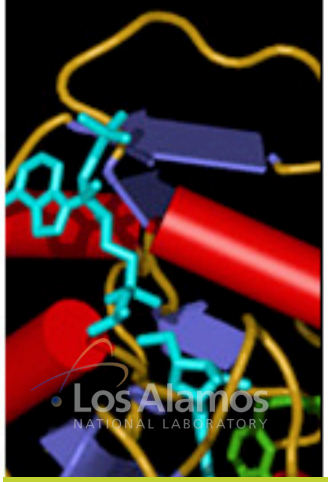
AOT & LANSCE The Pulse

September 2012






# Biennial national neutron scattering conference features strong Lujan Center presence


*Claire White receiving the Prize for Outstanding Neutron Scattering Student Rsearch from Bruce Gaulin, president of the Neutron Scattering Society of America.*

The 2012 American Conference on Neutron Scattering was held recently in Washington, D.C. and featured a number of presentations by Los Alamos researchers.

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

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

Other Lujan Center researchers presenting invited talks included Thomas Huegle discussing "Triphenylmethane and its potential applications in moderator design," Monika Hartl, "Small angle scattering of methane dissolved in water," and Saurabh Singh, "Influence of capping layer rigidity on properties of supporting temperature sensitive hydrogel polymers using neutron reflectivity."

*Technical contact: Mark Bourke*

# From Alex's Desk



Colleagues,

Let me take this opportunity to give you a quick summary of the August 27th inadvertent spread of technetium-99 that took place at LANSCE's Lujan Center in the HIPPO (High-Pressure-Preferred Orientation) flight path, which is located in ER-1. It is paramount to emphasize that based on the level of technetium-99 spread and the resulting contamination that workers and the public were not exposed to a health risk. Technetium-99 is a particular type of beta radiation. Beta emitters occur naturally in the environment, can travel through several feet of air, but are generally stopped by clothing and skin. Due to off-site contamination and because the Laboratory had to mobilize DOE's Radiological Assistance Program (RAP) teams, however, the perception of this event varied from many different viewpoints.

During this whole process—from the Laboratory establishing the Emergency Operations Center (EOC) during the first couple of days after the event discovery to now, during the recovery phase—LANSCE has received a great amount of support. It is important to recognize that considering the complexity of the accelerator, along with the various types of experimental facilities, the LANSCE facility continues to maintain a high level of safe operations. For the past six years, based on the rates for Total Recordable Cases (TRC) and Days Away Restricted-Transferred cases (DART), LANSCE's injury and illness metrics are comparable to any national lab facility with the same level of complexity—an important metric proving once again the dedication and attention to safety and security we have at TA-53. And it is thanks to our integrated and dedicated scientific, technical, and operational personnel that we are able to continue delivering beam and hosting users to the other four of LANSCE facilities: IPF, WNR, pRad, and UCN.

**'During this whole process... LANSCE has received a great amount of support.'**

We are now in the process of providing documentation for a DOE investigation that's taking place. The procedures we have had in place for many, many years--as far as work control, materials handling, and mentoring of employees, students, and postdocs--are good, but have room from improvement. The Laboratory Director has put forward a set of guidelines with clear expectations on how to collectively improve and maintain the quality and the safety of mentoring and work space. Based on that, TA-53 management is diligently performing extensive MOVs (Management Observation and Verification) of work and office spaces, in addition to work authorization at all levels. I fully understand and appreciate that the MOVs are taking place in the middle of the run cycle and in addition to the programmatic work we need to get done. Consider it as part of the job.

In the MOVs I participated in so far, there are many places where housekeeping was reasonable for a safe and secure work environment. There were others, however, where improvements are needed. We are in the process of collecting data and determining the level of support needed to improve some spaces. There are others, however, where just some level of a graded approach and

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# From Howard's Desk

Los Alamos National Laboratory and Sandia National Laboratories jointly hosted this year's Accelerator Safety Workshop (ASW) in Santa Fe (at the Eldorado hotel), held Sept. 25-27. This was the first time that NNSA (via Office of Science) labs hosted this event. The ASW brought together people from across the DOE complex to discuss safety issues related to accelerators and accelerator facilities. One point of emphasis this year was finalizing updated content for the Accelerator Safety Order Guide. The organizing committee at LANL was led by Patty Vardaro-Charles with help from me, Linda Zwick, Rosemary Romero, and Mike Duran.

