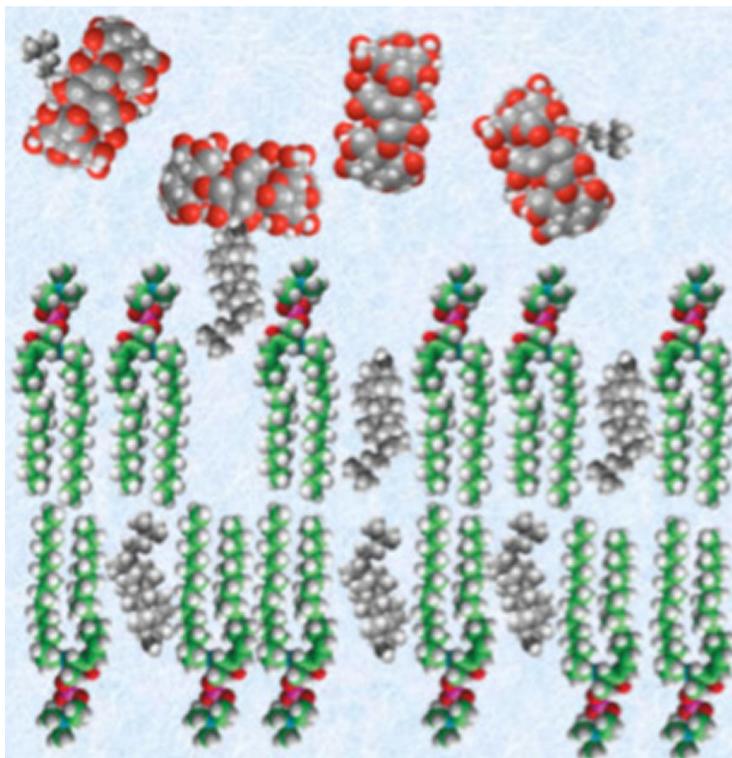
the amount of material removed from the SM/Chol bilayers. Unlike X-ray scattering, neutron reflectivity does not alter membrane structure. These are the first neutron scattering studies of the interactions between β -CD and SM/Chol bilayers.

The scientists demonstrated the presence and stability of the 2:1 sphingomyelin (SM)/Chol complex. While β -CD has no effect on membranes at or above the stable complexation ratio (2:1), it removes all uncomplexed Chol from membranes below the stable complexation ratio. The removal of Chol from lipid membranes shows that β -CD has the appropriate molecular dimensions to form inclusion complexes with sterol molecules. In contrast, double-chained phospholipids have a cross-sectional area that exceeds the dimensions of the β -CD cavity. Therefore, β -CD cannot complex sphingomyelin.

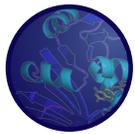
Reference: “Effects of β -Cyclodextrin on the Structure of Sphingomyelin/Cholesterol Model Membranes,” *Biophysical Journal* **99**, no. 5, September 2010 (in press).

The work benefited from the use of the Lujan Neutron Scattering Center, which the DOE Office of Basic Energy Sciences funds.

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● Schematic of selective cholesterol removal. The researchers investigated the interaction between β -cyclodextrin (β -CD, red cyclic molecules) and model membranes containing sphingomyelin (green molecules)/cholesterol (Chol, gray molecules) complexes.



Probing Local Dipoles and Ligand Structure in BaTiO₃ Nanoparticles

Katharine Page and Thomas Proffen (LANSCE-LC) and collaborators Markus Niederberger (ETH Zurich) and Ram Seshadri (University of California–Santa Barbara) have used total scattering neutron pair distribution function analysis to compare the structure of 5 nm particles of the canonical perovskite ferroelectric BaTiO₃ to the structure of the bulk material. The results revealed features of titanium-oxygen distances that are not well probed with X-ray scattering.

BaTiO₃ is a material of scientific interest because its high dielectric constant and room temperature ferroelectric behavior make it ideal for use in electronic components, such as multilayer capacitors and piezoelectric transducers. Moreover, high dielectric ceramics are currently in great demand because they can make materials lighter and smaller. BaTiO₃ has four crystallographic phases, each with a distinct dielectric behavior. Changes in symmetry arise from the displacement of titanium atoms from the center of the oxygen octahedra, causing spontaneous polarization. Ferroelectricity is frequently suppressed in BaTiO₃ architectures with one or more diminished dimensions. Because critical size effects will define the extent to which these materials can be incorporated into future generations of electronic devices, the scientists investigated BaTiO₃ nanoparticles to determine the degree to which these materials can be downsized and remain functional.

The researchers used the Neutron Powder Diffractometer (NPDF) at the Lujan Neutron Scattering Center for neutron total scattering to study the dipole correlations in a sample of freestanding, capped BaTiO₃ nanoparticles. The research addressed structural off-centering, the molecular basis for the existence of switchable dipoles in polar materials, and whether it is turned off when particles become very small. The studies revealed the atomic correlations of the nanoparticle

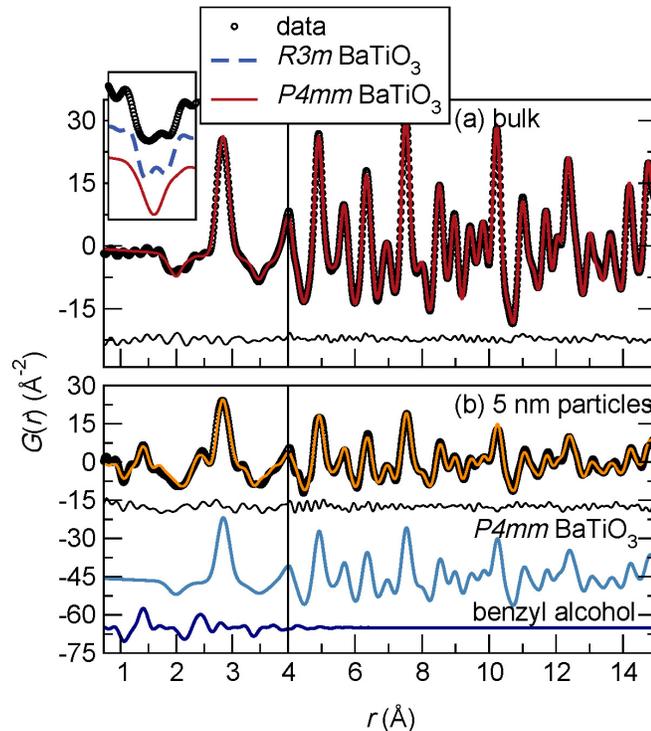
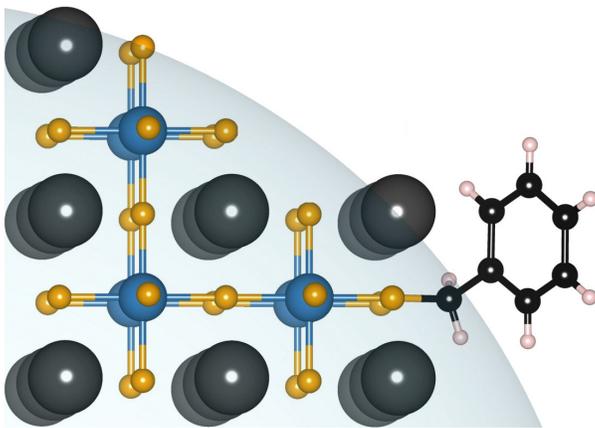
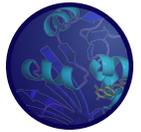
oxide and the capping benzyloxy ligand groups, and allowed careful comparison with the structure of bulk BaTiO₃. Even at these small sizes, titanium is locally strongly off-centered. The results revealed that small BaTiO₃ particles are more cubic, because of decreased dipole-dipole correlations, while retaining the tetragonal distortion similar to bulk BaTiO₃ locally.

The demonstrated probing of both the atomic structure of the oxide core and organic capping components with neutrons heralds a closer examination of other hybrid organic-inorganic systems and the roles that size dependence, defect structure, surface chemistry, and other effects play in determining material properties in numerous functional nanosystems. These effects are of fundamental interest because they will define the extent to which nanomaterials can be incorporated into future generations of electronic devices.

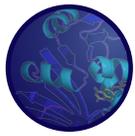
Reference: “Probing Local Dipoles and Ligand Structure in BaTiO₃ Nanoparticles,” *Chemistry of Materials* 22, 4386 (2010); doi: 10.1021/cm100440p.

The DOE Office of Basic Energy Sciences funds the work.

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● Neutron pair distribution function $G(r)$ analysis of (a) bulk and (b) 5 nm BaTiO_3 . Experimental data are displayed as points and fits and differences with lines. In panel (a) bulk BaTiO_3 is well described by the $P4mm$ structure, except for the nearest neighbor Ti–O distance near 2 Å displayed in the inset, which is split in a manner reminiscent of the structure of rhombohedral $R3m$ rather than tetragonal $P4mm$ BaTiO_3 . The peak is negative because of the negative scattering length of Ti. The nanoparticle $G(r)$ requires contributions from $P4mm$ BaTiO_3 as well as benzyl alcohol to fit the experimental data. The schematic image below depicts part of the nanoparticle, near the surface, with a single capping benzyloxy group.



Electric-Field Modification of Magnetism in a Thin Film

Researchers from Los Alamos and the University of California-San Diego used polarized neutron reflectometry to perform depth-resolved measurements of electric field-induced changes of the saturation magnetization in a thin ferromagnetic film. Their results further the understanding of spin electronics, a vibrant field of science and technology due to the strong interplay of electric field and magnetism at nanometer length scales. The findings provide quantitative information to test theoretical models of the magnetoelectric effect.

The use of an electric field (E) to actuate a magnetic response has been limited to materials with low Curie temperatures (T_c) or to low temperatures at which the effect is observable owing to the generally weak interaction between electric field and magnetism. Although T_c of 3d transition metals and their alloys can occur well above room temperature, these materials are conductors. Therefore, the influence of E fields on magnetism is severely constrained. Despite these difficulties, control of magnetism with E fields is attractive, because E fields can be localized to nanometer length scales and require less energy to produce than magnetic fields. An electrochemical cell can be used to influence surface magnetism directly with E fields (see schematic).

Mikhail Zhernenkov, Michael Fitzsimmons, and Jaroslaw Majewski (LANSCE-LC); Jerzy Chlistunoff (Sensors and Electrochemical Devices, MPA-11); I. Tudosa and E. E. Fullerton (University of California – San Diego) modified the magnetization depth profile by applying a large electric field (greater than approximately 10^8 V/m) to the sample surface using an electrochemical cell filled with propylene carbonate electrolyte. The scientists measured the E -induced modification of the magnetic properties of SiO_2/Ta (4.7 nm)/ $\text{Co}_{50}\text{Pd}_{50}$ (18.5 nm) thin films

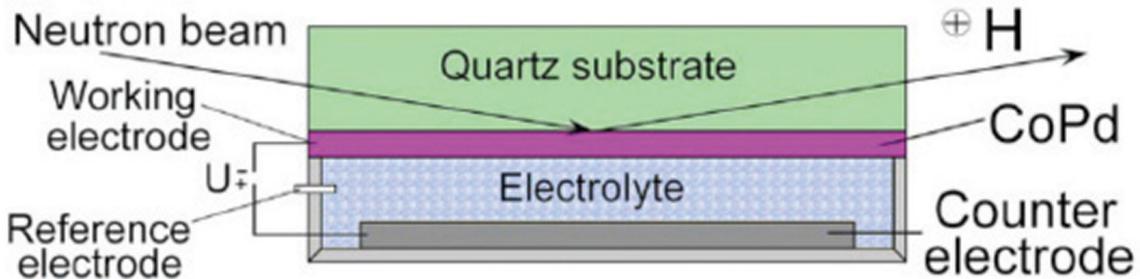
on the Asterix reflectometer at the Lujan Center.

The researchers applied a magnetic field of 3 kOe parallel to the sample's surface. They performed the experiment at three values of applied voltage U in the sequence of -0.32 V, -0.15 V, and 0 V. Analysis of the neutron scattering data revealed a linear increase of the magnetization as a function of applied potential within the top 7.2 nm region of the film closest to the surface. The 7.2 nm thickness of the E -field-affected-magnetic layer is comparable to the magnetic exchange (“healing”) length λ_0 for a wide range of ferromagnets. This result may be a manifestation of the spin-capacitor effect—the change of magnetization due to the accumulation of spin-polarized charges close to the surface. In a ferromagnetic material, the electron density of states near the Fermi surface is spin-polarized. Therefore, the net accumulation of charge due to the applied E field is also spin-polarized. A perturbation to Fermi level may change the net magnetization accordingly (see illustration).

Reference: “Electric-field Modification of Magnetism in a Thin CoPd Film,” *Physical Review B* 82, 024420 (2010); doi: 10.1103/PhysRevB.82.024420 and *Virtual Journal of Nanoscale Science & Technology* (August 2 issue).

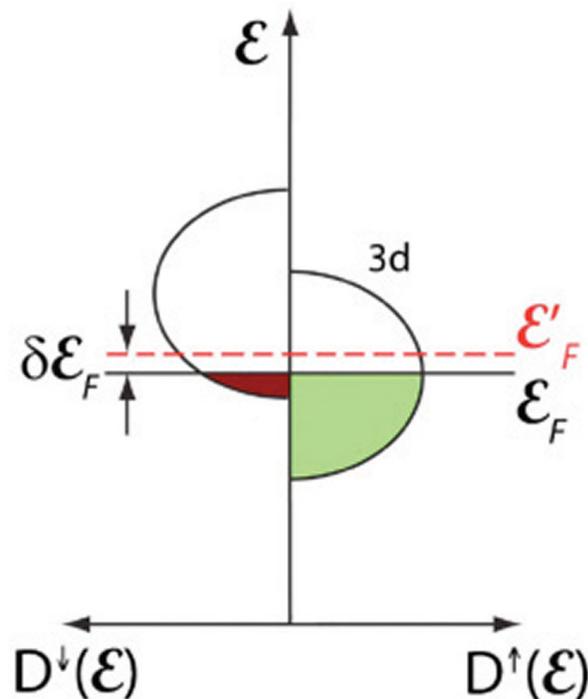
The DOE Office of Basic Energy Sciences funded the work.

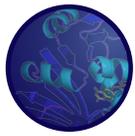
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 Schematic of the electrochemical cell.

 Illustration of the density of states $D_{\uparrow\downarrow}(\Sigma_F)$ of a ferromagnet near the Fermi level Σ_F . The difference of $D_{\uparrow\downarrow}(\Sigma_F)$ integrated from the bottom of the band to Σ_F is the net (spin) magnetization. The integrated densities of the state for spin-up and spin-down electrons are shown by green (right) and red (left) areas. Shift of Σ_F to Σ'_F changes the green and red integrals differently, thus changing the magnetization. With sufficient electric field E , the Fermi level and density of states $D_{\uparrow\downarrow}$ can change the magnetization M .





Discovery of New Physics in Lead-Zirconium-Titanium Voltage Bars

A scientific team of LANL researchers working at the Lujan Center with collaborators from Sandia National Laboratories (SNL) and academia has discovered important new physics in lead-zirconium-titanate (PZT) ceramic voltage bars that scientifically underpins reliable operation of neutron generators. Among the new insights is a neutron-diffraction-based crystal structure that unexpectedly overturns decades of X-ray studies. The increased body of knowledge established through neutron scattering experiments substantially decreases the risk in SNL's neutron generator production.

PZT voltage bars in neutron generators are small prisms of ferroelectric ceramic in which substantial electrical energy can be “frozen” into a low-pressure ferroelectric phase. They are used as an ultra-long-life battery that can be called upon reliably to deliver high voltage and large current on split-second demand under extreme environmental conditions at any time over more than a decade. This voltage accelerates deuterons in the neutron tube—a vacuum tube inside the neutron generator—to high enough energy to produce deuterium-tritium fusion in a tritium-loaded target. The fusion reaction produces copious neutrons. These single-use neutron generators are activated by an explosively driven shock wave propagating along the ceramic bar. At a certain pressure in the shock, the ferroelectric phase transforms to paraelectric and releases massive charge.

As part of nuclear reconfiguration, Pinellas-based neutron generator production was moved to SNL. Meeting annual production goals of SNL's new low-voltage neutron tube relies on synthesis of qualified PZT material. High voltage breakdown, resulting from materials flaws, can degrade the voltage pulse and leave the neutron flux outside design margins.

