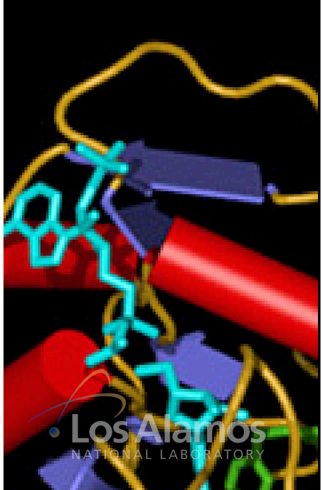
AOT & LANSCE The Pulse

May 2012

INSIDE



Martha Zumbro and Subrata Nath

Accelerating the pace of scientific research

By Diana Del Mauro
ADEPS Communications

As joint Accelerator Operations and Technology (AOT) deputy division leaders, Subrata Nath and Martha Zumbro are doing double duty.

Together, they're keeping the Los Alamos Neutron Science Center (LANSCE) humming while prepping for the creation of MaRIE, (Matter-Radiation Interactions in Extremes), the Laboratory's proposed experimental facility that will bring transformational materials solutions to national security challenges.

Both started their careers at LANSCE and have paired up before on high-visibility projects, including the Dual Axis Radiographic Hydrodynamic Test (DARHT) facility.

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

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

Tried and true leadership

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

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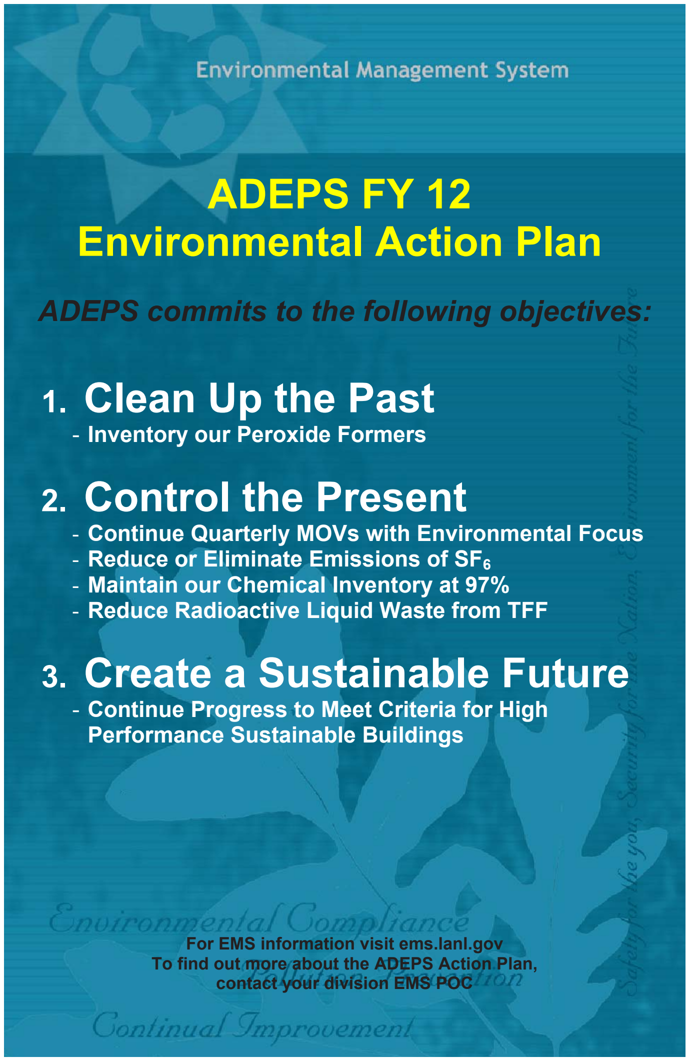
From Steve's Desk

It's time to come up to speed on the Directorate's implementation of the FY12 Environmental Action Plan (EAP) that was developed in support of the Lab's Environmental Management System. The ADEPS team responsible for developing and disseminating the plan includes Steve Glick from P Division (also serves as the Directorate Point of Contact), Jim Coy from MST, Cathy Padró from MPA, and Frances Aull from LANSCE.