*Howard Nekimken, LANSCE-DO*

**Desk . . .** organization will go a long, long way. Properly disposing of no longer needed material / equipment was a constant theme during this exercise. The bottom line is, if you have not used for the last 3 years, you probably will not need in the future. The same goes for empty boxes and packing material; don't just keep it around your labs and/or offices.

I also would like to take this opportunity to thank the LANSCE–Lujan Center members. Their level of engagement, at all levels, is to be applauded. And thank you all for helping—and welcoming—Lujan Center members with offices and meeting places.

Last, but not least the 2011 LANSCE Activity Report is now posted at lansce.lanl.gov. Thank you again for your contributions.

*LANSCE Deputy Division Leader Alex Lacerda*

*New experimental capabilities at Lujan Center*

# Development of high pressure-temperature cell to study interface processes

Solid-liquid interactions have controlled the success or failure of many attempts to engineer Earth's subsurface for energy and/or environmental applications, yet these interactions are not well understood nor can they be optimized effectively, except using Edisonian approaches. Mineral growth or dissolution and well-bore corrosion at geologic carbon sequestration sites, corrosion and scaling in nuclear reactors and geothermal systems, and hydrocarbon extraction from conventional and unconventional oil and gas reservoirs are controlled by interactions at solid/fluid interfaces at elevated pressure-temperature (P-T). Maintaining or restricting porosity to extract hydrocarbons in deep-gas fields, stimulating geothermal reservoirs, and maintaining porosity and seals in geologic carbon sequestration reservoirs all require accurate predictions of the dissolution and precipitation of solids in dense, often supercritical, mixed-volatile ($H_2O$-$CO_2$–hydrocarbon) fluids. Because such interface processes are important, they have been the subject of a great deal of R&D primarily at ambient P and T, and are reasonably well understood at such conditions. However, investigations at high P-T, the critical regime for many energy applications, are much more limited.

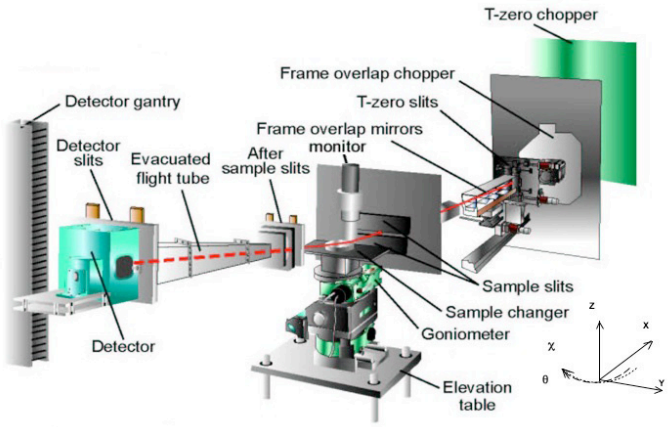


*Figure 1. Schematic of SPEAR neutron reflectometer*

Neutron reflectometry (NR) is a powerful technique for examining fluid properties, particularly density, within a few nm of interfaces because of the ability of neutrons to penetrate high P-T cells and to interrogate buried structures, combined with their sensitivity to $H_2$($D_2$) in hydrocarbon-rich fluids. NR thus represents a novel method for high P-T interface studies both for mineral systems and material systems in general. At LANSCE the time-of-flight SPEAR (Figure 1) reflectometer provides "state-of-the-art" NR capabilities to study solid-liquid interfaces. Recently an NR cell to conduct experiments at moderately elevated P-T (200 MPa and 200°C), (Figure 2), has been developed. This cell allows study of two-inch-diameter disks of minerals and other materials in contact with variety of fluids including $CO_2$-saturated liquids. Initial applications focused on corrosion of aluminum at elevated P-T and on calcite/fluid interfaces.