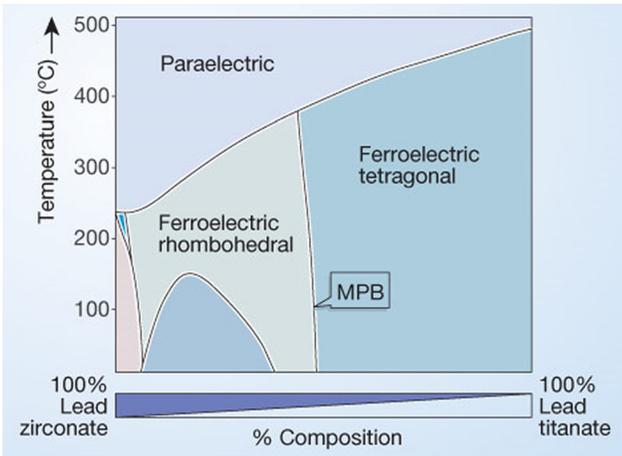
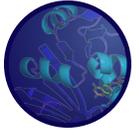
The team used neutron scattering to determine the true crystal structure for doped and undoped PZT. They detected a doubling of the unit cell, which for decades had eluded researchers who used only x-ray scattering to study the material. It is essential to know the precise chemical structure of material in manufacturing.

The team determined the fraction of ferroelastic strain—as opposed to lattice strain—in the PZT phase transition that develops charge in operation. They accomplished these measurements via a unique neutron scattering experiment under load. The team also measured nonideal lattice strain owing to ceramic grain alignment and intergranular stresses. This is the first time that neutron scattering of samples under load, combined with texture analysis, was used to examine ferroelectrics. The team validated the texture description of ferroelectric ceramics by comparing and consolidating measurements with X-rays and neutrons.

These insights inform both operation and production of neutron generators in DOE systems. The impact of this research underpins accelerated design and development of future implementations of this important limited-life component. More specifically, the risk in synthesizing batches of PZT is decreased by knowing the chemical structure and materials microstructure of qualifiable material.

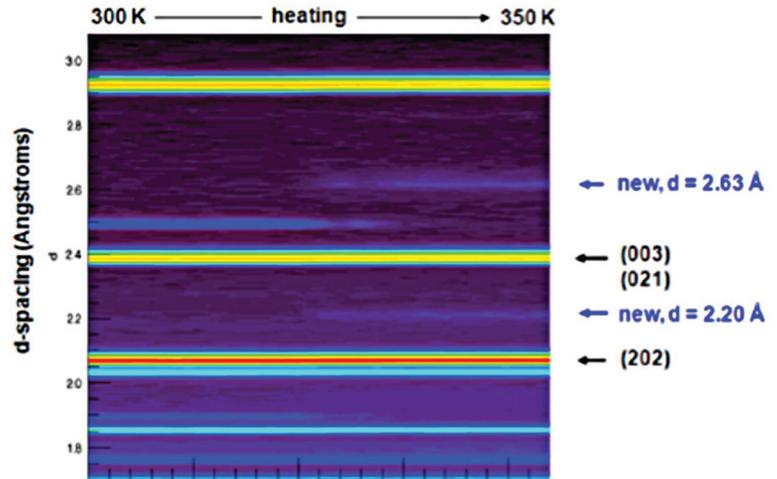
The team: Sven Vogel, Anna Llobet Megias (LANSCE-LC), Mark Rodriguez, Pin Yang (SNL), Jacob L. Jones (University of Florida), and Mark Hoffman (The University of New South Wales), received a Defense Programs Award of Excellence. Jones received a Presidential Early Career Award in Science and Engineering for research on ferroelectric materials, including this work.

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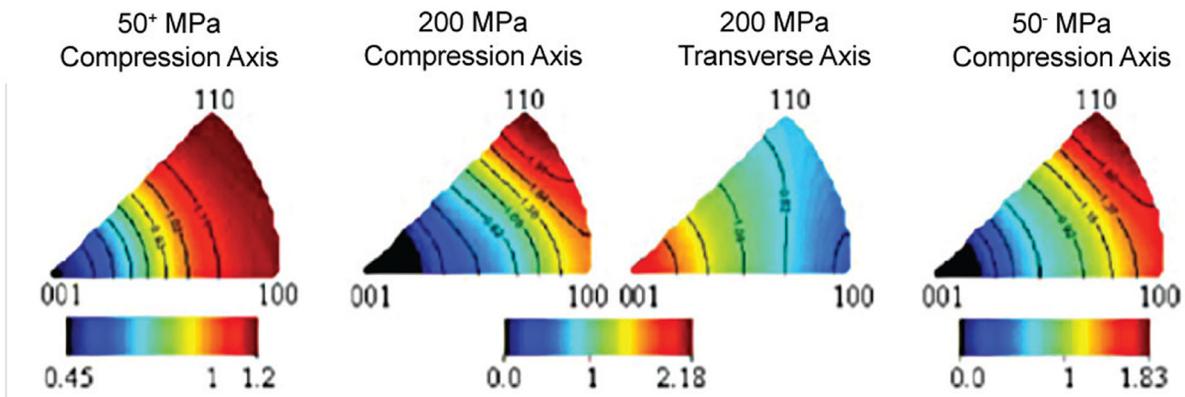


● Phase diagram for PZT ceramic showing the 95/5 composition line (blue dashes). The ferroelectric-to-paraelectric transition is similar to the pressure-driven transition that releases charge in neutron generators.

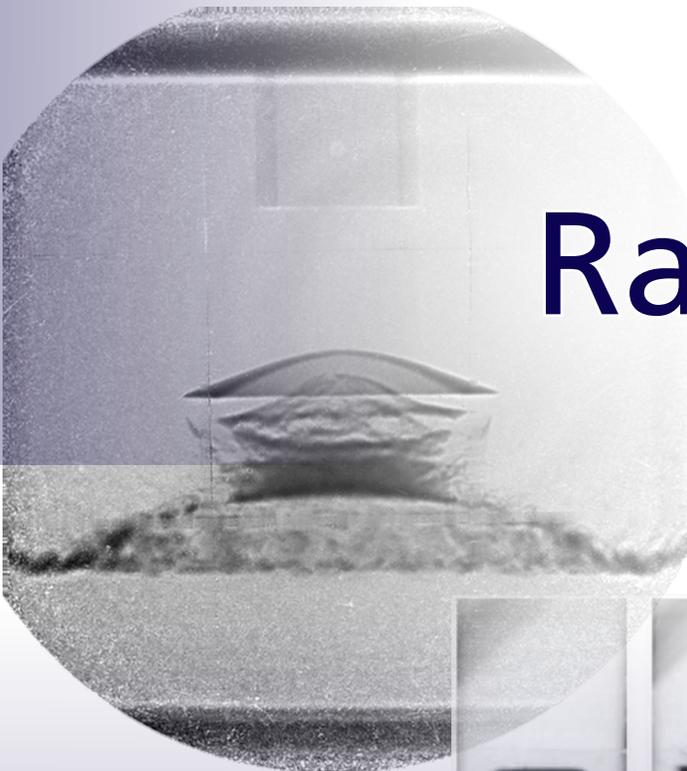
Reference: Materials science: "Lead-free at last," Eric Cross, *Nature* 432, 24-25(4 November 2004) doi:10.1038/nature03142.



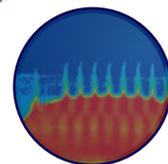
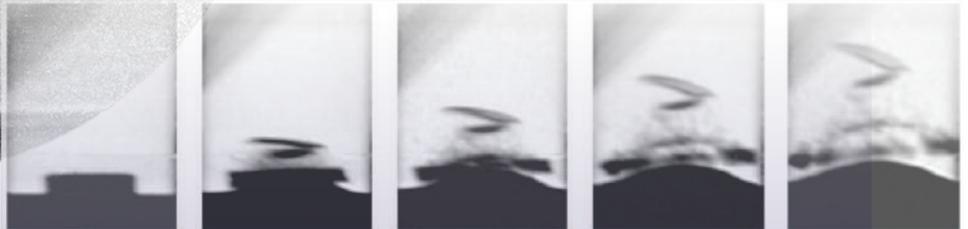
● Niobium-doped PZT 95/5 shows new neutron diffraction peaks when heated through the phase transition, an unsuspected cell doubling. The newly discovered structure of the high temperature phase revises decades of data from X-ray studies.



● Selected tetragonal inverse pole figures (stereographic projection) from neutron scattering are shown of the compression axis and transverse directions. Intensity reflects the diffraction pole density and helps determine the degree of ferroelastic strain.



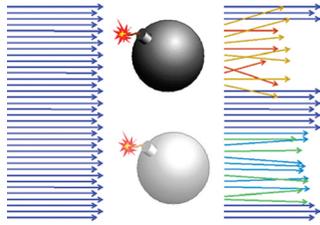
Proton Radiography 2010



pRad

Production

The interaction region is in a containment vessel specially designed to withstand the explosions that occur during experiments. Here, protons pass through the test object. This schematic illustrates (in an exaggerated manner) that protons traversing thicker or denser parts of the object lose more energy and are deflected more than those passing through thinner parts.

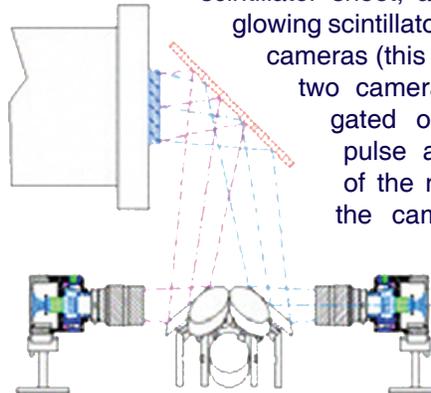


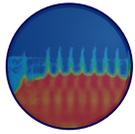
Strong magnets are used as lenses for the proton beam. In this picture, the magnets are the orange blocks—four magnets with drift regions make up one lens that images the interaction region. This imaging process gives protons huge advantages over Xrays for imaging: The image location is far enough from the interaction region that background noise from scattered protons is minimized and explosives from the experiment do not damage the detectors. Different lens configurations can be used to magnify the view— 3x and 7x magnifiers have been built and used at LANSCE. Highly radioactive objects can be imaged without their radiation “fogging” the image.



The magnetic lens system creates an angle-focus (Fourier) plane, a plane in the beam line where undeflected protons pass through the center and protons most deflected by the test object are near the edges of the beam. Introducing a collimator at this point preferentially removes protons that pass through the thickest parts of the object. Changing the aperture of the collimator changes the cutoff thickness—tuning the radiographs to best highlight features from a huge range of object densities from plastics to plutonium.

A gap in the vacuum beam pipe allows the protons to be imaged. The protons pass through a scintillator sheet, and the light from the glowing scintillator is viewed by multiple cameras (this schematic only shows two cameras). Each camera is gated on a different proton pulse and takes one frame of the movie. To the right of the camera station is seen another magnetic lens setup bringing the proton beam to another camera station so it can be imaged again. Currently, pRad is capable of taking 37 images in each experiment.





Study of High-Speed Surface Dynamics Using a Pulsed Proton Beam

Los Alamos is developing and implementing ejecta source and transport models for integration into the Laboratory's hydrodynamic computer codes. The underlying postulate for ejecta formation is that ejecta are produced by a special limiting case of a Richtmyer-Meshkov (RM) instability. Therefore, a key element of source modeling and transport centers on high-explosive shocked-tin proton radiography RM experiments at LANSCE.

The tin targets were machined with sine-wave patterns in the surface to seed the growth of the RM instability. The researchers examined growth of the RM instability into three environments: vacuum, neon (Ne), and xenon (Xe).

The vacuum data in Figure A show that the short-wavelength, large amplitude RM spikes travel the fastest, with the short-wavelength and small-amplitude traveling at a similar yet lower velocity as the long-wavelength and large amplitude. Bubbles are also evident and distinguishable from the free-surface velocity that is determined by the flat regions between the sinusoidal perturbations.

A comparison of the RM instability growth in the three environments shows that the RM spikes in the Ne gas behave much more like the vacuum series than do the spikes in the Xe gas (Figure B). This is interesting because the viscosity of Ne is about twice the Xe viscosity. Moreover, the density of Xe is about five times the density of Ne, so the kinematic viscosity of Ne is about ten times the kinematic viscosity of Xe. This result implies that the Weber number (ratio between the inertial force and the surface tension force) dominates the spike-breakup.

Particle breakup is important to particle transport in gases. Hydrodynamic models predict that the RM spike tips will not continue to grow thinner with time, but they will become blunted due to surface tension. This effect is nominally seen at around 11.6 ms in the vacuum series, which implies that the effect happens in the Ne and Xe series as well. Drag may be stripping liquid tin off the blunted tips, streaming the material toward adjacent neighbors. This assumption is supported by the fact that the RM spikes appear to break up in the middle of the spikes in the Ne gas at time 15.1 ms, and at time 12.1 microseconds in the Xe gas. Close inspection reveals evidence of the mass streaming from the fastest Ne spike tips, in the shape of a mach-stem, to their nearby neighbors at time 11.4 microseconds.

These observations can be used for code validation and verification studies. The collection of results will be used to inform FY10 experimental packages and test the Laboratory's working ejecta model. William Buttler and David Oro (Neutron Science and Technology, P-23), Guy Dimonte (Materials and Physical Data, XCP-5), Chris Morris (Subatomic Physics, P-25), Guillermo Terrones (Safety and Surety, XTD-1), Patrick Reardon and Felix Garcia (Polymers and Coatings, MST-7), and the proton radiography core team performed the work.

NNSA Campaign 1 (Bob Reinovsky, LANL campaign manager) funded the research.

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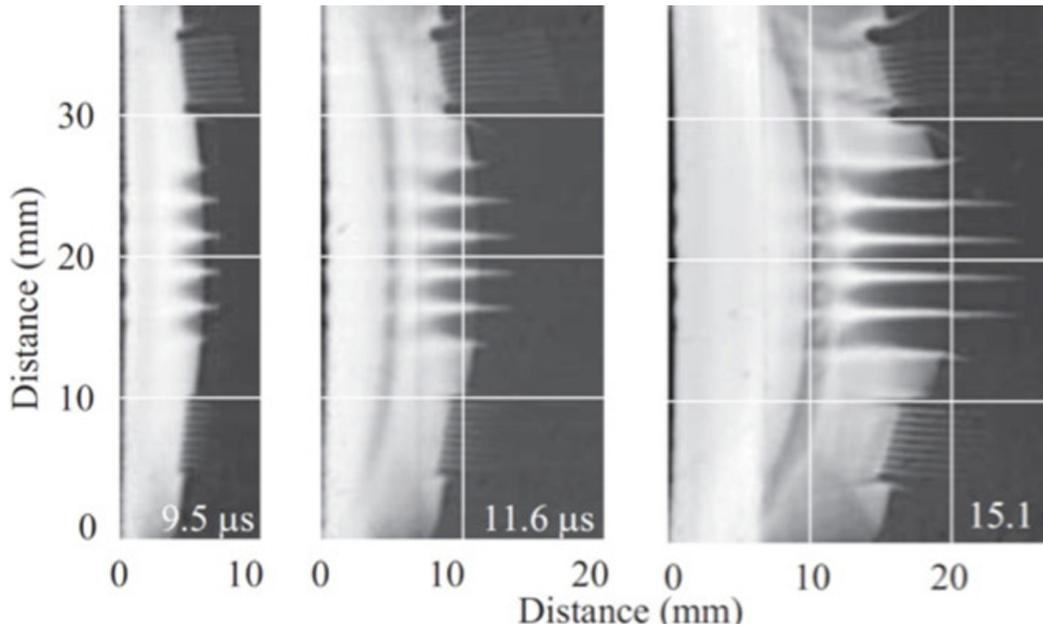


Figure A: Three of nineteen FY09 proton radiography RM images with image times. The instabilities are not fully resolved at this scale and contrast level. Salient features, including bubble and spike positions relative to the flat regions, are evident.