Our 2012 Environmental Action Plan addresses our impact on the environment. You have seen the poster: we will attack this from three angles—the past, the present, and the future.

Let's look at our objectives, and the specific targets we have developed to meet the objectives. These objectives parallel the LANL institutional objectives, with the targets fine-tuned to fit our Directorate's needs.



Objective 1 – Reduce Environmental Risks from Historical Operations, Legacy, and Excess Materials and Other Conditions Associated with Activities No Longer a Part of Current Operations (CLEAN UP THE PAST). Last year, we worked with the Lab's Environmental Team to understand our chemical waste generation profile so that we can establish long-term waste-reduction goals. Our focus this year is peroxide formers—we will perform a focused inventory of out-of-date peroxide formers to ensure proper testing and to identify potential disposal pathways.

Objective 2: Control and Reduce Environmental Risks from Current, Ongoing Operations, Mission, and Work Scope (CONTROL THE PRESENT). Managers will continue to emphasize environmental aspects during MOVs, we will conduct an annual chemical inventory, and we will disseminate information on the EAP using posters, group briefings, and e-mails. In addition, we are specifically targeting reduction or elimination of SF_6 releases. SF_6 is an extremely potent greenhouse gas and reducing or eliminating emissions is an institutional goal associated with the Site Sustainability Plan. Finally, MST Division was in line to receive institutional funding to reroute non-RLW (rad liquid waste) discharges at Target Fab Facility that currently go to the RLW Treatment Facility, but the project is on hold due to the funding being withdrawn.

Objective 3 – Reduce Environmental Risk from Customer Expectations and Regulatory Requirements Associated with Future Conditions, Managing these in Alignment with Short- and Long-Term Planning, Work Scope Projects, etc. (CREATE A SUSTAINABLE FUTURE). We will continue to work towards the requirements for High-Efficiency Sustainable Building recognition for the MS-OB (03-1415), including additional tenant education and the formation of a Green Team.

To succeed, we need everyone to "up" their awareness and take action. Turn off lights in offices, conference rooms, hallways, and labs when not in use. Get that leaking faucet/toilet/urinal fixed (contact your facilities coordinator). Turn off computer peripherals when not in use. Alter your purchasing habits–Purchase GREEN. Use the blue and green recycling bins. Share chemicals, minimize chemical inventories, purchase safer alternatives, recycle and dispose properly. Salvage all unnecessary or unused (and not needed) equipment. Nominate a deserving colleague for a P2 (Pollution Prevention) Award!!

Document, Record & Report all significant environmental actions that you take that positively affect the environment. Remember, if it's not recorded, it didn't happen. Please send your environmental action reports (e-mails are fine) to your Division contact: jcoy@lanl.gov for MST; padro@lanl.gov for MPA; aull@lanl.gov for LANSCE, and sglick@lanl.gov for P Division. This will ensure that our efforts continue to get the deserved recognition for our environmental efforts.

Steve Glick, ADEPS EMS point of contact

Zumbro and Nath . . . Zumbro's also responsible for the safe and effective day-to-day operation of the accelerator. She starts each day reviewing beam status and call-in logs from the night before to assess equipment operation. She and Nath meet every day to discuss concerns. "I worked in a user role at DARHT for awhile, reminding me of how it feels to be a user and the frustrations that can accompany being dependent on an accelerator for a successful experiment," she said.