The new experimental capabilities developed for probing high P-T interfacial properties are described in an upcoming publication of *European Journal of Physics Plus*. They can potentially be applied to a range of LANL mission areas where high P-T solid/fluid interface interactions are important, including deep-gas extraction, high P-T corrosion of nuclear fuels and cladding, performance of waste forms in repositories, and understanding and controlling a range of

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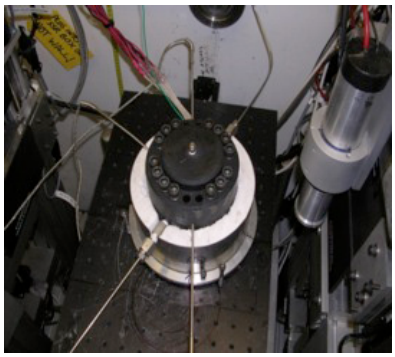

*Figure 2. The high P-T NR cell developed in the Lujan Center shown here on sample stage of SPEAR. From top: P-T cell with thermal insulation jacket; P-T cell with top half jacket removed; P generation and control board.*

***Development...*** engineered geosystems in extreme P-T environments. This work benefited from the funds provided by the LDRD-ER proposal "Determination of Fluid Properties at Carbonate Interfaces-An Integrated Experimental and Theoretical Approach," and the use of the SPEAR neutron time-of-flight spectrometer at Lujan Neutron Scattering Center (LANSCE-LC) at LANSCE funded by the DOE Office of Basic Energy Sciences and Los Alamos National Laboratory under DOE Contract DE-AC52-06NA25396.
*LANL technical contacts: Peng Wang, Don Hickmott, and Jaroslaw (Jarek) Majewski*

Reference:"High Pressure and High Temperature Neutron Reflectometry Cell for Solid-Fluid Interface Studies," by P. Wang (LANSCE), A. Lerner (Earth and Environmental Sciences Division), M. Taylor (LANSCE), A. Misra and J. Baldwin (Center for Integrated Nanotechnologies), A. Voter, D. Perez, and C.Y. Lu (Theoretical Division), R. Grubbs (Sandia National Laboratories), J. Majewski (LANSCE-LC), D. Hickmott (Earth and Environmental Sciences Division), accepted for publication in *European Physics Journal,* 2012.

# Role of elastic bending stress on magnetism of a manganite thin film studied by polarized neutron reflectometry

Los Alamos researchers and collaborators used polarized neutron reflectometry (PNR) to measure the neutron spin-dependent reflectivity from a single crystalline $(La_{1-x}Pr_x)_{1-y}Ca_yMnO_3$-δ (x = 0.52±0.05, y = 0.23±0.04, δ = 0.14±0.10) thin film as functions of applied stress and temperature. They unequivocally show that the application of elastic bending stress to the manganite film strengthens the ferromagnetic phase. Remarkably, 0.01% compressive strain produces a 20% increase of the saturation magnetization. This result suggests a means to improve the magnetic properties of complex oxide films. *Physical Review B* published the work.

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

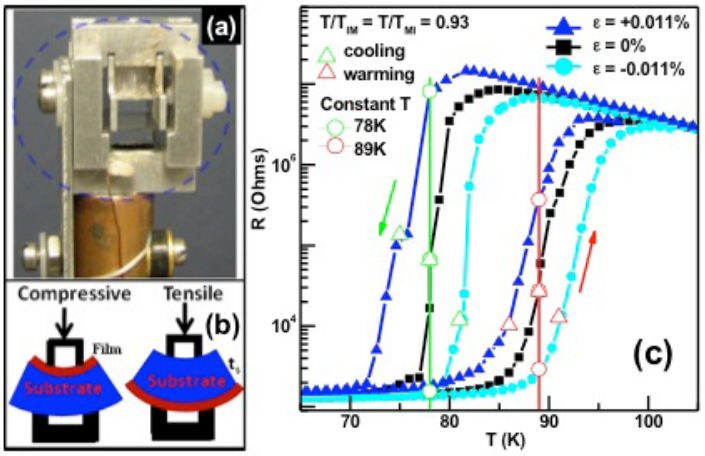


*Figure 3: End-view image of the four point jig (circled) mounted on a cryostat (a) and side-view schematic representation of applied bending stress (b). (c): Transport measurements of the film at different applied bending stress/strain, tensile (▲), compressive (●) and no strain (■). Open circles and open triangles represents constant T and constant T-ratio ($T/T_{IM} = T/T_{MI} = 0.93$) at which we simultaneously measured the neutron reflectivities.*

