the Lujan CENTER SCIENCE & PEOPLE

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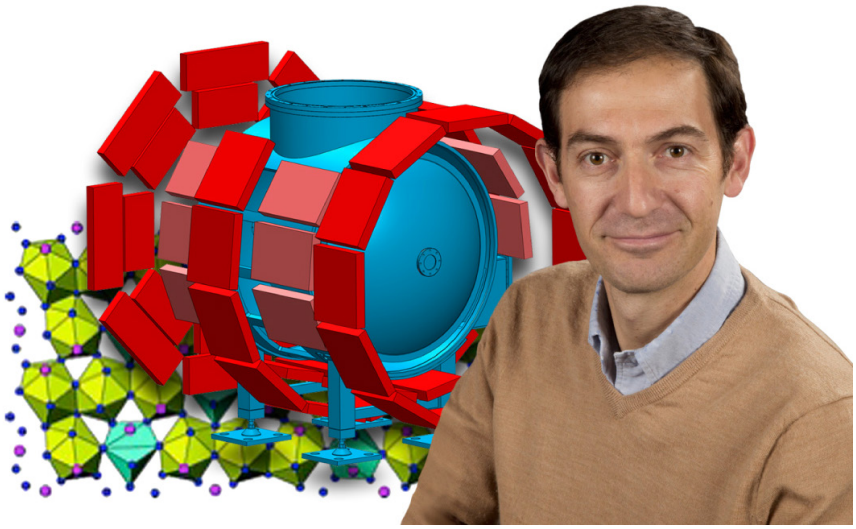

Photo by Sandra Valdez, IRM-CAS

A champion of neutrons for illuminating the properties and behaviors of materials, Olivier Gourdon uses neutron crystallography to study energy-related materials. Above, a schematic view of the High- Pressure-Preferred Orientation beamline at the Los Alamos Neutron Scattering Center. In the background, the atomic arrangement of a complex modulated intermetallic compounds of formulation $Zn_{212}Pd_{64}$ refined by Gourdon.

Olivier Gourdon

A crystallographer keen on showing off the revealing properties of neutrons

By Diana Del Mauro, ADEPS Communications

At Los Alamos's Lujan Neutron Scattering Center, crystallographer Olivier Gourdon shows visiting researchers some of the latest tricks that can be performed using this 100-year old multidisciplinary science, which has a spectacular record of demystifying materials as varied as DNA and Martian rocks.

"Crystallography has the image of an old science. I'm trying to refresh that," said Gourdon, an instrument scientist for HIPPO, the High-Pressure-Preferred Orientation Neutron Diffractometer.

> **"With neutron diffraction, we can learn much more than where are the atoms."**

Since the 1914 Nobel Prize-winning discovery that crystals can scatter the light waves of x-rays, thereby revealing how atoms are arranged in matter, scientists have used x-ray crystallography to great effect.

Neutron crystallography, a related experimental technique, debuted in 1946. Also known as neutron diffraction or neutron scattering, the method involves immersing samples in neutrons rather than x-rays. It tends to be underused, though, because generating neutrons requires a sophis ticated infrastructure, such as at the Los Alamos Neutron Science Center (LANSCE).

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GOURDON CONT.

Gourdon (Lujan Center, LANSCE-LC) is a proponent of both techniques as together they sometimes paint the most vivid picture of all. With HIPPO, he guides users through the process of bombarding ground-up crystals with intense neutron beams and afterward deciphering the data for high pressure-temperature, texture, liquid-amorphous materials, or reaction-kinetic studies.

"With neutron diffraction, we can learn much more than where are the atoms. We can, in some conditions, understand the dynamics and the vibrations of some atoms," Gourdon said. Neutrons, for instance, can determine the internal strains and structure of deformed metal, telling the story of why metals give before they break.

He also encourages scientists to use the Lujan Center's complementary techniques, not just crystallography. "There is not a magic instrument that will give all the answers," he said.