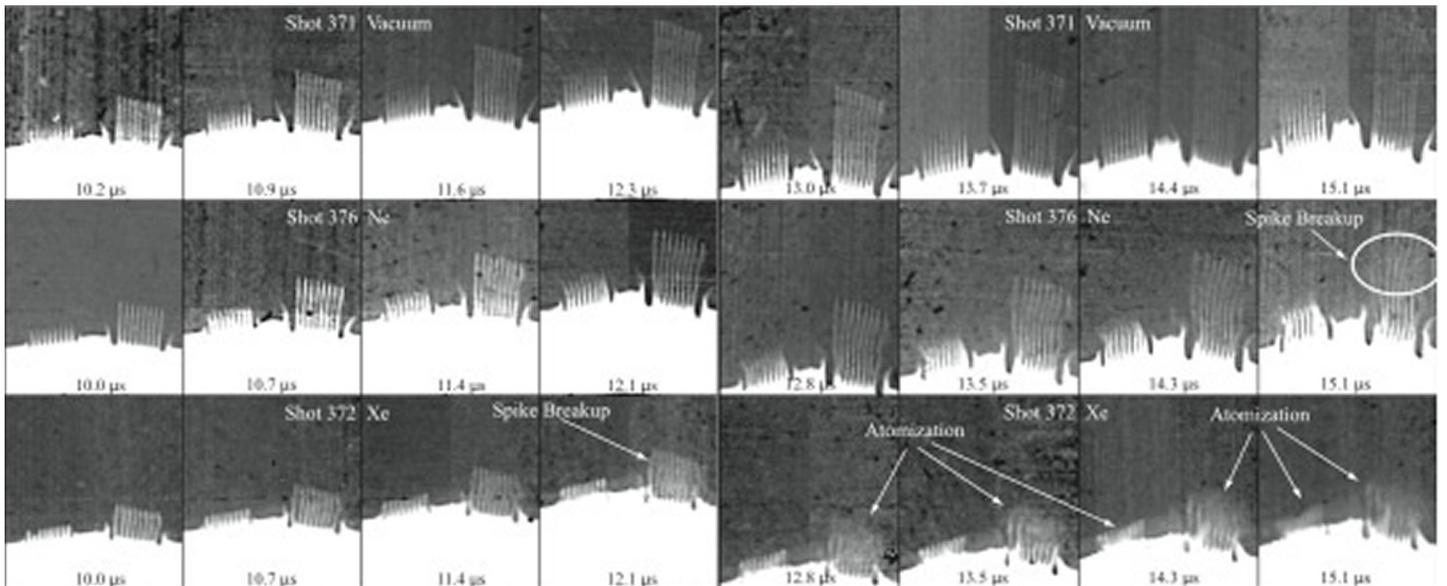
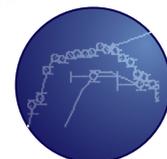


Figure B (right): Vacuum, Ne, and Xe proton radiography RM time-series data, beginning just after shockwave breakout. The tin is fully liquid on release, and the gas pressure was approximately four atmospheres for each pressurized experiment. Image times are closely matched.



Ultra-Cold Neutron Facility 2010

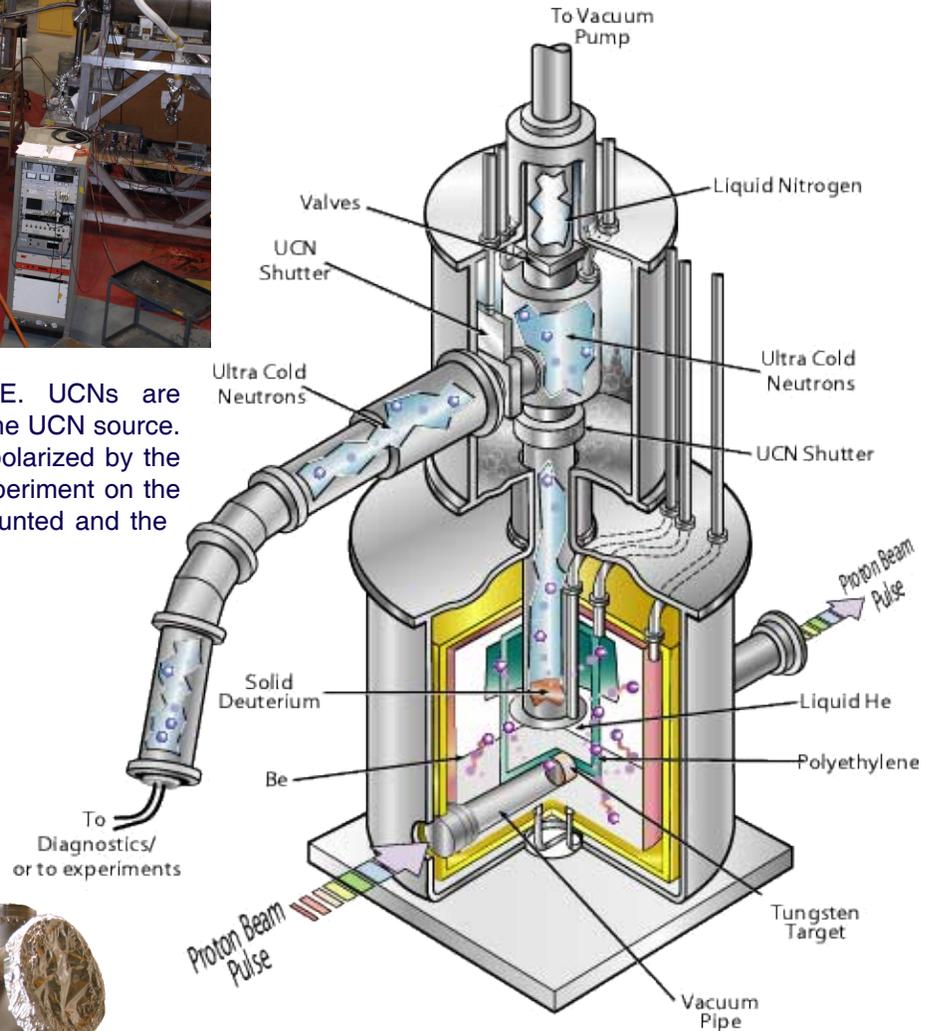


UCN

Production



The UCNA project at LANSCE. UCNs are created by the proton beam and the UCN source. Neutrons are piped across the room, polarized by the central magnet, then trapped in the experiment on the left. There, the decay electrons are counted and the A-correlation is measured.



Photograph and schematic of the ultra-cold neutron source. The neutrons are produced by the LANSCE proton beam striking a tungsten target; they are then moderated to cold temperatures by beryllium and polyethylene, then converted to ultra-cold temperature (~ 1 mK) by a solid deuterium converter. The UCNs are then transported out of the source and through pipes around corners to an experiment.



Ultra-Cold Neutron Accomplishments at LANSCE

The weak nuclear force is one of the four fundamental forces in nature, along with gravity, electromagnetism, and the strong nuclear force. Measuring the weak nuclear force parameters is one of the best ways to improve our fundamental understanding of the physics laws of the universe. Neutron beta decay provides one of the most accessible windows onto the weak nuclear force, enabling measurements at LANSCE with comparable precision to the Large Hadron Collider now starting operations at CERN, Switzerland.

The Ultra-Cold Neutron A project is an ongoing effort to measure the asymmetry in the beta decay of the neutron better than any previous experiments. UCNs are neutrons with energies low enough to undergo total external reflection from an effective potential energy barrier E_{Fermi} at some material surfaces, and thus can be stored in material bottles for experiments.

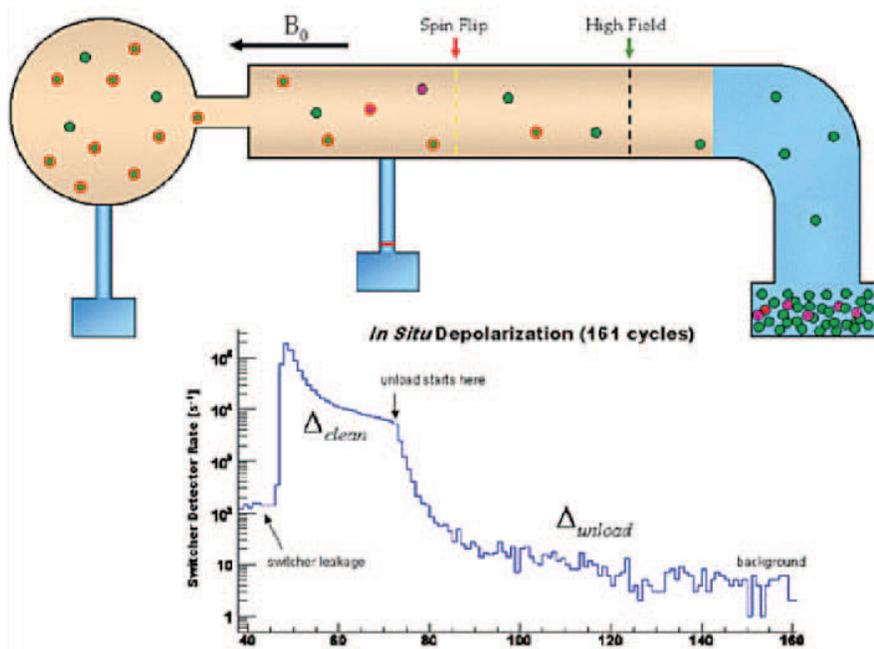
The project uses polarized ultra-cold neutrons produced at LANSCE because they offer systematic uncertainties smaller than and complementary to those of all previous experiments, which used cold neutron beams. In previous years, the project accumulated statistics for a 1% uncertainty on the decay asymmetry, which is comparable to the uncertainties on previous experiments. The ultimate goal of the project is to decrease the total uncertainty to about 0.25%. In order to do this, two things are necessary: a significant increase in the detected neutron decay rate over that seen in previous years, and measurement of the main sources of systematic uncertainty to prove that they are as low as originally thought. Both of these goals were accomplished during 2009. The decay rate approximately doubled, compared to 2008, by improving the ratio of detected decays to incident ultra-cold neutrons. All the leading systematic

uncertainties were studied and established to be sufficiently low to allow the ultimate goals of the project to be met.

The leading systematic uncertainties are the depolarization of the neutrons in the experiment, the energy loss of the decay beta particles while they are detected, and the undetected backscatter of the decay beta particles from their detectors. All three of these effects were studied in depth in 2009. As a result of the engineering run during 2009, the UCNA project is positioned to achieve the world's best measurement of the neutron beta decay asymmetry during the next accelerator cycle in 2010. An additional 3 million decay events were detected at the higher rates needed for the statistics of the final measurement.

The DOE Office of Science funds the research.

AOT and LANSCE - The Pulse, April 2010.
LALP-10-020



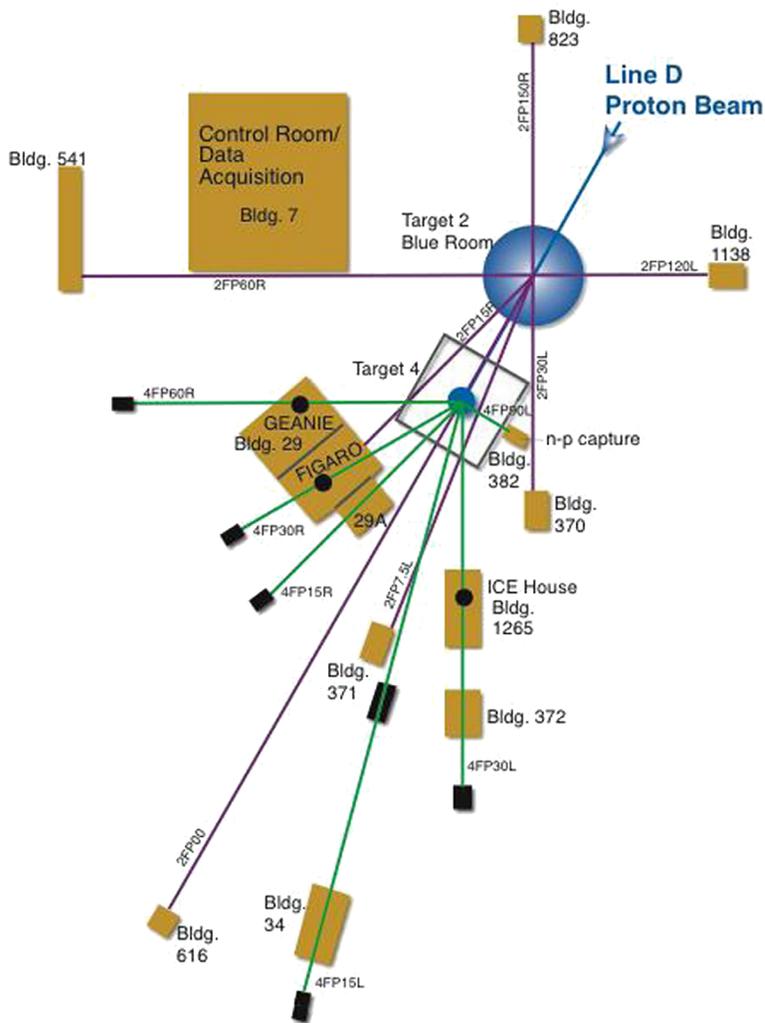
 Schematic of a test measurement of neutron depolarization. The experiment is shown as the circle on the left. The neutrons (depicted as dots) flow through the experiment and into a detector on the right.

(Bottom): The graph shows a typical depolarization measurement, which traps depolarized neutrons in the experiment while cleaning out the properly polarized ones. Any depolarized neutrons would show up as a peak under the label Δ_{unload} . The number of detected depolarized neutrons was consistent with zero, with sufficiently high precision to show that depolarization will not limit the precision of the final project results.

Weapons Neutron Research Facility 2010



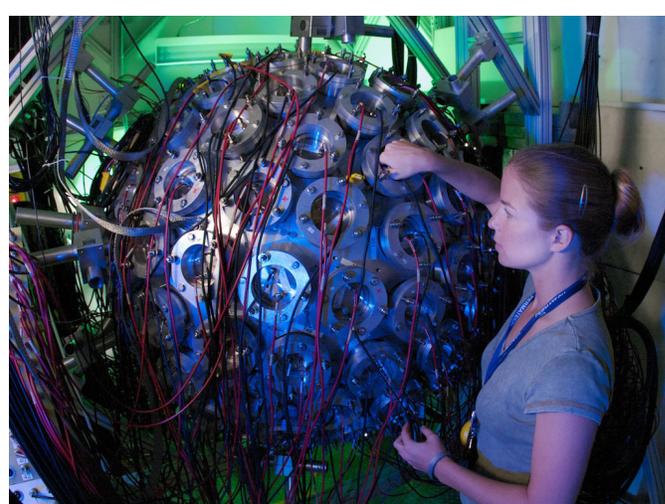
WNR



● WNR's GEANIE spectrometer consists of approximately 26 compton-suppressed, high-resolution germanium gamma-ray detectors. GEANIE is located on an approximately 20-meter-long flightpath.

● Schematic of the Target-1 and Target-2 flight paths.

● Detector for Advanced Neutron Capture Experiments (DANCE) is a 4p detector array that consists of up to 160 elements of barium fluoride crystals. It is designed to study capture reactions on small quantities of radioactive isotopes (down to 1 mg or up to 1 Ci), which are of interest to studies in nuclear astrophysics and stockpile stewardship science.





First Beam Tests With the Time Projection Chamber

Nuclear cross sections are fundamental in modeling the behavior of nuclear systems in weapons and nuclear power reactors. In certain cases, uncertainties in some key cross sections limit the predictive power of simulations. In these cases, sensitivity studies are used to identify cross sections where greater accuracy is needed. As part of the Laboratory's national security mission, scientists determined that the ^{239}Pu fission cross-section should be known to within 1% uncertainty or less.