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

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

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

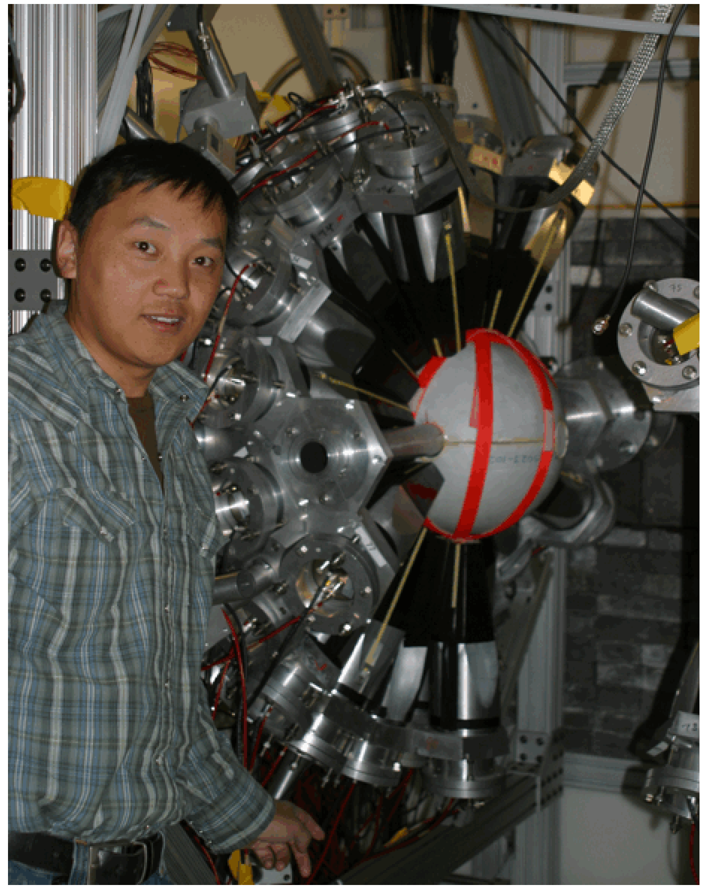
"Subrata brings a tremendous breadth of knowledge from several accelerator facilities and a wealth of experience in working to develop technology," Erickson said.

Returning to LANSCE

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

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

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



B. Baramsai with the DANCE detector.

Experiments hint that the atomic nucleus still holds some surprises

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

The statistical parameters depend on a quantum-mechanical property of the excited nucleus called spin. Recently, a novel method for determining excited-state spins by counting the number of gamma rays emitted in a nuclear reaction has been developed. In a paper in *Physical Review C*, B. Baramsai (North Carolina State University [NCSU] postdoctoral researcher, resident at LANSCE) and co-workers at NCSU, in collaboration with LANL and Lawrence Livermore National Laboratory, presented an elegant technique

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Nucleus… to use DANCE as a "spin-meter" through statistical pattern recognition techniques. When they tested the technique in a new and precise determination of excited-state properties in reactions on gadolinium-155 (155Gd), they obtained results in substantial agreement with previous measurements. This method has the advantages that there is no need to select prototype resonances, the maximum amount of information is used, and a confidence level is obtained for the correctness of the spin assignment. These results demonstrate that the new pattern recognition method is a valuable addition to methods of determining the quantum numbers of resonances studied with the DANCE calorimeter. The scientists have planned measurements on nuclei where existing data is incomplete or contradictory. Reference: "Neutron Resonance Parameters in 155Gd Measured with the DANCE γ-ray Calorimeter Array," *Physical Review C* **85**, 024622 (2012). Los Alamos coauthors include A. Couture, R.C. Haight, J.M. O'Donnell, and J.L. Ullmann (Neutron and Nuclear Science, LANSCE-NS); T.A. Bredeweg, M. Jandel, A.L. Keksis, and R.S. Rundberg (Nuclear and Radiochemistry, C-NR).

A paper published in *Physical Review Letters* by P.E. Koehler (Oak Ridge National Laboratory) in collaboration with Los Alamos researchers, hints that nature may still have some surprises. One of the consequences of the theory of random systems is that the average properties and their distribution should not change appreciably with small changes in excitation energy. The scientists used the DANCE detector and a "spin meter" technique to make accurate measurements of the probability for gamma-ray emission following the capture of neutrons by samarium-147 (^{147}Sm). The results revealed abrupt changes in the average properties of highly excited states in the product nucleus 148Sm for neutron energies above and below 300 electron volts. This result was not anticipated by the standard theory that underlies several models used to calculate nuclear reaction probabilities for applications in nuclear energy and defense. The new results indicate that the standard theory may be incomplete under certain conditions. Such effects could have important consequences for applications such as nuclear astrophysics and nuclear criticality safety, in which models often are used to calculate important quantities beyond the reach of measurement. Reference: "Abrupt Change in Radiation-Width Distribution for ^{147}Sm Neutron Resonances," *Physical Review Letters* **108**, 142502 (2012. Los Alamos researchers include J.M. O'Donnell and J.L. Ullmann (LANSCE-NS), R.S. Rundberg, D.J. Vieira, and J.M. Wouters (C-NR).