Scientists used the Lujan Center's Asterix polarized neutron reflectometer, which is intrinsically sensitive to interfacial magnetism, to examine the magnetism occurring across the thin dimension of a $(La_{1-x}Pr_x)_{1-y}Ca_yMnO_3$-δ single crystal film. To apply elastic stress, the scientists developed a four-point bending jig especially designed for neutron reflectometry (Figure 3). The jig was also designed to allow the scientists to measure the resistance of the film during the experiment (Figure 3). Data corresponding to the two polarization states of the neutron beam were obtained at selected temperatures (Figure 4, upper). From these data the saturation magnetization M depth profile was obtained

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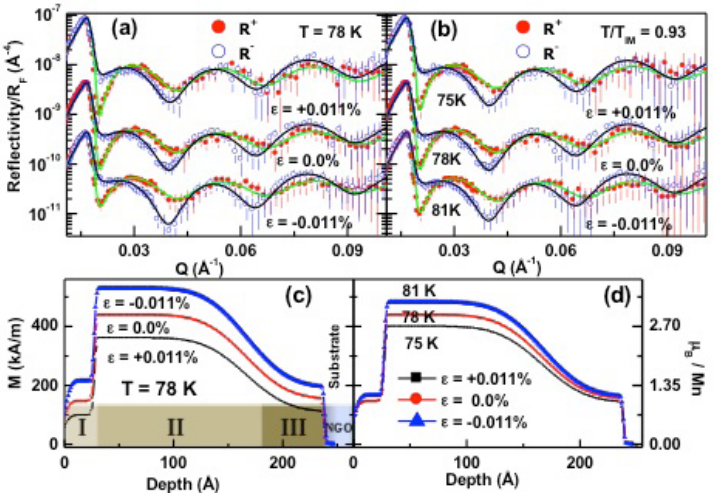


*Figure 4: PNR measurements from LPCMO film for different applied strain at constant temperature (a) and constant $T/T_{IM}$ (b) while cooling. Reflectivity data at different applied stress/strain are shifted by a factor of 5 for the sake of clarity. (c) and (d) show the magnetization (M) depth profile corresponding to (a) and (b) respectively.*

***Elastic bending . . .*** (Figure 4, lower). The result shows that independent of the film's chemical composition (which changes across its thickness), compressive strain increases the *M* by ~20%, while tensile strain decreases *M* by the same value. The influence of strain on the ferromagnetic phase of manganite films has been decidedly mixed until now. With the development and application of the four-point-bending-jig to neutron scattering we have the opportunity to turn just the "elastic strain knob." The jig and neutron scattering protocol are likely to have an impact on a broad range of important materials, including piezeomagnetic and multiferroic materials.

Los Alamos researchers include Surendra Singh, M.R. Fitzsimmons (Lujan Center, LANSCE-LC), and T. Lookman (Physics of Condensed Matter and Complex Systems, T-4). Collaborators are H. Jeen, A. Biswas (University of Florida), M.A. Roldan (Universidad Complutense de Madrid, Spain), and M. Varela (ORNL). Reference: "Role of elastic bending stress on magnetism of a manganite thin film studied by polarized neutron reflectometry," *Physical Review B* **85**, 214440 (2012). The DOE Office of Basic Energy Sciences supported the LANL portion of the research. The Lujan Center is a national user facility supported by DOE Basic Energy Sciences. The work supports the Lab's Energy Security mission area and the Materials for the Future and Science of Signatures science pillars.
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## Celebrating service

Congratulations to the following AOT Division employees celebrating service anniversaries recently:

| | |
|---|---|
| Bruce Carlsten, AOT-HPE | 30 years |
| Philip Chacon, AOT-IC | 10 years |
| Dennis Ortiz, AOT-OPS | 10 years |

# HeadsUP!

## TA-53 WSST: A strong and active presence on the LANSCE mesa

By Jean Trujillo
TA-53 WSST secretary

With 25 members representing four divisions, the TA-53 Worker Safety and Security Team is actively engaged in improving the safety and security of the workers on the LANSCE mesa. As just one example of its efforts, in reponse to residents' feedback the WSST coordinated the trimming of tree limbs blocking the view of the crosswalk near TA-53, Bldg. 1, resulting in increased pedestrian visibility.