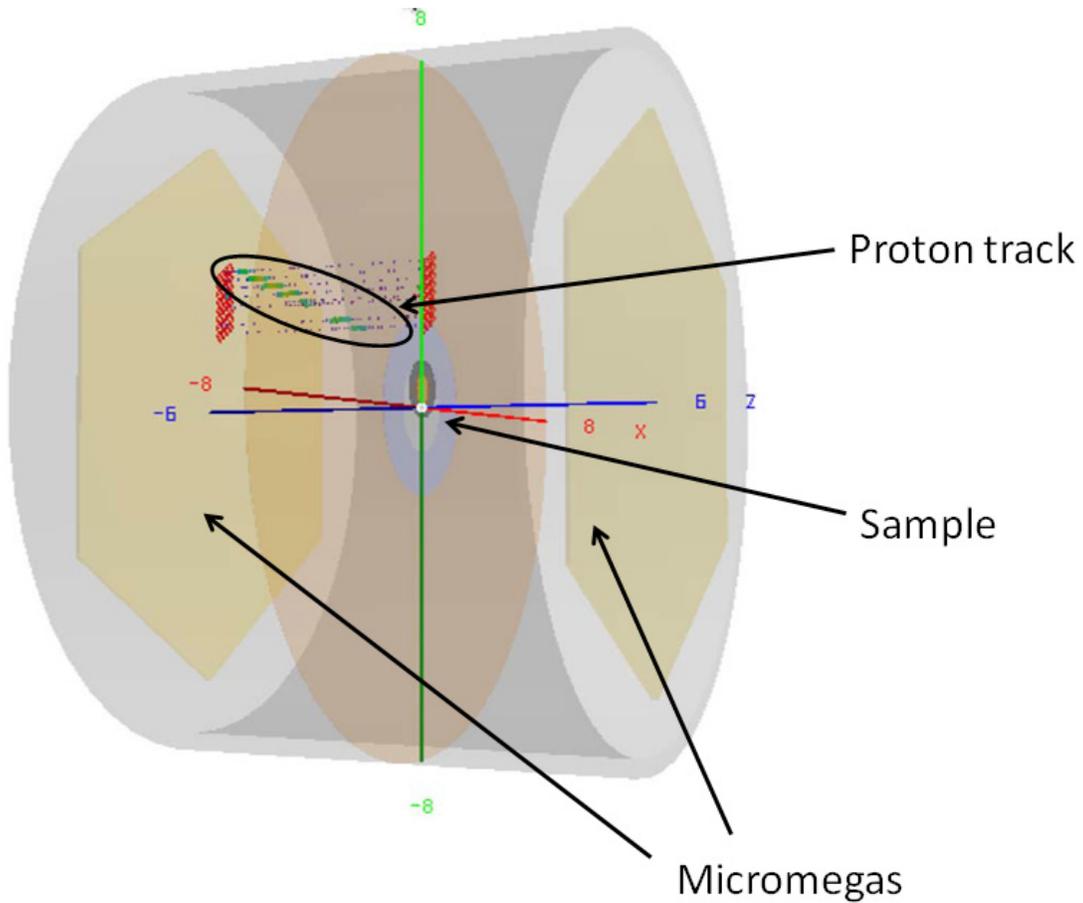
Because conventional techniques for measuring fission cross sections are limited to 3%–5% uncertainty, scientists proposed a new approach—a Time Projection Chamber (TPC)—to meet the uncertainty requirement. The Neutron Induced Fission Fragment Tracking Experiment (NIFFTE) collaboration, which includes Lawrence Livermore National Laboratory (LLNL), Los Alamos National Laboratory (LANL), Idaho National Laboratory (INL), and six university partners; is developing the detector.

The time projection chamber was invented in the late 1970s, and is used in high-energy physics. The NIFFTE TPC is unique because it is the first ever used for fission studies. A TPC uses segmented readout pads and drift time information to generate three-dimensional images of particle tracks within the active volume of the detector. This tracking information can greatly decrease systematic uncertainties in cross section measurements. The TPC will also reduce the uncertainties by providing excellent particle identification, eliminating the ambiguity between fission and decay background. It will allow the fission cross section to be measured relative to the $\text{H}(n,p)$ cross section, which is better known than the $^{235}\text{U}(n,f)$ cross section standard.

A prototype TPC was shipped from LLNL to LANL in July, and was installed on a beam line at LANSCE. The prototype has two out of 192 segments instrumented, which allows 64 channels to be read out. The first beam data collected in mid-August met a level 2 milestone for the weapons program. The figure depicts an example of a physics event collected at LANSCE. Proton recoil induced by the neutron beam interacting with the gas in the TPC chamber created the measured track. After observing these types of events for the first test, researchers loaded a ^{238}U sample into the TPC for fission track measurements.

Following the commissioning of the TPC, a production version will be used to measure ^{239}Pu fission. This measurement is important both to the weapons program and nuclear energy applications, and a suite of different measurements are expected to follow. In addition to cross sections, the TPC opens new and possibilities for studying the fission process, and it will contribute to a better understanding of this complex nuclear process. Fredrik Tovesson (LANSCE-WNR) led the team of Alexander Laptev (LANSCE-WNR), and students Lucas Montoya (University of New Mexico), Dana Duke (California Polytechnic State University), Nicholas Fuller (Houghton College), Daniel Pamplin (Abilene Christian University) and Nathan Pickle (Abilene Christian University). NNSA Science Campaign 1 (Robert Reinovsky, LANL Program Manager) and the DOE Nuclear Energy Fuel Cycle R&D program (Stuart Maloy, LANL Program Manager) support the work.

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● Particle track observed with the fission TPC. The Los Alamos Neutron Science Center Weapons Neutron Research facility's neutron beam interacts with the chamber gas, resulting in proton recoils. The TPC uses a type of gas ionization detector known as Micromegas (Micro-MEsh Gaseous Structure) for readout.

