AOT & LANSCE The Pulse

November 2011

INSIDE

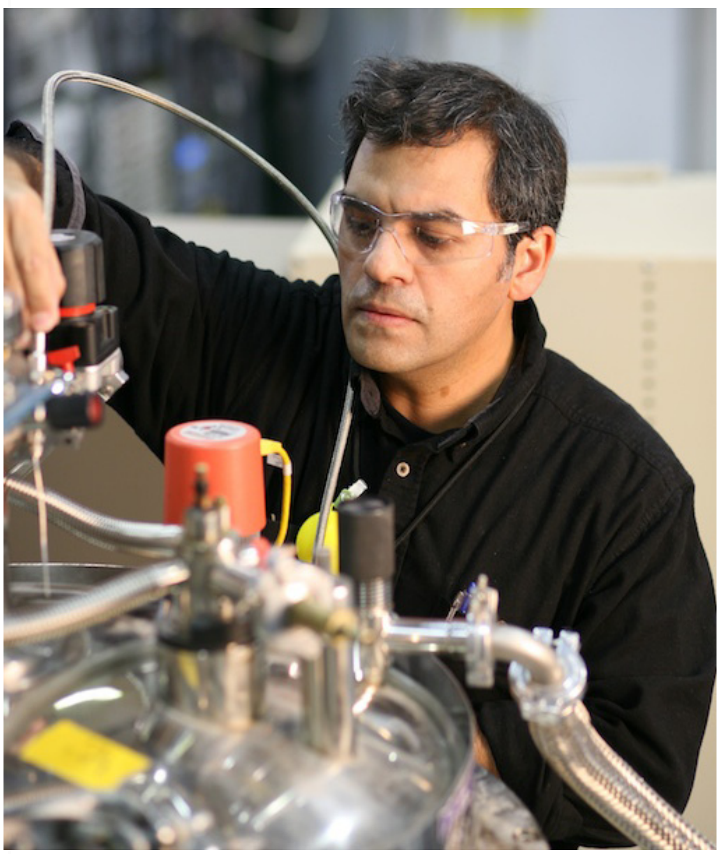


# Victor Fanelli

## *Building the tools for tomorrow's science*

By Diana Del Mauro
ADEPS Communications

Inside the Lujan Neutron Scattering Center, Victor Fanelli is busy preparing a superconducting magnet. In a series of delicate steps, he transfers liquid nitrogen and liquid helium to different reservoirs in the magnet and generates a magnetic field.



Fanelli can barely leave the equipment for even a few minutes, or else the magnet might slip out of its superconducting state, produce heat, vaporize all the helium, and exhale a huge cloud of gas. And he would lose precious time.

In a matter of days, a visiting scientist will arrive with a sample for an important experiment—and Fanelli wouldn't dream of missing the deadline.

As part of the Los Alamos Neutron Science Center, the Lujan Center attracts an average of 500 users a year from around the world. Here, scientists study the behavior of materials, at the microscopic level, in extreme conditions. As lead scientist for sample environments, Fanelli sets the stage for the scientists who wish to run experiments. If a Lujan Center user would like to explore some behavior of matter where no capability exists, he designs equipment to do it. "This is science driving the development of new capabilities– and at the same time, if we have these new capabilities, we can drive science," Fanelli said.

Fanelli, a physicist, has traveled to four U.S. neutron scattering facilities and others abroad, for 15 different experiments of his own. He understands the expectations and time constraints that Lujan Center users have. Some come for two days,

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# From Alex's Desk

Colleagues,

Challenging times (world wide) and with that some unique opportunities. At a time of uncertainty like this the tendency is to increase anxiety and to worry even more. All are understandable reactions and we should do our best to manage the best way possible. Yet it may be hard to accept the situation and just hope for the best.

A different approach, however, is to acknowledge the situation, focus on the job to be performed, and contribute to the future. As far as LANSCE is concerned there are new opportunities that we, as a facility, are pursing most vigorously.

As an example we are on the path to move forward in responding to a recent NNSA call related to experimental facilities for the future. Part of LANL's response is a major project related to the nuclear science complex, where TA-53 and our colleagues and collaborators from Chemistry Division will see a positive impact. Coupled to that, LANSCE will host a focused User Meeting where current and potential LANSCE users are encouraged to participate in the one-and-a-half day event. This topical users meeting will allow the user community a means to affect a unique opportunity for significant improvements to the LANSCE scientific infrastructure.The workshop is designed to solicit user input on four major research areas: new directions in local structure research, neutron radiography capability, nuclear science, and material dynamics.