Gourdon first experienced neutron crystallography as a 2004 Lujan Center postdoctoral researcher supporting users on the new HIPPO instrument and studying magnetic structures and hydrogen storage materials. Next, as an Oak Ridge National Laboratory instrument scientist for its neutron powder diffractometer POWGEN, he investigated structure-property relationships in materials for energy sources, such as batteries and fuel cells. And at Pennsylvania's International Centre for Diffraction Data, Gourdon built a materials database using neutron diffraction patterns as fingerprints and created software for diffraction data analysis.

Longing to return to hands-on science, Gourdon rejoined the Lujan Center in September. "He is without a doubt an extremely valuable addition to the Lujan Center and the HIPPO user program in particular," said HIPPO co-instrument scientist Sven Vogel, noting his former protégé's expertise in modeling crystal structures, fabricating samples, and analyzing neutron diffraction data. "His previous tenure [at HIPPO and POWGEN] allowed him to immediately contribute to our program."

When the LANSCE beam is on–about half the year–Gourdon dedicates himself solely to users. "We see so many kinds of people and so many kinds of science," he said. When the beam is off, he conducts energy-related research based on oxides and intermetallics. "Neutrons are more suitable than x-rays for studying batteries," he said, "since this ray can screen lightweight and heavy elements simultaneously."

Though Gourdon's first love was mathematics, he earned a PhD in materials chemistry and structural chemistry from the University of Nantes in France. "At the end of the day, crystallography is geometry, so it's math," he said. "I am somewhere between mathematics, physics, and chemistry. That's why the Lujan Center suits me well."

Seeking design rules for efficient lighting sources

In the search for more efficient general lighting, downconversion strategies based on inorganic light sources and phosphor conversion have emerged as a front-runner. Advantages include durability, long life, color stability, and an environmental footprint free of toxic heavy metals. In research published in Chemistry of Materials, scientists have examined the desirable properties of phosphor materials.

The oxide garnet $Y_3Al_5O_{12}$ (YAG), when substituted with a few percent of the activator ion Ce^{3+} to replace Y^{3+}, is a luminescent material that is nearly ideal for phosphor-converted solid-state white lighting. The local environments and distributions of the small number of substituted Ce^{3+} ions critically influence the optical properties of the phosphor, yet crystalchemical guidelines for finding new and efficient phosphor compounds have not been developed. A user group, led by the University of California, Santa Barbara, and staff of the Lujan Neutron Scattering Center employed a combination of state-of-the-art scattering and spectroscopy techniques to determine the nature of these local environments and correlate them with the macroscopic luminescent properties of Ce-substituted YAG.

This study demonstrates the deep understanding that can be obtained for the composition-structure-property relationships of solid-state phosphors. This knowledge could aid the development of rational design strategies for the syntheses of efficient thermally stable light-emitting compounds with tunable colors. The researchers established the rigidity of the garnet structure, which plays a key role in the high quantum yield and in the resistance toward thermal quenching of luminescence. Local structural probes reveal compression of the Ce^{3+} local environments by the rigid YAG structure, which gives rise to the unusually large crystal-field splitting and yellow light emission. The results suggest that effective design rules for finding new phosphor materials require rigid, highly three-dimensionally connected host structures with simple compositions that manifest a low number of phonon modes, as well as low activator ion concentrations to avoid quenching.

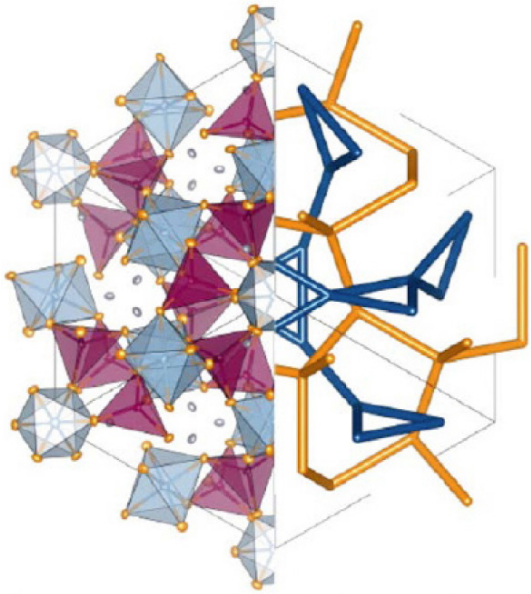
Reference: "Local Environments of Dilute Activator Ions in the Solid-State Lighting Phosphor $Y_{3-x}Ce_xAl_5O_{12}$," *Chemistry of Materials* 25, 3979 (2013). Researchers nclude Katharine Page and Anna Llobet (LANSCE-LC), Nathan C. George, Bradley F. Chmelka, and Ram Seshadri

Continued on page 3

DESIGN RULES CONT.