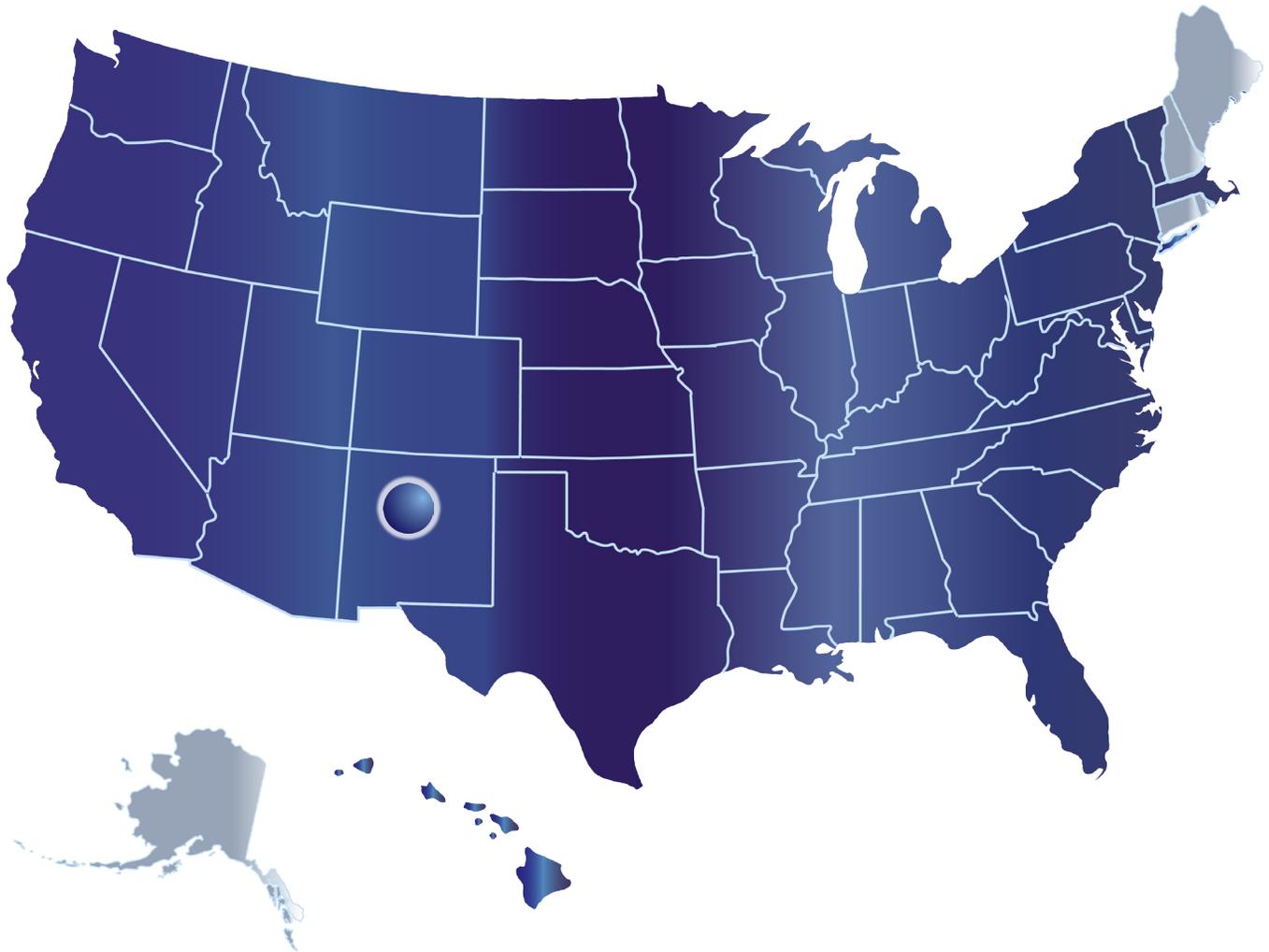
User Program 2010





User Demographics

User Program

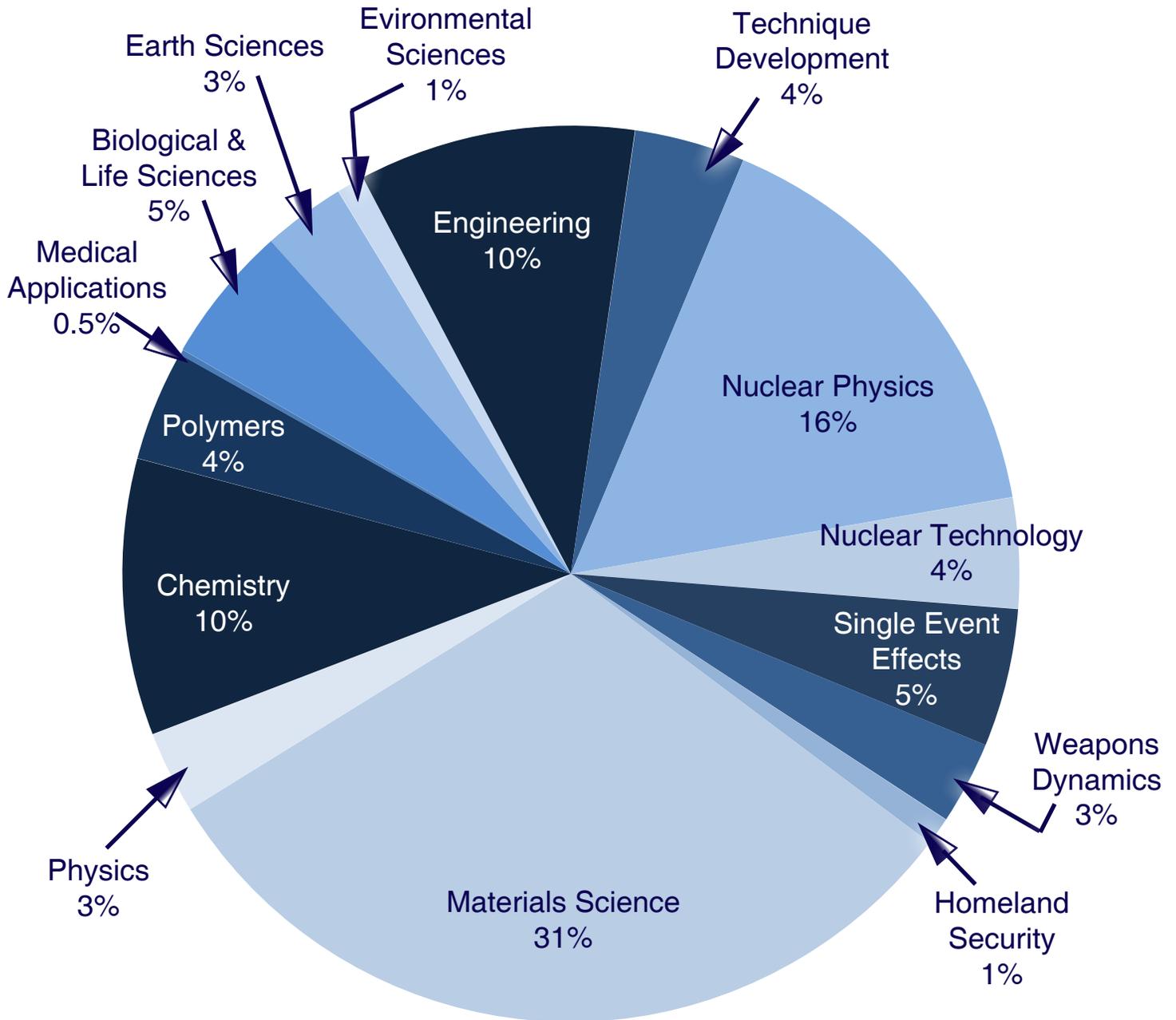


 U.S. States Represented by LANSCE Users

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

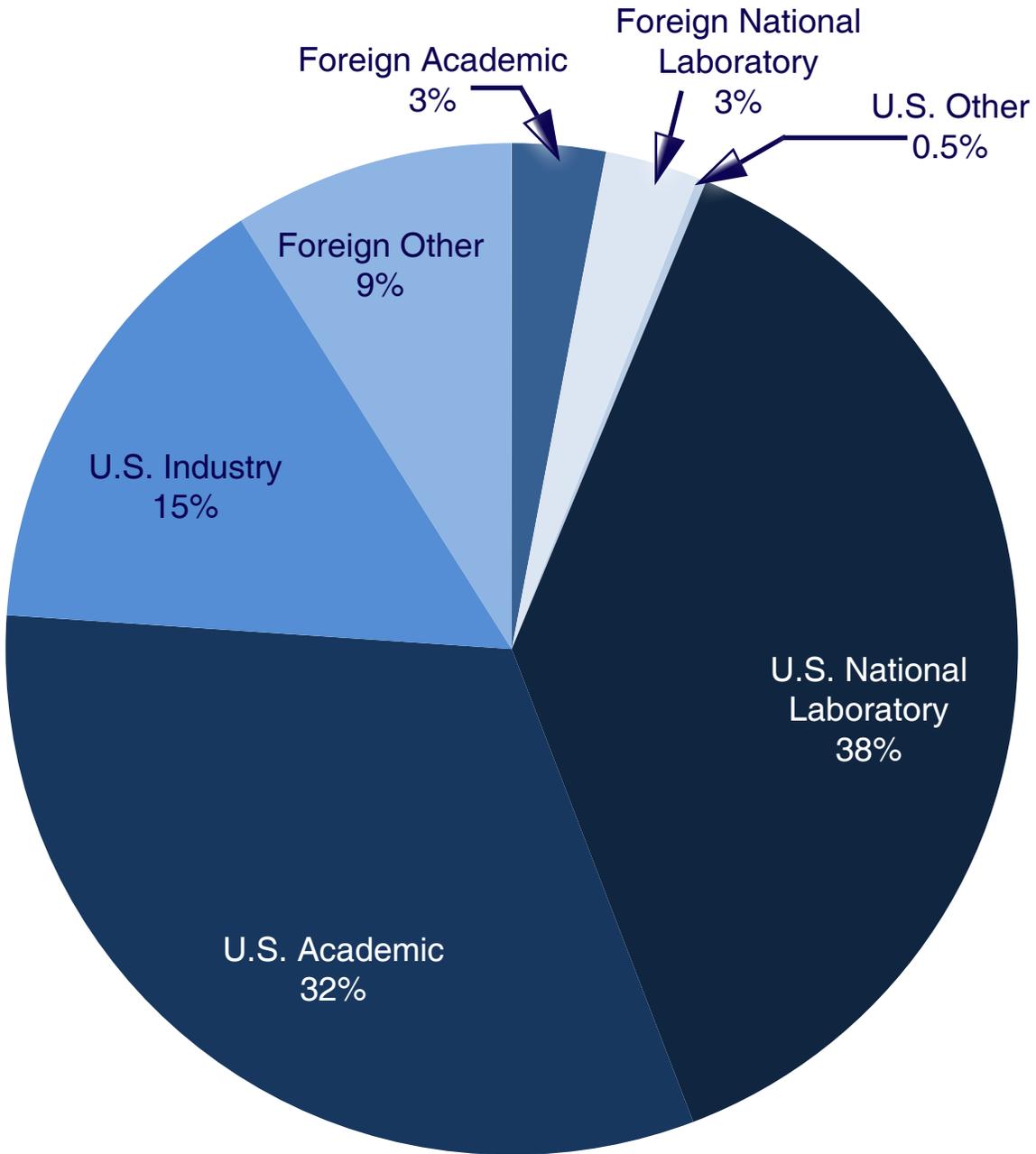


User Discipline



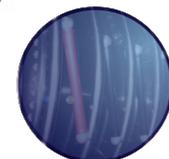


User Institutions

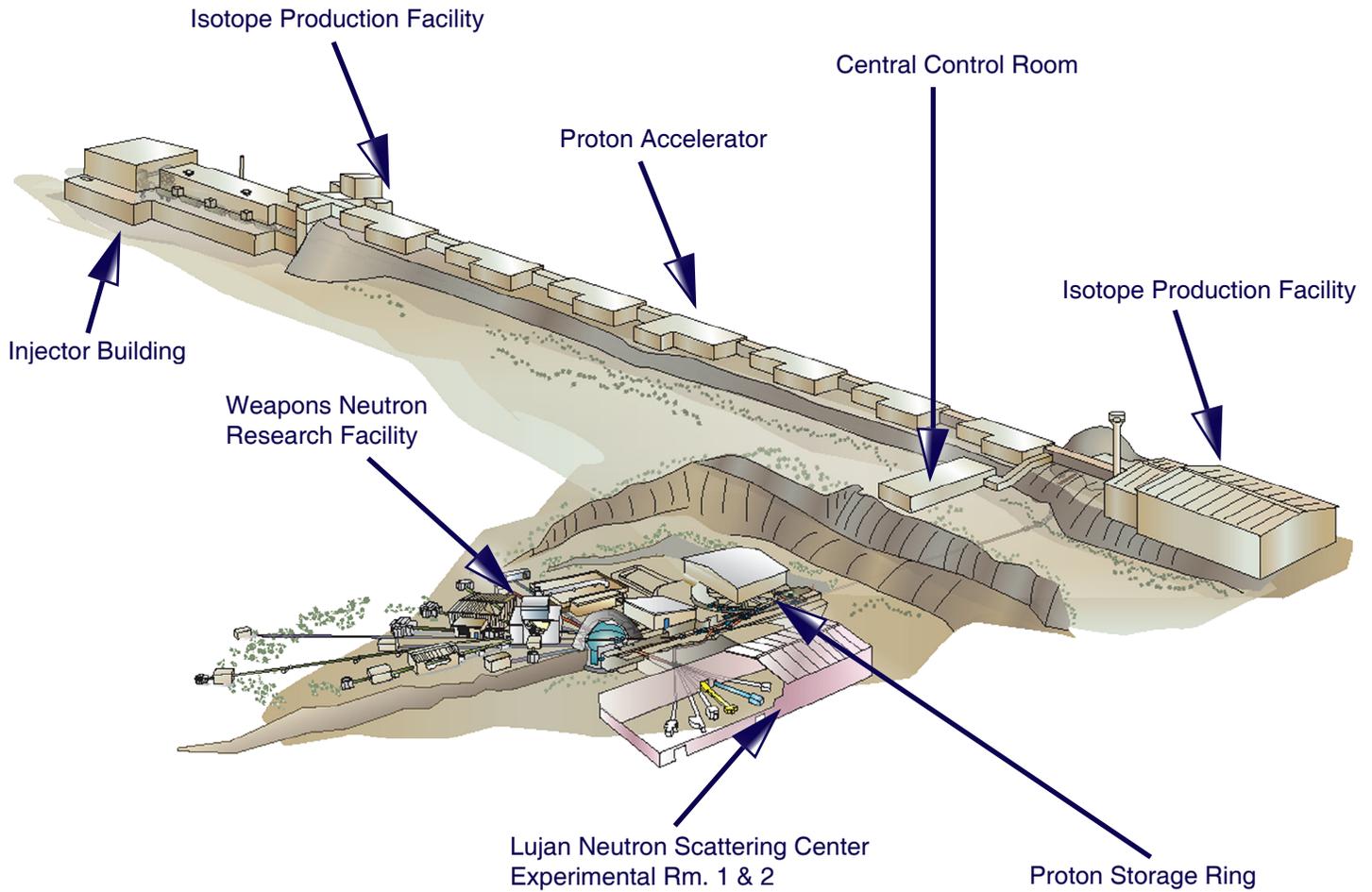




Accelerator Operations Technology 2010



AOT



 Schematic of LANSCE's Beam Delivery



Mark III Spallation Neutron Target Completed

On June 9, shortly after 5 a.m., the first proton beam hit the new “Mark III” spallation neutron target at the Lujan Center. All systems are green and already it is producing higher neutron flux than expected relative to numerical simulations.

Beginning in 2004, the neutronics design for the Mark III was developed by the Spallation Physics Team at the Lujan Center. Guenter Muhrer led the team of Michael Mocko and Charles Kelsey (LANSCE-LC), with substantial input from the instrument scientists. Researchers performed proof of principle experiments at the Weapons Neutron Research facility in partnership with the Neutron and Nuclear Science (LANSCE-WNR), Mechanical Design and Engineering (AOT-MDE), and Accelerator Operations (AOT-OPS) groups. The engineering design was conducted by Joe O’Toole (lead), Tony Gomez, Mike Borden, James O’Hara, Eric Olivas, Ray Valicenti, and Keith Woloshun (AOT-MDE); Mike Baumgartner and Eron Kerstiens (AOT-OPS); Curtt Ammerman, Gretchen Ellis, and Joe Schillig (Mechanical and Thermal Engineering, AET-1); and John Erickson (Accelerator Operations and Technology, AOT DO).

The new target design (the Mark III target) was installed in April 2010 by a multiorganizational team headed by personnel from the Accelerator Operations and Technology Division.

The Mark III has several innovations promising the highest performance yet, especially for cold neutron wavelengths greater than 4 Å. Used for reflectometry, small-angle scattering, and magnetism studies, cold neutrons will benefit from a new cold beryllium-reflector-filter that is projected to double the usable cold neutron (long wavelength) flux for three instruments. A gain of up to 10% is expected for the upper-tier liquid-hydrogen moderator as a result of changes in the moderator-reflector system. All the

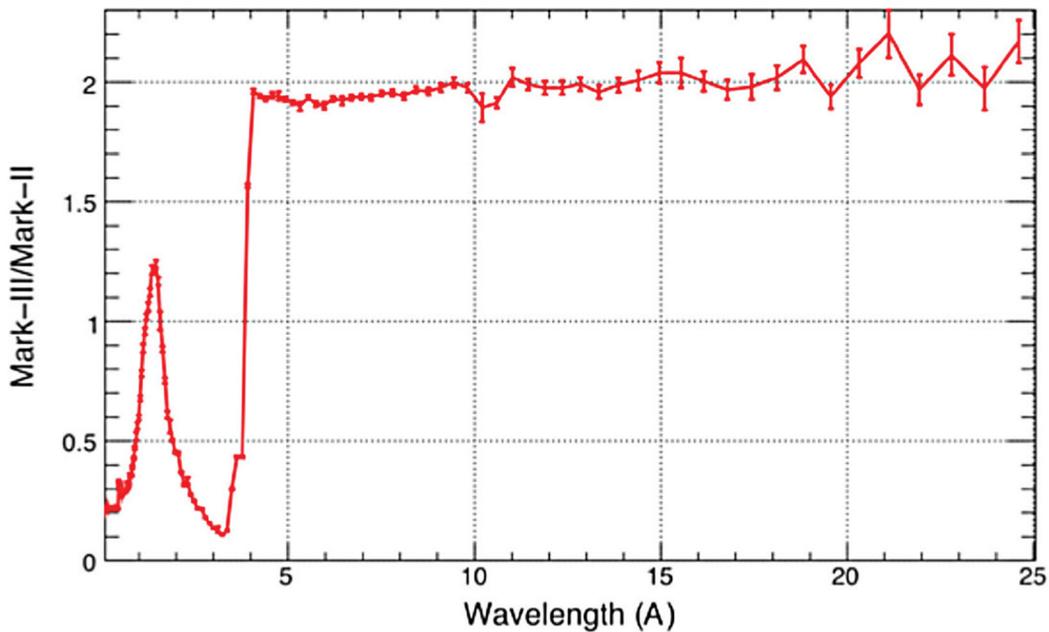
lower-tier moderators, both liquid hydrogen and water, will have “premoderators”—12 cm slabs of water placed nearby to soak up the excess thermal energy and to reduce high-energy background.

During the week of June 14, 2010, following the ion source recycle and after the radiation surveys are completed, the shutters for Lujan instruments were opened. Researchers began assessing the neutron beam flux on several instruments. NNSA’s Readiness in Technical Base and Facilities (RTBF) program provided \$10M funding for the Mark-III project.

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Photos: (Left) Mark II target removal.
(Right): Mark III target installation.



Calculated ratio of the neutron flux provided by the previous-generation (Mark II) and the current-generation (Mark III) target system installed at the Lujan Center, plotted as a function of neutron wavelength. The cold neutron flux is projected to increase by up to a factor of 2 for the lower-tier liquid hydrogen moderator.



LANSCCE Beam Facts

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

Pulses of 800-MeV negative hydrogen ions are employed at the Proton Radiography Facility to image dynamic events related to nuclear weapons performance and are also sent to heavymetal targets at the Weapons Neutron Research Facility, 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. It is also operated as a user facility visited annually by approximately 300 investigators.

The negative hydrogen ions are injected into a 90 m Proton Storage Ring that compresses the 625 ms pulses into a 250 ns intense burst of protons, which, through nuclear spallation, produce bursts of neutrons for neutron scattering studies of material properties at the Weapons Neutron Research Facility and Lujan Center. The Lujan Center is a major national research center annually hosting more than 300 scientists from around the world who perform materials science research and low-energy neutron nuclear physics studies using a variety of uniquely designed instruments.

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

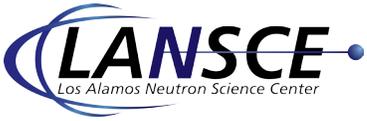
The ultra-cold neutrons then travel through a guide tube and are detected by a helium-three detector, allowing research of fundamental nuclear physics to test the standard model of elementary particles.

2010 Beam Reliability Summary

Production Delivery Statistics

Area	Scheduled Hours	Delivered Hours	Reliability
IPF	4165.0	3659.8	87.9%
Lujan	3389.9	2868.0	84.6%
pRad	820.5	765.9	93.4%
UCN	1799.7	1625.2	90.3%
WNRT2	498.7	440.6	88.4%
WNRT4	3040.9	2635.2	86.7%
Total	13714.7	11988.7	88.6%

 At the core of the LANSCE international user facility is a highly flexible linear accelerator system, which is overseen by the Beam Delivery Team. The DOE Office of Science/Basic Energy Sciences considers a reliability standard of 85% to be “world class.”



LANSCCE Beam Reliability Achieves World-Class Ranking • Mark III Outperforming Simulations • Los Alamos

News 2010





News Briefs

Funding for New Flight-Path Semiconductor Testing

The Los Alamos National Security Board of Governors has approved funding for a new building that enables another flight-path for semiconductor testing. The new flight path will be 30 degrees to the right of the proton beam and will provide the same neutron spectrum as the present ICE House which is located at 30 deg. to the left of the proton beam.

This new endeavor will double the amount of beam time for industry, university, and Laboratory users. This is a good example of LANL's leadership involvement with LANSCE's facilities and confidence in our future as a major player in the field.

LALP-10-02

Los Alamos Lends its Scientific Expertise to Clean Energy and Carbon Sequestration Projects

Department of Energy Secretary Steven Chu recently announced that as part of the Department of Energy Fossil Energy Program, the agency is funding large, complementary projects that will focus on clean energy and carbon sequestration. Los Alamos National Laboratory is deeply involved in two of these projects—the Clean Coal Center and the Carbon Capture and Storage Simulation Initiative.

Los Alamos is part of the winning proposal for the Clean Coal Center, named the U.S.-China Advanced Coal Technology Collaboration (U.S.-China ACT).

Los Alamos will lead the risk analysis task and provide scientific support for the subsurface simulation of CO₂ injection and coupled processes, site characterization and assessment for geological sequestration, and novel capture technology development tasks. The Laboratory also will leverage its carbon sequestration expertise, programs, and collaborations, such as DOE's National Risk Assessment Partnership (NRAP) and regional sequestration partnerships. Philip Stauffer (Computational Earth Sciences, EES-16) is the Los Alamos principal investigator for the Clean Coal Center project. Los Alamos researchers from Computational Earth Science (EES-16), Earth System Observations (EES-14), Lujan Neutron Scattering Center (LANSCE-LC), and Materials Chemistry (MPA-MC) will participate in the work.

LALP-10-02

LANSCE Research Featured in American Physical Society Calendar

The American Physical Society (APS) features graphics of physics research for its calendars, which the APS distributes to its approximately 47,000 members. For the month of October in the 2010 calendar, the APS chose an image of a polymer supported lipid membrane from LANSCE LC researchers and their collaborators.

The polymer gel layer provides a realistic, controlled environment to study biomembranes. As the polymer swells, it promotes both in- and out-of-plane fluctuations of the supported membrane that mimic the properties of living cellular membranes. The promotion of membrane fluctuations offers far-reaching applications as a surrogate biomembrane. This polymer-membrane system may facilitate otherwise difficult studies of lipid-protein interactions, transmembrane ionic transport, membrane structure, and membrane-based biosensors that previously have not been possible because of the limitations of existing models to in-plane studies.

Reference: "Model lipid membranes on a tunable polymer cushion," *Physical Review Letters* 102, 228102 (2009). The American Physical Society also selected the research to appear in the Virtual Journal of Biological Physics Research. LALP-10-02

DOE Recognizes Laboratory's Lighting Research

DOE recognized a team of researchers from Materials Physics and Applications and the Los Alamos Neutron Science Center for their research to develop new materials to lower the cost of organic light emitting diode (LED) manufacturing. Anthony Burrell, Eve Bauer, and Tom McCleskey (MPA-MC); Hongmei Luo (LANSCCE-LC); and Quanxi Jia (MPA-CINT) were honored at "Transformations in Lighting," the seventh annual U.S. DOE Solid-State Lighting Research & Development Workshop. The team was one of nine recognized by DOE for significant breakthroughs and achievements in 2009, representing research in light-emitting diodes and organic light-emitting diodes conducted at industry, universities, and research institutions.

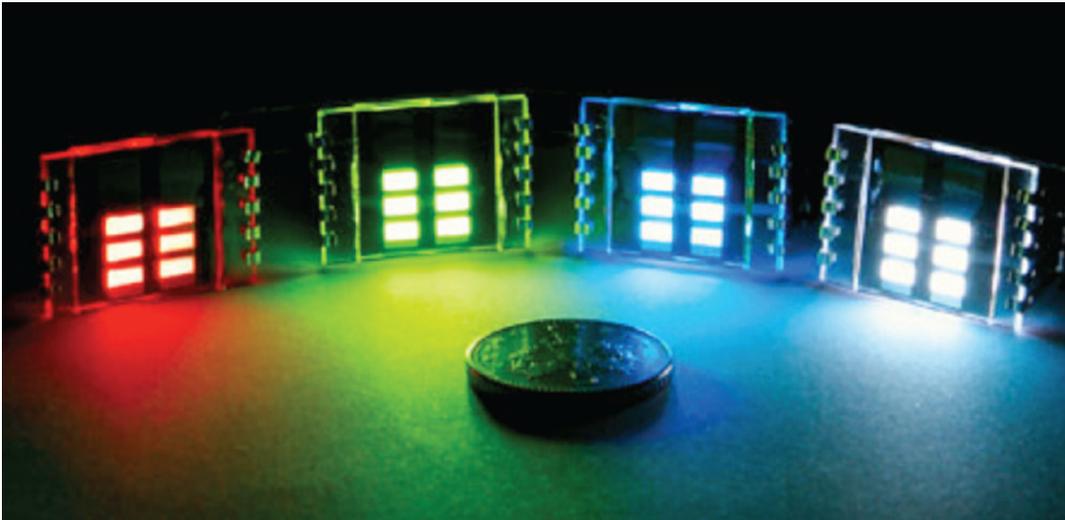
Lighting consumes about one-fourth of the electricity produced annually in the U.S. Potentially more efficient and environmentally friendly than current lighting sources, organic light-emitting diodes could conceivably replace both fluorescent and incandescent lights as the primary lighting source. The organic light-emitting diodes make light by the controlled movement of electrons, not by heating up a wire filament, as in incandescent lights. Therefore, these diodes use much less energy than conventional lights. Organic light emitting diodes also have unique properties that make them attractive for lighting applications, including making it possible to electrically control the spectral properties of the light emitted and the ability to be arranged over large areas in various shapes. These diodes are thin, flexible, and produce bright color. However, cost and long-term application are major issues of this new lighting technology because the indium used in these diodes is a limited resource.

Transparent conducting oxides are key components of organic light-emitting diodes. Their properties and production methods are vital to the future of solid-state lighting. Indium tin oxide is the most popular transparent conducting oxide for organic light-emitting diodes applications because of its high transparency and work function. However, indium is a rare material available from only a few places in the world. The consumption trend for indium may exceed production due to the increasing use of this material in flat panel displays and televisions.