NNSA Defense Programs supports the LANSCE accelerator, and the NNSA Defense Programs Science Campaigns fund the DANCE spectrometer. The work supports the Lab's Nuclear Deterrence and Energy Security mission areas and the Science of Signatures and Materials for the Future science pillars.

Technical contact: John Ullmann (LANSCE-NS).

Spin and orbital ordering in $Y_{1-x}La_xVO_3$

Many important technological devices are based on transition-metal oxide materials. These materials often possess strongly correlated electrons which give rise to highly desirable physical properties such as high-T*c* superconductivity in layered cuprates, colossal magnetoresistance (CMR) in perovskite manganites, to the coexistence of magnetism and ferroelectricity–termed multiferroicity. Understanding how to manipulate strongly correlated electron systems allows scientists to develop new and better tunable functional materials with which are often stable under high temperatures and chemically extreme conditions.

In research published in *Physical Review B*, scientists from Ames Laboratory and Iowa State University in collaboration with Anna Llobet (Lujan Neutron Scattering Center, LANSCE-LC) have studied the $Y_{1-x}La_xVO_3$ family of compounds in order to understand the interplay between the strongly correlated spin-orbital-lattice degrees of freedom. The orthorhombic RVO_3 perovskites (*R*=rare earth or yttrium [Y], V=vanadium, O=oxygen) are a family of compounds in which all the atoms have the same configuration of electrons regardless of which atom is used in the *R* site. In the V^{3+} ions ($t_{2g}^2e_g^0$) a preferential occupation of the electron orbitals can lead to a distortion of the VO_6 octahedra called a Jahn-Teller distortion where some of the V−O bonds elongate and others

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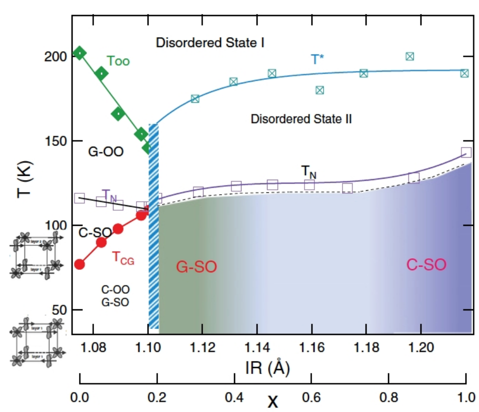

Figure 1a (top) Spin and orbital-ordering phase diagram for $Y_{1-x}La_xTiO_3$. (This work).

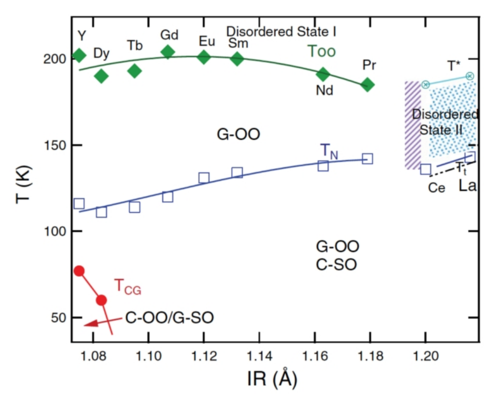

Figure 1b (bottom) Spin and orbital-ordering phase diagram for RVO_3 (R = rare earth and Y) perovskites. (Previously published work.) G/C-type orbital ordering is labeled as G/C-OO, G/C-type AFM magnetic spin order is labeled as G/C-SO. G-OO/C-SO and C-OO/G-SO states are schematically represented in Figure 1a.