**'(The January) topical users meeting will allow the user community a means to affect a unique opportunity for significant improvements to the LANSCE scientific infrastructure.'**

The 2012 Topical User Workshop will be held January 9-10. Registration for the workshop is now open; please see lansce.lanl.gov/users/lug/lugregistration.shtml.

Last, but not least the 2010 LANSCE Activity Report is now available online at lansce.lanl.gov/news/activity.shtml.

This issue covers major activities and accomplishments during CY2010. We hope you enjoy reading it as much as we did preparing the report.

*LANSCE Deputy Division Leader Alex Lacerda*

***Fanelli . . .*** others for two weeks. When users show up with their sample, the equipment must be in topflight working order and fit the experiment's specifications. If something malfunctions during the experiment, Fanelli or his counterpart better know how to quickly fix it.

With instruments ranging from helium cryostats, helium dilution refrigerators, superconducting magnets, and furnaces, Fanelli imagines new possibilities, such as testing a material at high pressures and low temperatures while also under magnetic fields. But since he just started this job in March, he has much to learn, he says.

Frans Trouw, with 31 years of experience in neutron scattering, is one of Fanelli's chief mentors. The two scientists met six years ago when Fanelli was a graduate student executing a challenging experiment at the Lujan Center. Right off, Fanelli impressed Trouw as a "very smart guy" and "a very hard worker."

Fanelli began his college education in his native Argentina. By 2005, he was stationed at the National High Magnetic Field Laboratory (NHMFL)-Pulsed Field Facility in Los Alamos while he was a graduate research assistant at the University of California, Irvine. In 2009, Fanelli advanced to postdoctoral research associate at the magnet lab, where he ran experiments and built equipment for visiting senior scientists and students.

Today, Fanelli counts himself lucky to be a full-fledged Los Alamos National Laboratory staffer. "It was a very well received surprise," he said.

What Fanelli learned about cryogenics and magnets at the NHMFL "definitely fulfills a niche" at the Lujan Center, Trouw noted. And when it comes to meeting the needs of users, equally important are Fanelli's conscientiousness, trademark politeness, and good people skills.

"Users can be demanding," Trouw said. "He's more patient than I am."

Fanelli, meanwhile, still devotes 25 percent of his time to basic research at the magnet lab.

"My dream experiment would be to perform an inelastic neutron scattering to look for magnetic moments in plutonium at low temperatures," Fanelli said. The Pharos instrument, a chopper spectrometer that measures phonon and spin-wave dispersions at the Lujan Center, is ideal for that.

### Victor Fanelli: My favorite experiment

**What:** Temperature dependence of the elastic properties of a plutonium alloy

**Where:** National High Magnetic Field Laboratory-Pulsed Field Facility (NHMFL-PFF)

**When:** 2006-present

**How:** The resonant ultrasound team at the NHMFL-PFF measured accurately the elastic moduli of plutonium, which are of central importance in assessing both theory and models of this element.

**Why:** We were interested in measuring elastic properties like the bulk and shear moduli of an alloy of plutonium with a certain amount of gallium which has shown a temperature independent atomic volume over a range of 200K.

We were very surprised when we found extreme variations of the elastic constants on this same range of temperature. How can the bulk modulus, which is basically the curvature of the interatomic energy with respect to the volume, change when the volume does not? This is not explained by current electronic structure models.

**The a-ha moment:** Our results, associated with the large thermal atomic displacements calculated from experiments performed here at the Lujan Center in 2000, made us think that these thermodynamic properties are not driven by volume but by thermally induced fluctuations in the electron structure. We were very excited to start this discussion with the scientific community during the "Plutonium Futures" meeting of the American Nuclear Society last year.

## Lujan Center research featured on cover of *Langmuir*

Work performed on SPEAR, the neutron time-of-flight reflectometer at the Lujan Neutron Scattering Center, is featured on the cover of a top-ranking scientific journal this month. The image, which appears in the Nov. 15 issue of *Langmuir*, shows a structural phase diagram of various cushioned membrane states for a supported biomembrane with polymer-decorated lipids that carry a sticky end.