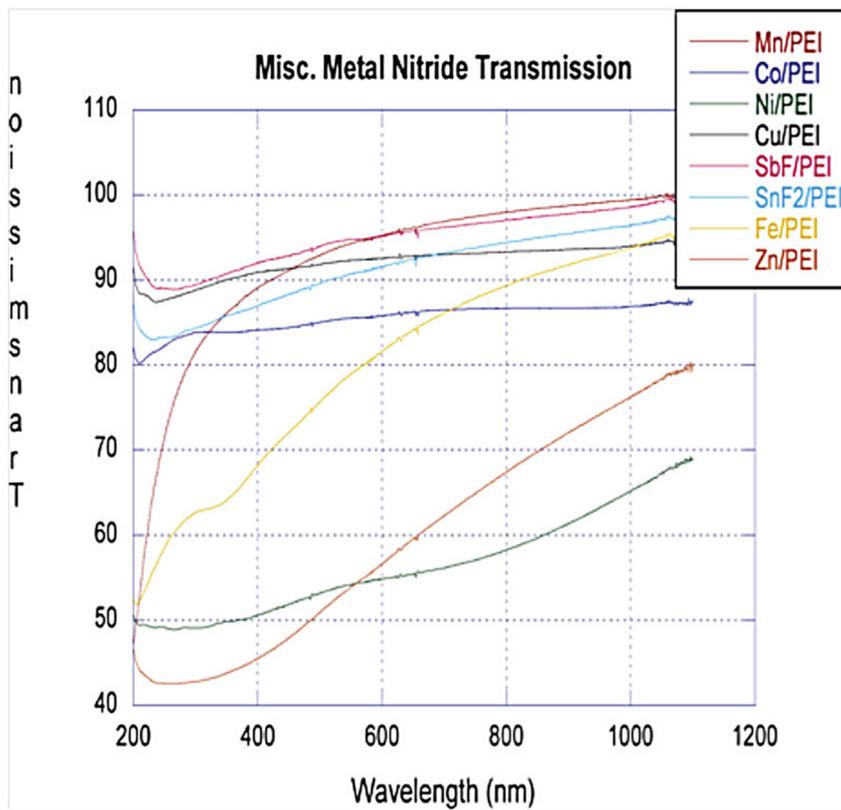
The LANL team identified new compositions that could be alternatives to indium tin oxide for use in organic light-emitting diodes (see figure). The scientists developed transparent thin film nitrides based upon vanadium nitride doped with first row transition metals. These metals are much more readily attainable and economical than indium.

The DOE Solid State Lighting program (Karl Jonietz, LANL program manager) funded the work.

AOT and LANSCE - The Pulse, June 2010.
LALP-10-020



● Organic LEDs



● Metal nitride transmissions for potential use in organic light-emitting diodes.

Mark III Outperforming Simulations

The new target-moderator-reflector system “Mark III” at the Lujan Center is producing higher neutron flux than expected relative to numerical simulations.

A recent absolute measurement of cold neutron flux at Flight Path-10, where the small-angle scattering instrument low-Q diffractometer (LQD) is sited, shows that the expected gain of about 2x in cold neutron flux is surprisingly 20% higher. This enhancement bodes well for experiments performed on cold-spectrum instruments LQD and its reflectometer cousins Asterix and SPEAR.

The fact that calculations underestimated the actual gain at long wavelengths on the hydrogen moderator is exceptionally good news for users and a delightful mystery for spallation physicists. It may be a surprise to know that the full neutron physics for the target assembly materials is not fully known. Essentially every new target assembly fabricated at spallation neutron facilities across the world breaks new ground, especially at the Lujan Center where innovative design has been the norm. Among the Lujan innovations now copied by others is the split-target flux-trap—a separation of target materials between two tiers with a vacuum in between where the hot-spallation neutron gas can be concentrated—and the partially coupled moderator—a way to increase neutron flux dramatically by allowing strong, coupled interchange of neutrons between moderator, reflector, and target components. Gary Russell (retired) and Eric Pitcher (LANSCCE-DO) were intellectual leaders of these innovations and had seminal input to the Mark III design team headed by Guenter Muhrer (LANSCCE-LC).

In Figure 1, the ratio of Mark III and the retired Mark II fluxes measured (red) and calculated (black) for FP-10 shows that extant theory reproduces features at short wavelengths almost exactly. A designed notch in Mark III’s flux spectral probability

density at 3 angstroms borrows short wavelength neutrons for higher flux at long wavelengths greater than 4 angstroms in order to probe soft matter more comprehensively. That notch, created by a new beryllium reflector-filter added to the liquid hydrogen neutron moderator, is well reproduced by Monte Carlo calculations. The full calculated spectrum for the old and new targets is shown in Figure 2.

Observations at other beam lines at Lujan Center show improved flux with Mark III. Instruments viewing water moderators, optimized for short wavelength neutrons useful in diffraction, are seeing—at a minimum—a return to design-level flux after experiencing a multiyear decay of intensity from the Mark II, apparently due to tungsten target degradation. Preliminary measurements of intensity from Mark III exhibit enhanced flux relative to design on two flight paths, to be confirmed.

One variable that could explain some of the early, promising results is the ortho-para hydrogen ratio in the hydrogen moderator. Because protons are fermions with either spin up (+) or spin down (-), a hydrogen molecule adopts either excited (++) or ground-state (+-) spins; the neutron cross section is 100x higher for the excited ortho-hydrogen state, making it the more efficient moderator. Through natural conversion mediated by interactions between hydrogen molecules and walls, the equilibrium ortho-to-para fraction approaches zero within nine days without beam at 20 K. When the beam is on, the steady-state fraction of 25% excited hydrogen is desirable but ill-controlled. Mark II measurements published by Japanese collaborators in 2006 inferred a steady state fraction of 35% however that fraction has never been directly measured; there are plans to do so with Mark III in the coming months.



Clever redesign of the Lujan Center target and moderator system has resulted in a cold neutron flux rivaling the highest power pulsed spallation sources in the world while using one-tenth of the proton beam power. The increased cold neutron flux will allow experiments on longer length scales and longer times scales than previously possible.

This work was funded by the RTBF program of DOE NNSA and by the Office of Basic Energy Sciences.

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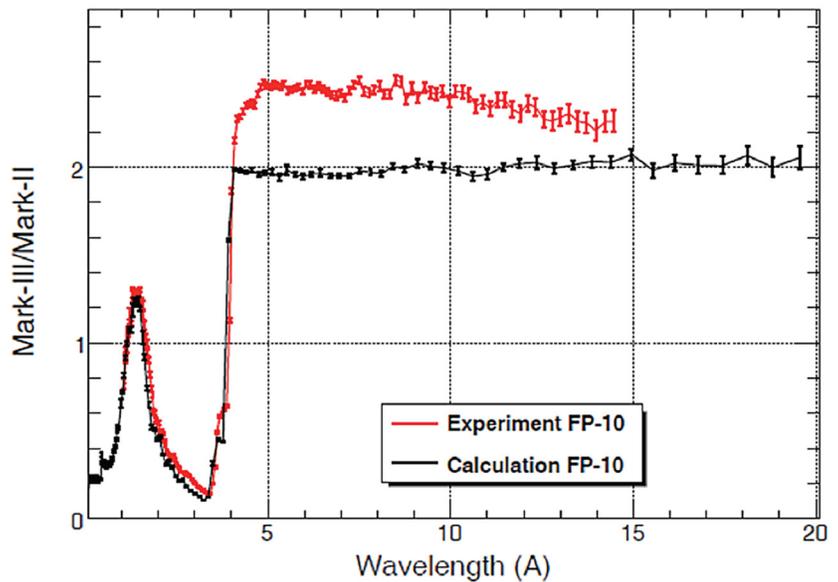


Figure 1. Ratio of neutron flux spectra for Lujan Center's new Mark III target to last year's Mark II target comparing calculated (black) and experimental (red) ratios. The Mark III moderator design optimizes for high flux of cold neutrons with wavelengths greater than 4 Å. While Monte Carlo simulations predicted a factor of 2 increase in neutron flux spectral density owing to a new Be reflector-filter, experiment shows a surprising factor of 2.4 owing to unexplained physics of the target assembly.

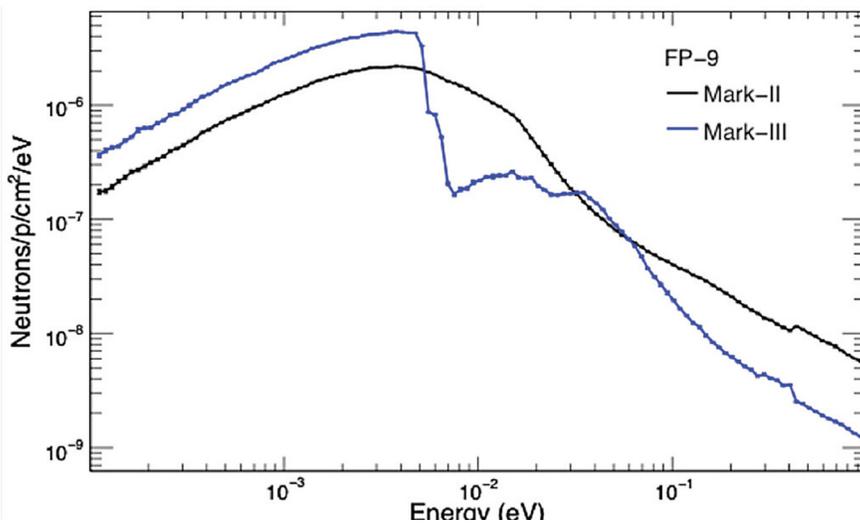


Figure 2. Measured (black) and calculated (blue) neutron spectral densities on the liquid hydrogen moderator serving Flight Path 9 at the Lujan Center.

Upgrade to Filter Difference Spectrometer Enables More Science

The Filter Difference Spectrometer (FDS) at the Lujan Center is undergoing an upgrade that will significantly improve its functionality and usefulness for scientific research. In neutron vibrational spectroscopy, FDS exploits the large incoherent scattering cross section of hydrogen to obtain the vibrational spectrum of hydrogenous materials (Figure 1). FDS is used mostly to study chemical bond dynamics in materials. The science addressed by the instrument includes heterogeneous catalysis and surface science, hydrogen bonding, organometallics, explosives, water in materials, hydrogen storage materials, hydrous minerals, and numerous other problems involving hydrogen. The instrument is particularly well suited to address scientific challenges relevant to the DOE hydrogen initiative, and use of the instrument within this context has increased dramatically over the past five years.

The principle of operation of the instrument is simple. Time-of-flight determines incident energy of the neutron. The final energy of the scattered neutron is set by a filter placed between the sample and the detector. Beryllium (Be) filters set the final neutron energy at 5.22 meV (nominally), and beryllium oxide (BeO) filters impose a final neutron energy of 3.76 MeV. These filters do not have a perfectly sharp transmission function, but the difference between the Be and BeO data sets produce a vibrational spectrum with a resolution of the order of 1 meV, hence the name "Filter Difference Spectrometer." Early on, the difference could be computed with a minimum of hardware. When more powerful computers became available, numerical deconvolution methods replaced the filter difference method. Be and BeO data sets could be deconvoluted separately to produce a spectrum with better resolution than the filter difference method. Currently, the typical energy resolution is 2% to 5% depending on the data

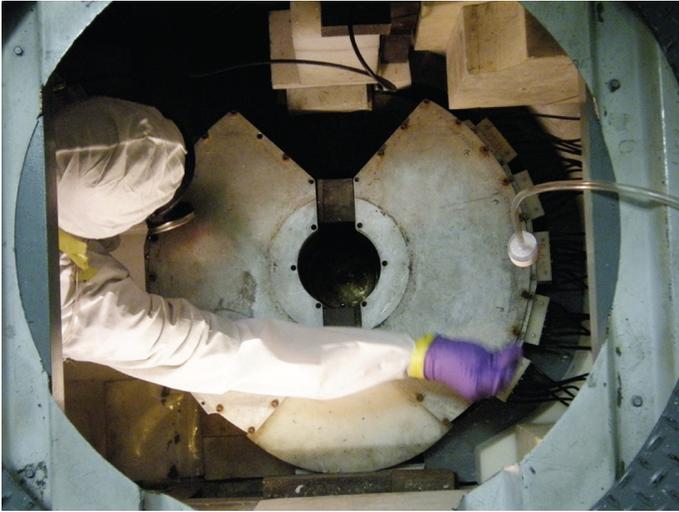
analysis method. Since BeO filters never lent themselves to reliable numerical deconvolution, users often ignored the corresponding data. Therefore, the Lujan Center is replacing the BeO filters with Be filters.

The FDS filters are located in an evacuated tank and cooled to 100 K to reduce phonon scattering. This tank had not been opened in more than 20 years. The scientists assessed the condition of the various components, including filters, inside the tank. This operation, which took place in February, revealed a perfectly clean system in pristine condition with minor (and inconsequential) oxidation on a few sheets of cadmium. Brush Wellman (OH, USA) produced the five new Be filters with high purity (> 99%) Be and near theoretical density. Each filter comprises three parts (photo 2), stacked on top of each other. This low-cost upgrade will make the entire FDS detector more useful and will double the count rate of the instrument. The increased decoupling between filters will also help reduce instrument background.

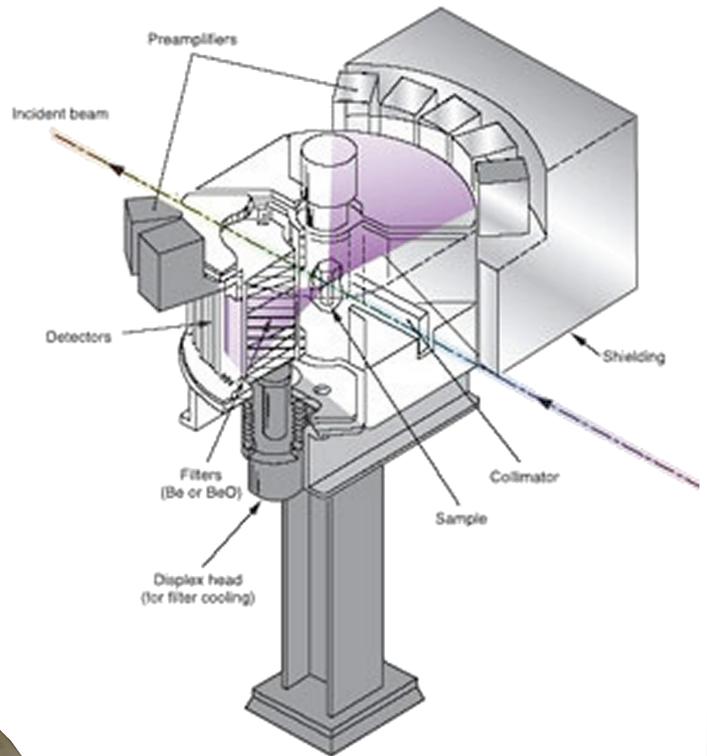
These upgrades will enable more science on FDS, such as use of smaller samples, greater sensitivity, the ability to conduct time-dependent experiments, faster measurements of unstable samples, and the capability to run more compositions or conditions. An upgrade of the data reduction software for FDS will provide users with additional graphical features, in addition to the two traditional data analysis methods of direct deconvolution and maximum entropy.

The capital funding component of the DOE Basic Energy Sciences - Lujan Center Operations supported the work.

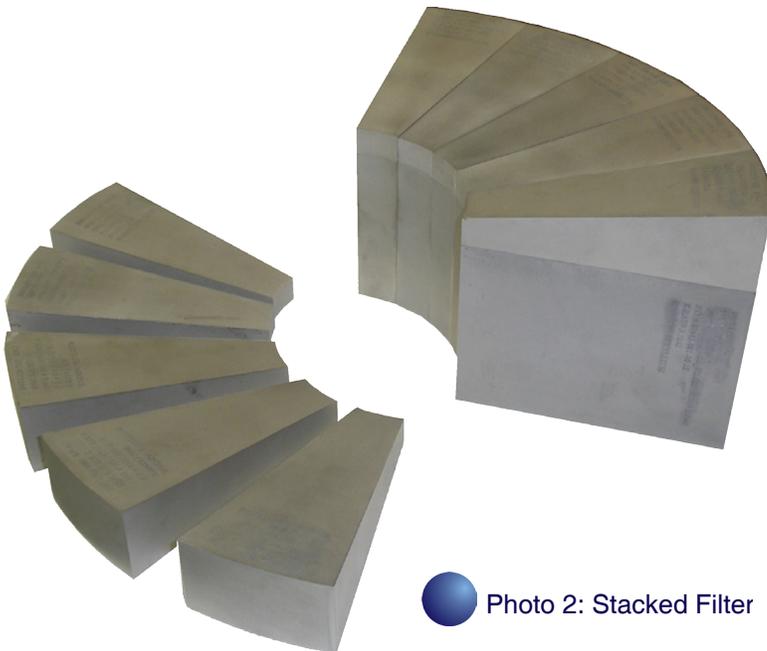
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LALP-10-020



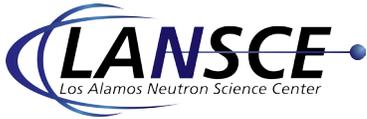
● Photo 1: Top view of the FDS filter tank. Samples reside in the 5 in. hole in the middle of the tank.