Spin . . . shorten. When a particular arrangement of the octahedral distortion coherently propagates through the crystal, an orbital ordered state emerges (OO). All RVO_3 members show multiple orbital orderings and ordering of the magnetic spins, thus providing a unique opportunity to study the spin-orbital-lattice coupling of π-bonding *t*-orbital electrons. To distinguish competing effects, the team focused on the $Y_{1-x}La_xVO_3$ system because (1) the La^{3+} and Y^{3+} ions carry no magnetic moment either to obscure the magnetic behavior of the VO_3 array or to interact with it, and (2) $LaVO_3$ and YVO_3 have a different sequence of spin and orbital ordering. In addition to the study of the magnetic properties, thermal conductivity, and specific heat, the scientists examined the corresponding crystal-structure changes associated with the spin and orbital ordering using a variety of techniques including neutron powder diffraction largely performed at the High Intensity Powder diffractometer (HIPD) at LANSCE. These extensive characterizations lead to the understanding of the evolution of the spin and orbital ordering and a full description of the phase diagram for all values of x in $Y_{1-x}La_xVO_3$.

Their results are summarized in Figure 1a where the phase diagram of $Y_{1-x}La_xVO_3$ as a function of the R^{3+}- ion average ionic radius (IR) or doping substitution *x* are shown and are compared to Figure 1b, which shows the phase diagram of the RVO_3 system (*R*=rare earth and Y). Magnetization and neutron powder diffraction measurements point to the coexistence below the magnetic order temperature T_N of the two magnetic phases in the compositional range $0.4<x<0.738$. Samples in the compositional range $0.20<x\leq1.0$ were also characterized by an additional suppression of a glasslike thermal conductivity in the temperature interval $T_N<T<T^*$ and a change in the slope of the temperature dependence of the magnetic susceptibility. The authors findings show that T^* represents a temperature below which spin and orbital fluctuations couple together via spin-orbit coupling (transition between Disordered orbital state I to Disordered orbital state II in Figure 1a). They also state that for $0.20\leq x\leq1.0$, competitive orbital ordering can be expected to introduce short-range orbital fluctuations of orbitally ordered regions that suppress the thermal conductivity by phonons (Disordered state II).

The dramatic difference between the two phase diagrams in Figure 1 is in sharp contrast to the strong similarity between the phase diagrams for $RTiO_3$ and $Y_{1-x}La_xTiO_3$ (previously published). This contrast can be traced to the different effect of the bias by the intrinsic site distortions, which give rise to a different orbital and magnetic ordering competition in vanadate versus titanate perovskites.

In conclusion, this study reveals the way an intrinsic site distortion of orthorhombic perovskites biases the development orbital ordering and unveils the development of short-range orbital fluctuations of orbitally ordered regions that suppress the thermal conductivity by phonons in $Y_{1-x}La_xTiO_3$.

Reference: "Spin and orbital ordering in $Y_{1-x}La_xVO_3$, " *Physical Review B* **84**, 214405 (2011). The DOE Office of Basic Energy Sciences, Division of Materials Sciences and Engineering funded the research. This work has benefited from the use of HIPD at the Lujan Center at Los Alamos Neutron Science Center, funded by DOE Office of Basic Energy Sciences. The work supports the Lab's Energy Security mission area and the Materials for the Future science pillar.

Technical contact: Anna Llobet

Probing manganite films chemical uniformity with polarized neutrons

Los Alamos researchers and collaborators used polarized neutron reflectometry (PNR) to measure the neutron spin-dependent reflectivity from a single crystalline $(La_{1-x}Pr_x)_{1-y}Ca_yMnO_{3-\delta}$ ($x=0.52\pm0.05$, $y = 0.23\pm0.04$, $\delta = 0.14\pm0.10$) thin film. They observed coexistence of magnetic phases as a function of depth. However, magnetic phase coexistence was correlated with variation of the chemical composition with depth. This work highlights a concern about chemical uniformity (or lack thereof) in manganite films. *Physical Review Letters* published the work.