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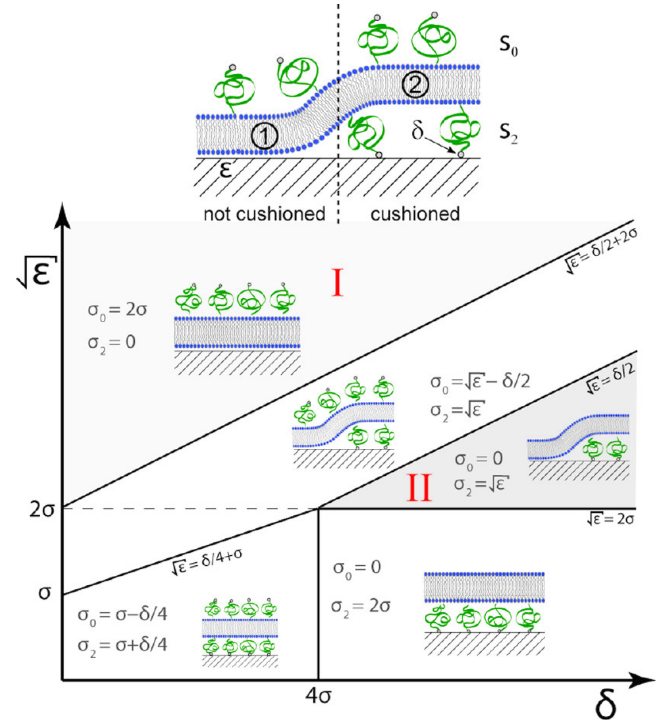
***Lujan . . .*** *Langmuir*, an interdisciplinary journal published by the American Chemical Society, ranks No. 2 in citations out of 121 journals in the physical chemistry.

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

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

Reference: "Structure and thermodynamics of lipid bilayers on polyethylene glycol cushions: Fact and fiction of PEG cushioned membranes," by Jaroslaw Majewski (LANSCE-LC); Chad Miller (Stanford Synchrotron Radiation Lightsource); Erik Watkins, Rita El-khouri, Brian Seaby, and Tonya Kuhl (University of California, Davis); and Carlos Marques (Université de Strasbourg, France). The National Science Foundation's Division of Chemistry supported the work. Neutron measurements were performed at the SPEAR reflectometer at the Los Alamos Neutron Scattering Center and the Advanced Photon Source, which are funded by the U.S. Department of Energy.

*Technical contact: Jaroslaw Majewski*




*Phase diagram of various cushioned membrane states as a function of the membrane adhesion energy to the substrate, ε, the binding energy of the reactive group to the substrate, δ, and the grafting density of the lipopoymers, σ. For the case of nonreactive lipopolymers $\delta \approx 0$ and $\varepsilon > 0$, the membrane system is in state I. In the reactive lipopolymer case, $\delta > 0$, however, ε is substantial and the membrane system is in state II.*

# Functional oxides under extreme conditions– quest for new materials

Functional materials, which exhibit detectable response (e.g., voltage) to an external change (such as pressure or magnetic field), are widely used in many technological applications. Examples include non-volatile memory cells based on ferroelectric materials, piezoelectric actuators in micromotors, pumps, and in cell phone microphones and speakers. For applications the essential feature is the coupling between two or more physical properties, such as the atomic-scale changes induced by applied hydrostatic pressure. In piezoelectric ceramics the response to external stress or electric field can be divided into intrinsic and extrinsic contributions. The former is essentially a single crystal response (i.e., is formed by

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**Oxides . . .** the ion displacements within a primitive cell of the crystal), whereas the latter covers the contribution due to grain boundaries, preferred orientation or texture of the grains, i.e., ferroelectric domains within the grains, and changes in crystal phase fractions. For applications the chemical composition of the material is chosen such that two phases co-exist in the vicinity of a first-order phase transition, the most famous example being the morphotropic phase boundary (MPB) in the classical piezoelectric lead zirconate titanate (PZT, $Pb(Zr_xTi_{1-x})O_3$). The importance of understanding the intrinsic and extrinsic contributions is not only related to the magnitude of the piezoelectric response but also to the reversibility-a key requirement for applications. Especially domain wall motion and two-phase co-existence, characteristics of the first-order phase transition often result in irreversible changes. Neutron scattering is an excellent tool for studying the complex changes occurring in oxides in response to pressure, heat or compositional modification due its unique ability to determine the oxygen positions together with the cation positions, phase fractions and magnetic ordering.