● Figure 1: Illustration of



● Photo 2: Stacked Filter



Conferences, Workshops & Tours 2010





LANSCCE-NS Hosts National Laboratories Fission Measurements Meeting

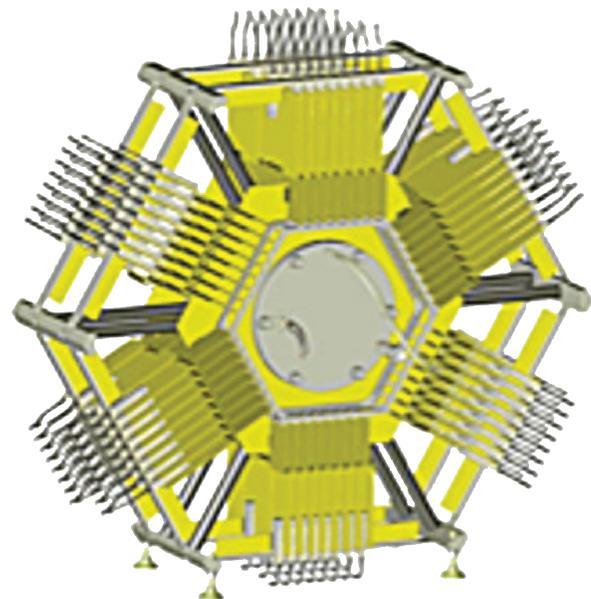
LANSCCE-NS staff recently hosted a planning meeting on neutron induced fission measurements. The meeting addressed ongoing collaborative projects to accurately measure the spectrum of neutrons emitted in fission and to attain an accuracy of less than 1% in the measured fission cross-sections. Both goals are priority items in the predictive capability framework of the Defense Programs Science Campaigns, and are important components of nuclear energy programs. Attendees included collaborators from LANSCCE-NS, C-NR, Lawrence Livermore National Laboratory (LLNL), and Idaho National Laboratory (INL). Portions of these efforts are funded by Campaigns 1, 2, and 4 of the weapons program and by the Nuclear Data program of the Nuclear Energy office.

Fission cross-sections and fission neutron output spectra are key quantities in modeling nuclear reactivity. As improvements are made in understanding materials properties and hydrodynamics of nuclear weapons, nuclear properties are a significant contributor to the overall uncertainty of predicted performance. The Chi Nu collaboration involving LANL, LLNL, INL, and university collaborators is developing techniques to measure fission neutron output spectra over the full incident and outgoing neutron energy ranges of interest. This work requires the new neutron detector arrays and associated digital data acquisition systems, which were a focus of this meeting.

A new approach to provide fission cross-sections with accuracies better than 1% uses a Time Projection Chamber that can track and identify all charged particles emitted from fission and from other reactions. This technique allows removal of

backgrounds that limited the accuracy of previous measurements and enables a better understanding of systematic errors. The Time Projection Chamber was developed in collaboration between LANL, LLNL, INL, and six universities. The chamber was assembled at LLNL, and operation was tested using a radioactive source. The researchers will install the first prototype Time Projection Chamber at LANSCCE in the upcoming accelerator beam cycle to start the commissioning phase. Tests of the time projection chamber in the LANSCCE neutron beam are scheduled for the upcoming accelerator-running period. The participants evaluated and updated the multiyear project scope and progress at the meeting.

AOT and LANSCCE - The Pulse, May 2010.
LALP-10-020



 Schematic of the Time Projection Chamber. The readout contains many thousands of channels of electronics that digitize the ionization tracks produced by charged particles of the gas in the chamber.

LANSCCE-NS Hosts NNSA Academic Alliance Center of Excellence Leader

Professor Jolie Cizewski of Rutgers University is on sabbatical as a Visiting Scholar and working with Neutron and Nuclear Science (LANSCCE-NS) staff. Cizewski, who was a postdoctoral researcher at Los Alamos from 1978 to 1980, is the leader of an NNSA Stewardship Science Academic Alliance Center of Excellence.

Cizewski's work focuses on understanding neutron capture reactions and developing alternative experimental and theoretical techniques to determine neutron capture reaction rates where direct measurements are difficult or not possible. Knowing these reaction rates, particularly for small and unstable samples, is important in understanding past nuclear weapons tests as well as understanding the creation of elements in stars. She is leading an experiment at LANSCCE using high-resolution gamma-ray detectors to gain insight into spin distributions following neutron capture. These data, compared with data obtained with alternate reactions that probe the same nucleus, will allow evaluation of the accuracy of alternate reaction techniques.

Several postdoctoral researchers and students are participating in the experiment in collaboration with Cizewski and LANSCCE-NS staff.

AOT and LANSCCE - The Pulse, December 2010.
LALP-10-020



● Professor Jolie Cizewski (front center) with collaborator Bill Peters and postdoctoral researchers Meredith Howard and Remi Adekola.



LANSCE hosts NNSA Academic Alliance Workshop

Researchers from the NNSA Academic Alliance Rutgers University Center of Excellence for Stewardship Science recently visited LANSCE for a workshop. The Center of Excellence is a collaborative effort between Rutgers University, Oak Ridge Associated Universities, the University Radioactive Ion Beam consortium, Los Alamos National Laboratory, and Lawrence Livermore National Laboratory. The goal of the center is to provide nuclear science data with applications to stockpile stewardship, nuclear structure, and nuclear astrophysics, and to help train the next generation of scientists for defense related programs. Jolie Cizewski of Rutgers University leads the Center.

Eighteen graduate students and postdoctoral researchers presented talks or posters on their work and attended lectures on defense-related nuclear science at Los Alamos. Two university faculty members also gave talks. Topics presented by the visitors included the potential use of alternate reactions to deduce nuclear reaction cross sections on unstable nuclides that are difficult to measure directly; development of a neutron detector array for use in radioactive beam research; development of a time projection chamber for neutron measurements; nuclear structure studies; and simulations of new experiment designs.

Kurt Schoenberg (ADEPS), Bob Haight, (LANSCE-WNR), Shannon Holloway, Patrick Talou, and Takehito Watanabe (T-2); Kevin John (SPO-SC); and Chris Morris (P-25) gave lectures that covered the broad nuclear science program at LANL, including neutron induced capture, fission, and neutron and charged particle emission reactions, level density studies, nucleosynthesis, isotope production and

proton radiography. A tour of LANSCE facilities capped the visit.

AOT and LANSCE - The Pulse, February 2010.
LALP-10-020



 The Center of Excellence visitors in front of the Weapons Neutron Research Facility Control Room building at LANSCE.

LANSCCE Neutron Scattering School Focuses on Structural Materials

The 2010 Lujan Center Neutron School in Structural Materials will be held August 5-13 at the Lujan Neutron Scattering Center. The school will describe how neutron scattering methods can provide unique insights to diverse areas of interest including shape memory alloys, to intermetallics, to super-alloys to bulk metallic glass composites. Lecturers of international stature will cover introductory material and describe exciting new opportunities deriving from new DOE-funded instruments and from the next-generation spallation neutron source. Introductory talks will cover the theory of neutron diffraction and Rietveld analysis, then specific areas of interest will include composites, texture, and residual stresses. A series of case studies will illustrate in practical terms how scattering experiments contributed insight to disparate problems. The complementarity of neutron and synchrotron X-ray measurements as well as with other characterization techniques will also be described. The lectures will be complemented by “hands-on” experiments using the SMARTS, HIPPO, NPDF and LQD neutron scattering instruments at the Lujan Center.

The students will gain experience with a variety of tools to study the behavior of structural materials, and interact with advanced polycrystalline plasticity models developed at LANL. Don Brown (Structure/Property Relations Group, MST-8) is the Chair of the Neutron School Organizing Committee, Jim Rhyne (LANSCCE-LC) is the School Director and Heinz Nakotte (NMSU) is the School Co-Director.

LANL lecturers include: Don Brown and Carlos Tome (MST-8); Bjørn Clausen, Thomas Proffen, and Sven Vogel (LANSCCE- LC).

The school is limited to 30 participants, who should be full-time graduate students or postdocs, early career industrial researchers, or advanced undergraduate students in an appropriate physics, materials science, or related scientific discipline. The National Science Foundation and the DOE Office of Basic Energy Sciences support the LANSCCE Neutron Scattering School. Tuition is free, and assistance for travel, lodging, and subsistence is available.

The National Science Foundation and the DOE Office of Basic Energy Sciences support the LANSCCE Neutron Scattering School. Tuition is free, and assistance for travel, lodging and subsistence is available.

lansce.lanl.gov/neutronschool

AOT and LANSCCE - The Pulse, September 2010.
LALP-10-020



● Small groups of students are involved in five or six different experiments. As part of the hands-on exercises, students learn how to analyze the data taken on different instruments under the guidance of the instrument scientist. The student groups then give presentations on the instrument of their choice and the analysis from the experiment.

Institutions and Number of Visits

Institutions (A - Dep.)	Number of Visits
AKIMA Construction Services	2
Amalgam Industries	1
American Indian Science & Engineering Society	1
Argonne National Laboratory (ANL)	2
Army Research Laboratory (ARL)	1
ATC New York	1
Atlantic Technical Center and High School	1
Barranca Mesa Elementary School	1
Bechtel Corporation	1
Beckman Couller	1
Bergoz Instrumentation	1
Boy Scouts of America - Troop 59	1
Brookhaven National Laboratory (BNL)	2
California State University	1
Carnegie Institution of Washington	1
Canada Health Infoway	1
Central Michigan University	1
Centro Nacional de Investigaciones Metalurgicas	1
CERN European Organization for Nuclear Research	1
Charles University	1
Chevron Corporation	3
Chrysler Group LLC.	1
Cochiti Community Center	1
Cochiti Community Development Corporation	1
Colorado College	2
Colorado State University (CSU)	2
Columbia University	1
COMPA Industries	1
Cornell University	1
COSMOS California State Summer School for Mathematics & Science	1
Cuba High School	1
Defense Threat Reduction Agency (DTRA)	2
Deutsches Elektronen-Synchrotron (DESY)	1
Department of Energy (DOE)	3



Institutions and Number of Visits

Institutions (Dep. AL - Ka)	Number of Visits
Department of Energy - Administrative Litigation (DOE AL)	1
Department of Energy - Headquarters (DOE HQ)	1
Department of Energy - Nevada Test Site	1
Department of Energy - Office of the Chief Information Officer	1
Department of Energy - Office of Science (DOE SC)	1
Diamond Light Source	1
Diaz & Associates	1
Dimtel Inc.	1
Dupage Medical Group	1
Electric Power Research Institute (EPRI)	1
Fermi National Accelerator Laboratory (Fermilab FANL)	3
Ford Motor Company	1
Frances Marion University	1
General Motors (GM)	1
German Aerospace Center	1
Georgia Institute of Technology	1
Gesellschaft für Schwerionenforschung	1
Girl Scouts of New Mexico	1
GSI Heimholtzzentrum	1
GMW Associates	1
Hamilton Sundstrand	1
Harvey Mudd College	2
Heidelberg Ionenstrahl-Therapie Centrum (HIT)	1
Health Canada Infoway	1
Idaho National Laboratory (INL)	2
Illinois Institute of Technology	1
Illinois State University	1
Instrumentation Technologies	1
Institut de Recherche sur les Lois Fondamentales de l'Univers (CEA)	1
Jefferson Lab	1
Johann Wolfgang Goethe-Universität Frankfurt	3
John Hopkins University Applied Physics Laboratory (JHUAPL)	1
Jülich Forschungszentrum	1
Kansas City Plant	1

Institutions and Number of Visits

Institutions (Ke - Of)	Number of Visits
Keck Graduate Institute	1
Lawrence Berkeley National Laboratory (LBNL)	3
Lawrence Livermore National Laboratory (LLNL)	6
Lopez Engineering	1
Los Alamos Chamber of Commerce	1
Los Alamos County	2
Los Alamos Family Strengths Network	1
Los Alamos High School	1
Los Alamos Site Office (LASO)	4
Louisiana State University	1
Massachusetts Institute of Technology (MIT)	2
Massachusetts Institute of Technology - Lincoln Laboratory	1
Metzgers	1
Michigan State University	1
Michigan State University National Superconducting Cyclotron Laboratory (NSCL)	1
Mississippi State University	1
MITRE Corporation	1
Mountain View College	1
National Conference of State Legislatures	1
National Instruments	1
National Jewish Health	2
National Network of Digital Schools (NNDS)	1
National Nuclear Data Center of BNL	1
National Nuclear Security Administration (NNSA)	8
New Mexico Public Education Department	1
National Security Technologies (NSTEC)	4
New Mexico State University (NMSU)	3
Northern New Mexico College (NNMC)	1
Northwestern University	1
Oak Ridge National Laboratory (ORNL)	3
OASIS	1
Office of Senator Jeff Bingaman	1
Office of Senator Tom Udall	1



Institutions and Number of Visits

Institutions (Oh - Te)	Number of Visits
Ohio State University	1
Pacific Northwest National Laboratory (PNNL)	1
Petersburg Nuclear Physics Institute	1
Phoenix Nuclear Labs	1
Piper High School	1
Pohang Accelerator Laboratory (PAL)	1
Private	8
Pro2Serve	1
Pueblo of Cochiti	1
Photonis	1
Proctor & Gamble (P&G)	3
Physics Today	1
Princeton Plasma Physics Laboratory (PPPL)	1
Red Rock Pictures	1
Regis University	1
Rensselaer Polytechnic Institute	1
Rg Construction Service LLC	1
RIKEN	1
San Ildefonso Pueblo	1
Sandia National Laboratory	9
Santa Fe Indian School	1
Santa Fe Public Schools	1
Science & Technology Facilities Council Accelerator Science and Technology Centre (ASTeC)	1
Self Help Inc.	1
SLAC National Accelerator Laboratory	2
Sigma-Aldrich ISOTEC	1
Southwestern College	1
Stanford Linear Accelerator Center	1
Struck Innovative Systeme	1
Summit Engineering	1
Technology Integration Group (TIG)	1
Texas A&M University	3
Technische Universität Dortmund	1

Institutions and Number of Visits

Institutions (Un - Up)	Number of Visits
Universidade Federal de Goiás	1
University of Nevada, Las Vegas	1
University of Notre Dame	1
United States Air Force	1
United States Air Force Academy	1
United States Army	2
United States Council for Automotive Research (USCAR)	1
United States Office of Management and Budget	1
United State Senate	1
United Way of Northern New Mexico	1
University of California Office of the President	1
University of California-Berkeley	2
University of California-Davis	2
University of California - Los Angeles	3
University of California - Merced	1
University of California - Riverside	1
University of Central Florida	2
University of California - Santa Cruz	2
University of California - San Francisco	1
University of Idaho	1
University of Liverpool	
University of North Dakota	1
University of Southern California	1
US Investigative Services	1
University of Michigan	1
University of New Mexico - Hospital	1
University of New Mexico - Los Alamos	1
University of Tennessee	2
University of Texas at Austin	1
University of Texas El Paso	1
University of West Florida	1
University of Wisconsin	1
University of Wisconsin - Madison	1
Uppsala Universitet	1



Institutions and Number of Visits

Institutions (V - Z)	Number of Visits
Varian Medical Systems	3
Washington University	1
Yale University	2
Yonsei University	1
Young Presidents' Organization	1
Ztec Instruments	5

Celebrations 2010





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

AOT, LANSCE Division Staff Members Awarded Defense Programs Awards of Excellence

AOT and LANSCE Division members were among the recipients of several Defense Program Awards of Excellence, presented by NNSA Deputy Administrator for Defense Programs Don Cook. The LANSCE Operations Team demonstrated extraordinary dedication and commitment to providing beam time to user of the LANSCE facility. The reliability goal for the accelerator beam delivered to the DP users is 85%. Beam reliability at or above 85% is considered world class for a facility such as LANSCE.

The annual awards recognize significant achievements in quality, productivity, cost savings, safety, or creativity in support of NNSA's Defense Programs. The awards also demonstrate how the Laboratory's capabilities support the Lab's nuclear deterrence mission.

LALP-10-020

LANSCE, AOT Division Members Recognized with Pollution Prevention Awards

Numerous LANSCE and AOT Division members are recipients of Pollution Prevention Awards for their efforts in pollution prevention and cleanup projects.

The awards recognize individuals or teams whose efforts over the past fiscal year have eliminated or minimized waste or pollution; conserved resources; procured green or environmentally preferred products; applied sustainable design principles; or identified other ways to reduce risk, save money, and enhance the Laboratory's mission.

LALP-10-020

Michal Mocko Recognized at Annual Technology Transfer Ceremony

Michal Mocko (LANSCE-LC) was among the recipients of the Programmatic Impact Award at the recent 12th Annual Technology Transfer Recognition and Awards reception. Mocko was a member of a Laboratory team honored for their efforts in the Stand-Off Radiation Detection System Program.