Improvements in sample fabrication capabilities have enabled the growth of increasingly complex materials with crystalline quality. This has allowed observation of exotic behavior, such as the coexistence of ferromagnetic metallic, orthorhombic

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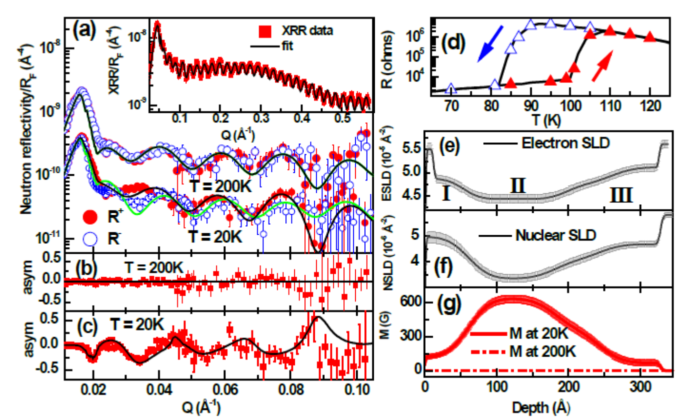

Figure 2 (a) PNR data (inset: x-ray reflectivity). (b) and (c) Difference between the two spin states, R+ and R- normalized to their sum. (d) Resistivity of the sample measured during the experiment showing the metal-insulator transitions. (e) and (f) Electron and nuclear scattering length density depth profiles obtained from the x-ray and neutron reflectivities, respectively. (g) The saturation magnetization depth profile.

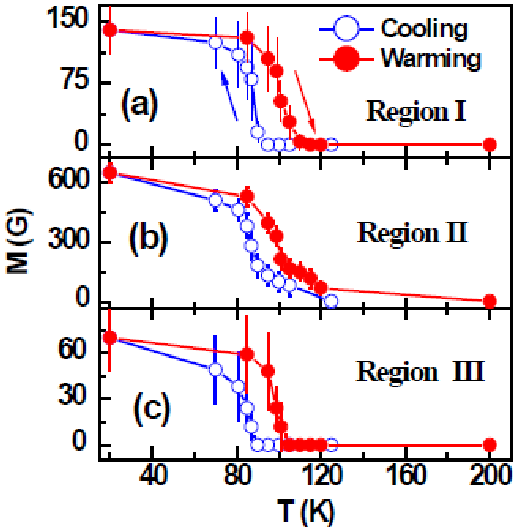

Figure 3. The temperature dependence of the saturation magnetization for the different regions of the sample identified in Figure 2.

Probing . . . antiferromagnetic charge ordered insulating and pseudo-cubic paramagnetic insulating phases. Commonly, the behavior is assumed to occur in chemically uniform material. However, given the small length scales over which coexistence occurs, typically tens or hundreds of nanometers, an outstanding challenge is to prove chemical uniformity over the same length scale.

The scientists used the LANSCE-LC Asterix polarized neutron reflectometer, which is intrinsically sensitive to interfacial magnetism, to examine the magnetism occurring across the thin dimension of a $(La_{1-x}Pr_x)_{1-y}Ca_yMnO_{3-\delta}$ single crystal film. Data of the neutron beam spin asymmetry ('asym') obtained at low temperature is shown in Figure 2. From these data the saturation magnetization *M* depth profile was obtained Figure 2(g). The result shows compelling evidence for suppression of the M near the surface and buried interface of the film. However, these regions also have different chemical and nuclear compositions (Figures 2(e, f)). Suppression of *M* is a clue towards understanding the origin of poor tunnel magnetoresistance of manganite films. *M* was also measured as a function of temperature (Figure 3) from which the dependence of the Curie temperature of the film (and hence phase coexistence of magnetism) on depth was measured.

Los Alamos researchers include Surendra Singh, M.R. Fitzsimmons, T. Lookman, and J.D. Thompson. Collaborators are H. Jeen, A. Biswas (University of Florida), M.A. Roldan (Universidad Complutense de Madrid, Spain) and M. Varela (ORNL). Reference: "Magnetic Nonuniformity and Thermal Hysteresis of Magnetism in a Manganite Thin Film," *Physical Review Letters* **108**, 077207 (2012). 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.

Technical contact: M.R. Fitzsimmons

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Questions about this training? Contact Ombuds Office at 665-2837.

Celebrating service

Congratulations to the following AOT and LANSCE Division employees celebrating a service anniversary this month:

Molly Herrera, AOT-MDE	30 years
Leo Bitteker, LANSCE-NS	20 years
James Abernathey, AOT-MDE	25 years
Matthew Fresquez, AOT-RFE	15 years
William Winton, AOT-IC	15 years
James Sedillo, AOT-IC	10 years

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