(University of California, Santa Barbara), Andrew J. Pell and Guido Pintacuda (Université de Lyon, France), Geraldine Dantelle (École Polytechnique, France), and M. Balasubramanian (Argonne National Laboratory). This work benefited from the use of the Neutron Powder Diffractometer (NPDF) and the High Intensity Powder Diffractometer (HIPD) at the Lujan Neutron Scattering Center, which the DOE Office of Basic Energy Sciences funds. The research supports the Laboratory's Energy Security mission area and Materials for the Future science pillar.

Technical contact: Katharine Page



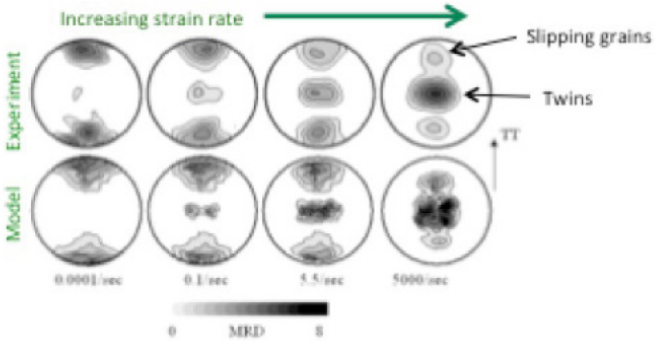
The crystal structure of YAG viewed down the (111) face of the unit cell with red, blue, gray, and orange spheres representing four-coordinate Al, six-coordinate Al, Y, and O atoms, respectively. The right half of the figure depicts the interpenetrating networks of Y and Al, which form a double-gyroid structure. The high connectivity of the lattice decreases the degrees of freedom available for phonon modes and enhances luminescence properties.

Rate-dependent deformation mechanisms in beryllium

Los Alamos National Laboratory scientists have developed and validated physics-based constitutive models of the deformation of beryllium, allowing for predictive computer codes that simulate how materials perform under conditions that cannot be reached experimentally.

Beryllium has applications for the aerospace industry, nuclear energy, and nuclear weapons. The technique of characterizing the twinned microstructure also has had an impact on research in magnesium, zirconium, and other lowsymmetry metals, which are relevant to the automotive and nuclear power industries, for example.

At the Lujan Neutron Scattering Center, scientists used data collected on the Spectrometer for Materials Research at Temperature and Stress (SMARTS) and the High Pressure –Preferred Orientation (HIPPO) diffractometer to characterize the deformed microstructure.



Experimental/model agreement achieved over 7 orders of magnitude in strain rate and 3 different starting textures.

Experiments were carried out over 7 orders of magnitude in strain rate. Three different starting textures provided strong validation for the constitutive model developed in the Theoretical Division. Deformation twinning goes from inactive at quasi-static rates to an important deformation mode at a rate of 5000/sec.

Researchers include Don W. Brown, Thomas A. Sisneros, Bjørn Clausen, Carlos Tomé (Materials Science in Radiation and Dynamics Extremes, MST-8) and Irene Beyerlein (Fluid Dynamics & Solid Mechanics, T-3).

Reference: "Role of twinning and slip during compressive deformation of beryllium as a function of strain rate" *International Journal of Plasticity*, 29 (2012).

This work benefited from the Lujan Neutron Scattering Center at Los Alamos Neutron Science Center, funded by the DOE Office of Basic Energy Sciences and Los Alamos National Laboratory under DOE Contract DE-AC52-06NA25396.

The work supports the Advanced Scientific Computing initiative by providing model validation data.