The neutron diffraction experiments conducted in LANSCE were focussed on two perovskite oxides, ferroelectric lead titanate ($PbTiO_3$) and manganese modified strontium titanate ($Sr(Ti_xMn_{1-x})O_3$). Both lead titanate and strontium titanate are classical perovskite oxides. The high-pressure (up to 8 GPa) neutron powder diffraction experiments and density functional theory computations carried out for lead titanate show that it is the competition between two factors which determines the morphotropic phase boundary. The first is the oxygen octahedral tilting, favoring the rhombohedral *R3*c phase, and the second is the entropy, which in the vicinity of the morphotropic phase boundary favors the tetragonal phase above 130 K. If the two factors are in balance over a large temperature range, a steep phase boundary results in the pressure-temperature plane which is desirable for application. The advantageous feature of the *R3c* phase is its ability to be compressed efficiently by tilting the oxygen octahedra, in contrast to symmetries prohibiting oxygen octahedral tilting.

The predicted oxygen octahedral tilting under high-pressure in $PbTiO_3$ served as a motivation to look for crystal symmetries of magnetic ion modified $SrTiO_3$. The neutron experiments revealed that small substitution (2 at. percent Mn for Ti) in a classical cubic perovskite $SrTiO_3$ is sufficient for decreasing the symmetry from cubic to orthorhombic, already at room temperature, see Fig. 1. The corresponding oxygen octahedral tilting is shown in Fig. 2. Interestingly, already this small amount of Mn-doping was able to cause a magnetic anomaly between 70 and 80 K, accompanied by an anomalous behavior in lattice parameters at 50 K. These results show that novel multiferroic materials, being piezoelectric and magnetic, can be introduced by looking for systems possessing octahedral tilting and magnetic ions, such as manganese. The present research efforts at LANSCE are dedicated to high-pressure neutron studies of PZT with composition in the vicinity of the morphotropic phase boundary at which two phases, *R3c* and *Cm* (which is in practice pseudo-tetragonal), co-exist. The characteristic feature of the morphotropic phase boundary compositions is that the *electromechanical coupling coefficient*, the most important figure-of-merit of a piezoelectric material, peaks at these compositions. The nature of the phase transition has been under keen studies for 40 years yet no consensus about the nature of the phase transition exists. The goal is to determine the temperature and pressure dependent changes in phase fractions and atomic scale structures. The experiments serve as a test to the *ab-initio* computational studies conducted at the Aalto University, which predict that the rhombohedral phase is favored above 9 GPa pressures.

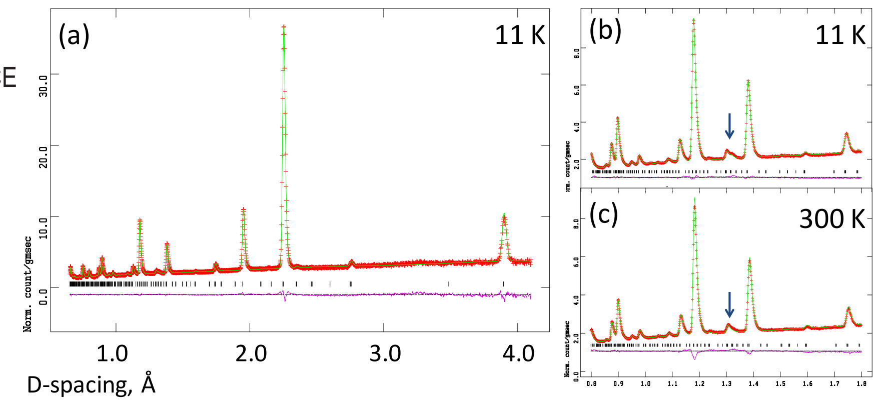


*Fig. 1. Neutron powder diffraction patterns collected for $Sr(Mn_{0.02}Ti_{0.98})O_3$ sample at 11 K and 300 K. Panel (a) shows larger region diffraction pattern measured at 11 K. Panels (b) and (c) show a detailed picture of the diffraction pattern at 11 and 300 K. The arrows point the reflections which are the clearest indication of a symmetry lowering from the cubic symmetry present already at room temperature. The space group symmetry was Pbnm. Rietveld refinements were carried out using the GSAS software.*

The researchers include Johannes Frantti, Yukari Fujioka and Risto Nieminen (all Aalto University), Jianzhong Zhang, Sven Vogel, Yusheng Zhao, Luke Daemen, Zhijun Lin, Matt Reiche, and Adrian Losko (all Lujan Center, LANSCE-LC).