The TA-53 Worker Safety and Security Team also recently held a successful vehicle safety check. Forty-one vehicles were inspected in lower parking lot of Building 6 for simple maintenance issues such as lights, tires, windshield, and wipers that contribute to a safe driving experience. TA-53 WSST members who participated included Eric Larson, Kristy Ortega, Jean Trujillo, Damian Romero, Marlon Castle, Nathan Okamoto, Jason Burkhart, and Victor Vigil. Karen McHugh (TA-48) and Alice Trujillo (TA-48) assisted with the vehicle safety check. The event also featured the distribution of free gift bags and prizes. We are planning to have a winter vehicle check in October.

For more information about the TA-53 WSST, please see int.lanl.gov/org/padste/ade/accelerator-operations-technology/worker-safety-security-team/index.shtml

## UI Division call center activated

Utilities and Institutional Facilities (UI) Division has activated a call center to help improve and more closely work with tenants to meet their maintenance and facility operation needs. The call center provides another method for requesting services and is a communication tool to clarify delivery expectations that UI can meet and deliver. The call center number is 667-2488. Through the UI call center, employees can make requests from UI for reporting facility-related problems; request routine maintenance or repairs; or request office furniture or equipment moves. Employees can still make requests through the Facility Request System. Questions? Contact Martin Aguilera, MSS-UI maintenance manager at 5-4720.

## Worker Safety and Security Teams

WSST stands for worker safety and security team; the key word being "worker." Although one might think WSSTs are just another of the many "safety things" we are required to do and dismiss them as trivial, WSSTs are, however, an opportunity to have a say in how we treat safety and security at the Lab. This is what the "worker" in WSST means. We are a team run by the workers in collaboration with management.

In December 2005 Los Alamos National Security (LANS) was awarded the contract to manage and operate Los Alamos National Laboratory. As part of the proposal, LANS set as a goal attaining Department of Energy Voluntary Protection Program (VPP) Star Status. Star recognition is the highest achievement level in the VPP and recognizes outstanding safety and health programs. VPP's main tenant is that management and workers come together to solve long-standing, as well as short-term, safety and health problems present in the everyday workplace. As part of working toward VPP certification, the institutional WSST was formed late in 2006.

The worker is the expert at how to improve safety and security in his or her workplace. These improvements may include easy access to needed tools, well-maintained parking lots and sidewalks, or repair and maintenance of the facilities in which we work. As workers we may be frustrated and discouraged at the perceived lack of interest in our workplace's condition and the difficulties in our ability to address these problems. We seem to be required to read more and more documents to address safety compliance, but have seen little participation in actually solving existing problems.

Our directorate's WSSTs actively try to solve these problems. ADEPS management is active and supportive, and while financial constraints limit what can be done to solve problems, it has been effective in solving many problems in the past few years. Below are some of the many accomplishments due to WSST involvement.

Problems solved due to solutions teams' walk-arounds include

- Emergency lights are in the process of being installed in a lab at MST. The lab is very dark with the lights off and would be dangerous in the case of a power failure.
- Mystery circuit breakers in a lab were identified, supplying power for instruments in that lab.
- A faulty plug in behind a glove box was discovered and repaired.
- Electrical safety refresher courses were surveyed. The results were given to instructors in hopes that classes can be refurbished to better meet our needs.
- Crosswalk signage was placed in more obvious places at TA-53 to enhance safety.
- Trees that were intrusive to walkways have been trimmed. A dead tree in front of the Materials Science Laboratory was cut down after WSST intervention. It took further intervention to get it removed.
- Additional cell phone boxes were placed at TA-3 in a timely manner.
- WSST facilitated repair of exterior lighting along pedestrian path at TA-35 within 2 days.
- Coordinated with ice and snow removal teams to increase removal efforts in problem parking and pedestrian walk areas.
- After WSST intervention a mess of ice and mud left in the government vehicle parking spots left after fire hydrant repair was cleaned up.

These are just a few of the many accomplishments of the WSSTs in your directorate. We would like to add more to the list, which could be accomplished with more participation among the workers. Please get to know the WSST reps in your groups and work with them on problems that exist. They may be able to help you.

The photos on the next page are of your division reps. Can you match the name and face to your division? If you don't know the rep in your group, the face you see can tell you who he or she is. Get to know your group rep, or even better, become your group rep or alternate rep. With help from workers we can shed light on problems that need fixing at the worker level, and get some of them solved.

*The ADEPS WSST*

# Take the 'Know your Worker Safety and Security Team rep' QUIZ!

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7

KEY: A7, B4, C6, D3, E1, F2, G5