The Programmatic Impact Award recognizes individuals or groups who have made advancements to the Laboratory's programmatic mission through their interactions with industry partners.

LALP-10-020

Laboratory Communicators Recognized in International Competition

LANSCE Activity Report 2006 (Award of Merit) Clay Dillingham, Editor/Writer and Barbara Maes, Desktop Publisher and Brenda DeVargas, graphic artist (Communication Arts and Services, IRMCAS).

MPA Materials Matter, (Award of Merit), Karen Kippen and Robb Kramer (Experimental Physical Sciences Directorate, ADEPS) and Thomas King (Communication Arts and Services, IRM-CAS).

The Society for Technical Communication sponsored the 2010 International Technical Publications Competition. The international technical publications competition promotes, recognizes and encourages excellence in communication through printed media.

LALP-10-020

LANL Postdoc Association Wins Poster Award at National Postdoctoral Association Meeting

Katharine Page (LANSCE-LC) was among the recipients of The Los Alamos Postdoc Association (LAPA) which earned third place in the National Postdoctoral Association (NPA) Poster Competition for the poster "Combinatorial Strategies Adopted by Los Alamos Postdoc Association (LAPA) for Personal and Professional Growth of Postdocs." NPA presented the award at its annual meeting.

The NPA is a member-driven organization that provides a unique, national voice for postdoctoral scholars.

LALP-10-020

Frederik Tovesson Among Recipients of LDRD Day Poster Awards

Frederik Tovesson (LANSCE-NS) was among the recipients of a Best Poster Award at the recent second annual LDRD Day event. Tovesson was a coauthor of "A Novel Neutron Detector."

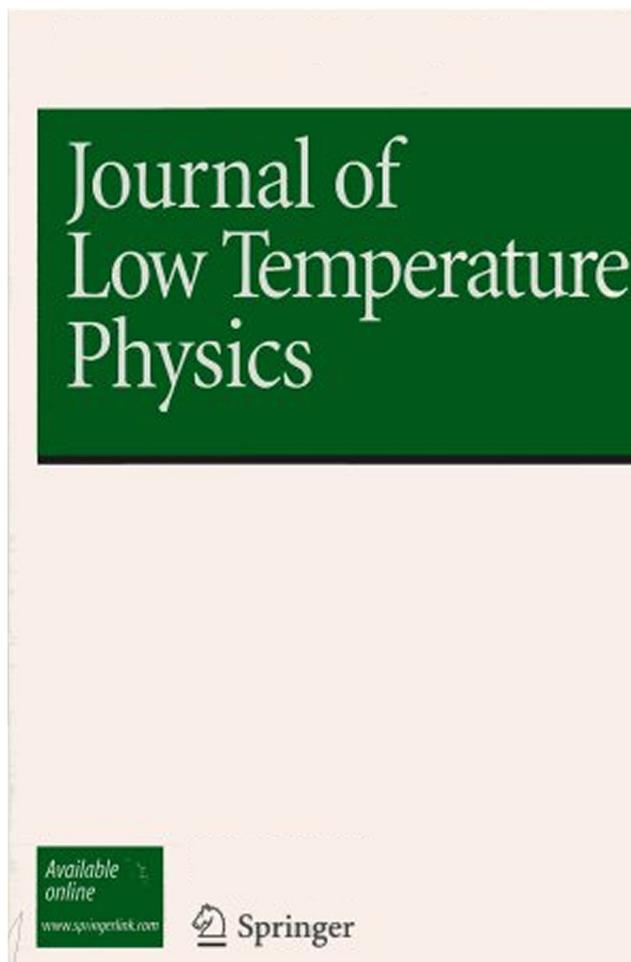
Laboratory Directed Research and Development (LDRD) invests in potentially high-payoff projects at the discretion of the Laboratory Director. These investments enable the Laboratory to anticipate and prepare for emerging national security challenges.

LALP-10-020

Alex Lacerda Joins Editorial Board of *Journal of Low Temperature Physics*

Alex Lacerda (LANSCCE-DO) has joined the editorial board of the *Journal of Low Temperature Physics*. The journal serves as an international medium for the publication of original papers and review articles on fundamental theoretical and experimental research developments in all areas of cryogenics and low-temperature physics. Subject areas include superconductivity, superfluidity, quantum solids, liquids and gases; matter waves; ultracold quantum gases; laser cooling; macroscopic quantum effects and coherence; magnetism and electronic properties; transport and phonon phenomena at low temperatures; quantum size effects and mesoscopic systems; low-temperature technology that concerns new areas of experimental research; and applications. Lacerda is a recipient of a 2006 LANL Distinguished Performance Large Team Award for the 100T project, a Japanese Society for Promotion of Science Fellowship, a 2009 LANL Women's Diversity Working Group Outstanding Mentoring Award, and has authored more than 190 publications.

AOT and LANSCCE - The Pulse, June 2010.
LALP-10-020





James Rhyne selected to be a Neutron Scattering Society of America Fellow

The Neutron Scattering Society of America (NNSA) selected James J. Rhyne to be a Fellow. He is cited “for extraordinary research on magnetic materials and thin films and outstanding leadership and support of major U.S. neutron facilities and research opportunities.” Rhyne is the deputy group leader for science in the LANSCE–Lujan Center (LANSCE-LC). His primary research interests are magnetic exchange, anisotropy, and magnetostriction effects in rare earth metals and compounds with particular emphasis on rare earth metallic superlattices. Rhyne has authored more than 230 papers in physics and materials science, has written 12 book chapters and invited review chapters, and has presented more than 30 invited talks at national and international conferences. He is a Fellow of the American Physical Society and was awarded the Doctor Honoris Causa from the Université Henri Poincaré in Nancy, France. Rhyne joined the Laboratory in 2003.

The main goal of the Neutron Scattering Society of America is to stimulate, promote, and broaden the use of neutron scattering in science, engineering and technology. Through the Fellows Program, the NNSA recognizes members who have made significant contributions to the neutron scattering community in North America in one or more of the following areas: advances in knowledge through original research and publication, innovative contributions in the application of neutron scattering, contributions to the promotion or development of neutron scattering techniques, and service and participation in the activities of the NNSA or neutron community.

Each year, election to fellowship of the NNSA is limited to no more than one half of one percent of the membership. The new Fellows will be recognized at the 2010 American Conference on Neutron Scattering to be held in Ottawa, Canada, in June.

AOT and LANSCE - The Pulse, May 2010.
LALP-10-020



Andrey Kovalevsky and Zoe Fisher recipients of Los Alamos Distinguished Postdoctoral Awards

The awards recognize individuals or small teams who have made an outstanding and unique contribution to the Lab's programmatic and scientific work during FY09. Their accomplishments display unusual creativity, innovation, or dedication.

Kovalevsky and Fisher (B-8) came to Los Alamos as a Director's Postdoctoral Fellow and a postdoctoral research associate, respectively. They received an award for the Protein Crystallography Station Team. The team is recognized for successfully running the Protein Crystallography Station (PCS) at the Lujan Center, as well as the effective application of X-ray and neutron crystallography to understand enzyme mechanisms related to three proteins.

The PCS is a neutron crystallography capability for the external structural biology community, funded by the Office of Biological and Environmental Research of DOE and run by the Bioscience Division as part of the LANSCE user program. Kovalevsky and Fisher provided full scientific and technical coverage for the PCS, coordinated the peer review process, and scheduled beam time. In the absence of senior and more experienced scientists to carry out this work, the team took responsibilities beyond duty calls and provided the services. In addition to presenting seminars and posters, the team's work on understanding the mechanisms of three different enzymes resulted in a number of publications, several in top-ranking journals such as the *Journal of Molecular Biology*, the *Journal of American Chemical Society* and the *Journal of Medical Chemistry*. Paul Langan (B-8) nominated them. The Deputy Director of the Lujan Center stated, "the scientific motivation and expertise of the two individuals is rarely found in other early career scientists."



 S. Zoe Fisher



 Andrey Kovalevsky

AOT and LANSCE - The Pulse, April 2010.
LALP-10-020



LANSCCE Summer Students Won Poster Award

As part of the Neutron Induced Fission Fragment Tracking Experiment (NIFFTE) project, two LANSCCE summer students, Dana Duke and Nicholas Fuller, won a poster award in the Physics Category at the recent Student Symposium for their research on the Time Projection Chamber (TPC)

gas handling system. The system remotely controls the flow of multiple gas sources into the TPC. Major components of the gas handling system include solenoid valves, pressure transducers, and mass flow controllers.

LALP-10-020

The NIFFTE TPC Gas Handling System
Dana Duke and Nicholas Fuller
Los Alamos National Laboratory, LANSCCE-NS, for the NIFFTE Collaboration

1. Motivation

The Neutron Induced Fission Fragment Tracking Experiment (NIFFTE) uses a time projection chamber (TPC) to determine the fission cross section of actinides. Although the cross section has been previously measured using various methods, the uncertainty can be reduced to sub 1% using a TPC. See Figure 1. Higher accuracy of cross section measurements will improve efficiency of nuclear reactor operations and will lead to better understanding of the fission process.

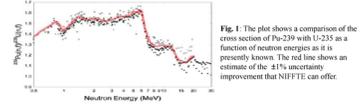


Fig. 1: The plot shows a comparison of the cross section of Pu-239 with U-235 as a function of neutron energy as it is presently known. The red line shows an estimate of the ~4% uncertainty improvement that NIFFTE can offer.

2. Fission Cross Sections

A cross section is a property of the target and projectile during a collision. The fission cross section extends this idea to nuclear fission to determine the probability of whether a fission event will occur. Fission cross sections vary with the energy of the incoming particle and is given by the equation:

$$C = N\sigma\phi$$

Located at the LANSCCE-WNR fast neutron beam at 90L, incident neutrons are directed at actinide targets. The neutron flux is given by ϕ , σ is the cross section, N is the number of target nuclei, and C is the number of fission counts. Cross sections are usually measured in a ratio with a U-235 cross section. Thus, higher precision in the measurement of U-235 will affect all cross section data.

2. The NIFFTE TPC

A TPC houses a target and gas. The TPC can be seen in Figure 2. When an incident neutron collides with a target plate, it may induce fission. Gas particles are ionized as they move through the chamber. The resulting electrons will drift towards detecting pad planes through an electric field. By reconstructing the trail, the particle identity, velocity, and trajectory are measured. See Figure 5 for an example of particle tracking using ionization.

The TPC will significantly reduce systematic errors associated with fission cross section measurements through use of a sophisticated detection system. This will ensure that each fission fragment will be identified, delivering fission cross sections with unprecedented precision.

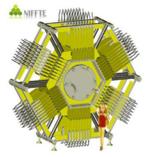


Fig. 2: A computer generated image of the NIFFTE TPC. The central chamber houses the gas and targets. It is surrounded by detector components. A doll is shown for scale.

3. The Gas Handling System

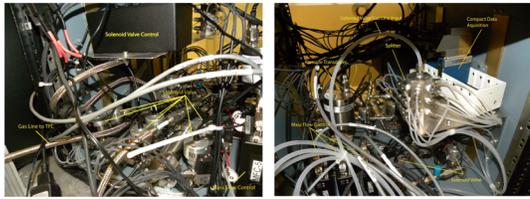


Fig. 3: The gas handling system hardware is shown from the left and right sides respectively. Major components are labeled. Gas lines to the TPC are not shown.

A gas handling system is essential for a TPC apparatus since its tracking method is based on gas ionization. The GHS is responsible for controlling the flow of gas and pressure within the TPC. The NIFFTE TPC is capable of measuring cross sections for gaseous targets and use them for normalization. The cross-section of elastic Hydrogen scattering will be measured for calibration purposes since the H(n,n) cross-section is known to a high degree of certainty.

The system will initially use P10 (90% Ar, 10% CH₄) for the drift gas until Hydrogen testing on solid targets is performed. In the future, gaseous Rb-83 will also be flowed through the system intermittently with the counting gases for calibration. One of the innovations of this GHS is its ability to flow multiple gas sources through the system. Additionally, the TPC can be calibrated regularly during data runs.

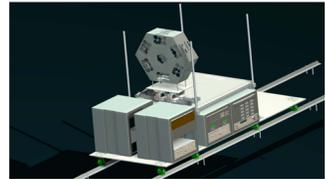


Fig. 4: A computer rendering of the TPC mounted on the adjustable table with slow controls and the gas handling system.

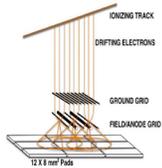


Fig. 5: A fission fragment travels along a path. It ionizes electrons which move through the electric field and strike the pad plane. By tracing these paths, the fragment's path in the xy-plane can be reconstructed. By knowing electron drift velocity in the gas medium and measuring time, the z-component of the fragment can be determined.

4. Hardware

In order to provide optimum control over various properties of the gas (e.g. flow rate, pressure, type of gas, etc.) the GHS uses several different forms of hardware. Mass flow controllers are used to regulate the amount of gas entering and exiting the system, thereby controlling the flow rate within the TPC. Solenoid valves control which gases flow and the pipes through which they travel. Pressure transducers measure the gauge pressure inside the system, and are also responsible for the relay that prevents overpressure in the GHS and TPC. See Figure 3 for a photograph of the assembled hardware for the system. A rendering of the experiment setup is shown in Figure 4.

5. Software

In order to control the GHS while the TPC is collecting data, a LabVIEW program has been developed. See Figure 7. This program uses RS-232 cables to enable the adjustment of the mass flow controllers, as well as the monitoring of pressure within the system. In addition, each individual solenoid valve can be opened or closed by using two modules connected to the compact data acquisition system (cDAQ).



Fig. 7: The front panel of the LabVIEW program. This is used to control the gas handling system by opening solenoid valves and varying the amount of gas through the MFCs. The pressure in the system can also be monitored.

6. Experiment Status

The gas handling system is being installed at LANSCCE as of July 2010. Prototype testing began in December 2009. Beam tests will begin on the NIFFTE TPC prototype in August-September 2010.

6. Acknowledgements

The NIFFTE collaboration involved three national labs: LANL, LLNL, INEL, and 6 universities. Also, thanks to Lucas Snyder, Fredrik Tovesson, and Jennifer Klay.

The NIFFTE Time Projection Chamber Gas Handling System Assembly poster as shown during the NIFFTE Collaboration.

Acknowledgements

The 2010 LANSCE Activity Report was produced with the valuable contributions of LANL all subject-matter co-authors, co-editors and select articles from the 2010 suite of *The Pulse*. Special acknowledgment to the ADEPS Communications Team, Karen Kippen (ADEPS), Clay Dillingham (IRM-CAS), Sheila Molony (IRM-CAS) and Guadalupe Archuleta (IRM-RMMSO) for their contributions and generous support.

This is the ninth report in this series.



 Aerial view of LANSCE looking east over the mesas of northern New Mexico.



LA-UR-11-05580

Approved for public release; distribution is unlimited.

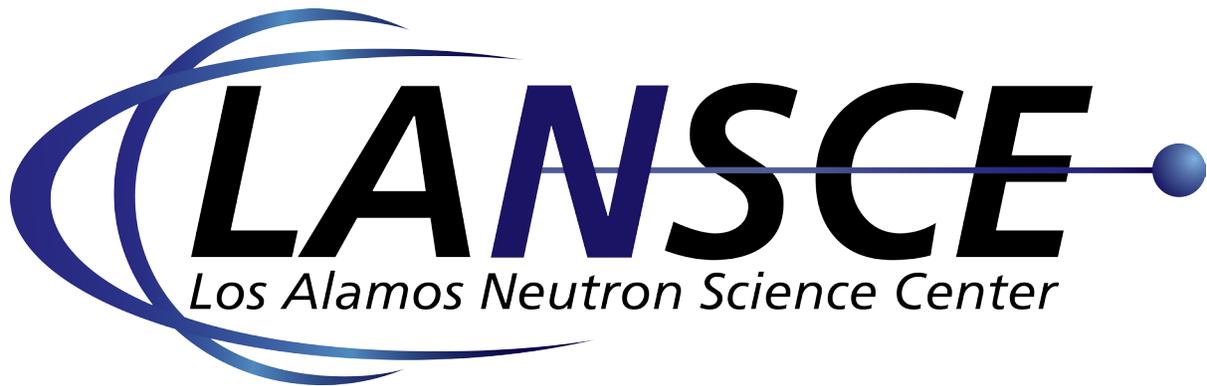
Issued: September 2011

LANSCe Activity Report 2010

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- Isotope Production Facility
- Lujan Neutron Scattering Center
- Proton Radiography
- Ultra-Cold Neutrons
- Weapons Neutron Research Facility
- LANSCE User Program