This work benefited from the use of the HIPPO diffractometer at Lujan Center. JZ, SV, YZ, LD, ZL, HR, AL and the Lujan Neutron Scattering Center at Los Alamos Neutron Science Center are funded by the DOE Office of Basic Energy Sciences and Los Alamos National Laboratory under DOE Contract No. DE-AC52-06NA25396. On the Finnish side the research work was supported

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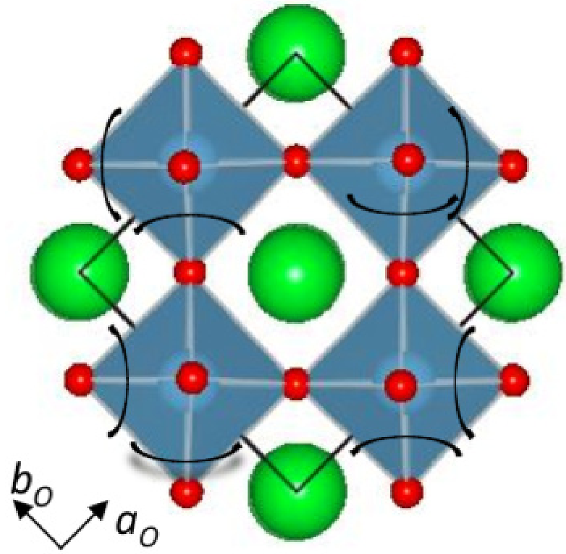


*Fig. 2. Oxygen octahedral tilting found in $Sr(Mn_{0.02}Ti_{0.98})O_3$ sample. Pbnm symmetry corresponds to the three-tilt system ($a^+b^-b^-$ in Glazer's notation). The octahedral antiphase tilts (the $b^-b^-$ tilts) in the orthorhombic ab-plane are indicated by arrows. Blue spheres are oxygen, light blue ones are the B-cations and the green ones are Sr ions. Figure was prepared by VESTA.*

***Oxides . . .*** by the collaboration project, started in June, between the Center of Excellence for Advanced Materials Research at King Abdulaziz University in Saudi Arabia (principal investigator from Saudi-Arabian side is Professor Abdullah M. Asiri) and the Aalto University in Finland (project leader in Finland is Professor Nieminen). The collaboration project focuses on the development of new functional oxide materials. The research was also supported by the Academy of Finland (Projects 207071, 207501, 214131, and the Center of Excellence Program 2006-2011).

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# HeadsUP!

## Prep your vehicle for winter

Driving in the winter has all of the hazards it does during the rest of the year—add wind chill, snow, ice, and darkness and we have even less margin for error. With days becoming ever shorter between now and the Winter Solstice, many of us will be commuting both ways in the dark. Cold and unpredictable weather will be the norm for the next few months. What should we be doing?

### Make sure your vehicle is ready:

- If you have all-season tires on your car or light truck, ensure they are not more than 40-50% worn to provide adequate traction in serious snow. Even all-wheel drive vehicles are only as good as the tread on their tires.
- Windshield wipers and all-season washing fluid must be ready to quickly clear filth, slush, and water from your field of view.
- Are all of your lights (headlights, running lights, tail lights, brake and turn signals) operating?
- Have you checked your heater and defroster?
- Do you have a small shovel and some sand and emergency supplies (flares, blanket, flashlight, emergency chains, cell phone) handy? Do you have a windshield scraper and snow remover and do you plan on clearing all your windows for safe visibility?

### Make sure you are ready, too:

- Are you thinking about how to handle winter driving? Do you have teens who will be driving to school? Have they thought about the information listed here?

  - Wear sturdy shoes or boots that do not slip and slide on snow.
  - Dig out your clothing suitable for sudden changes in weather.
  - If you take the bus, are you ready to walk in wind chill and on slushy or slippery sidewalks while remaining upright and visible?