Technical contact: Don Brown

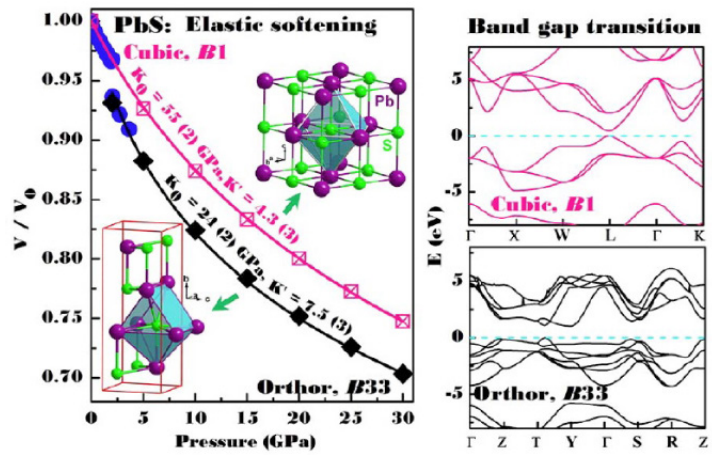
Improved understanding of a semiconductor used in infrared detectors

At the Lujan Neutron Scattering Center a combined study of high-pressure neutron diffraction, electrical resistance measurement, and first-principles calculation provides new insights into structural and electronic transitions in lead sulfide (PbS). PbS is a semiconductor used in infrared detectors. The material undergoes both structural and electronic phase transitions under pressure. However, the nature of the transitions remains a subject of debate. The experiments and complementary models published in the journal *Inorganic Chemistry* offer a description of the phase transition mechanisms and advance the understanding of lead-based semiconductors.

The researchers observed phase-transition induced elastic softening and direct to indirect band gap transition in PbS. First-principles calculations simulated the elastic properties and band structures of PbS. The scientists conclude that both cubic and orthorhombic phases are semiconductors, but they exhibit features of direct and indirect band gaps, respectively. Phase transition induced elastic softening in PbS is likely to be associated with enhanced metallic Pb - Pb bonding in the orthorhombic phase. Phase transition also leads to an anomalous drop in electrical conductivity in orthorhombic PbS, which the researchers attribute to the lower crystal symmetry and the enlarged band gap in the Cmcm phase. Based on the results and calculations, the team proposed a new model for the B1--> B33--> B2 phase transitions. They suggest that the phase transitions paths involve translation of a trigonal prism in the B1 phase and motion of the next-nearest neighbor Pb atom into {SPb7} coordination and subsequent lattice distortion in the B33 phase.

Reference: "Phase-Transition Induced Elastic Softening and Band Gap Transition in Semiconducting PbS at High Pressure," *Inorganic Chemistry* 52, 8638 (2013). Researchers include Jianzhong Zhang (LANSCE-LC), Shanmin Wang, Yi Zhang, Andrew Alvarado, Jeevake Attapattu, Liping Wang, Changfeng Chen, and Yusheng Zhao (University of Nevada, Las Vegas); and Duanwei He (Sichuan University, China). This work benefited from the use of the High-Pressure Preferred Orientation Diffractometer (HIPPO) instrument at the Lujan Neutron Scattering Center at LANSCE funded by the DOE Office of Basic Energy Sciences. The research supports the Lab's Energy Security mission area and the Materials for the Future and Nuclear and Particle Futures science pillars.

Techincal Contact: Jianzhong Zhang



(Left): Pressure-volume data from high-pressure neutron diffraction and ab initio simulations. (Right): Simulated band structures.

New instrument aids fission-fragment yield measurements

SPIDER benefits weapons program research

Uranium undergoes fission with thermal neutrons. The fissioning isotope, ^{235}U, splits into two asymmetric fragments. The distribution of the mass of these fragments–the mass yield–is an important test for different theoretical models of nuclear fission. In addition, it provides important data to nuclear weapons diagnostics, provides a way to determine the burn-up of nuclear fuel, and calculate the source-term for spent fuel waste stream analysis. Future measurements of ^{239}Pu fission yields will provide a definitive answer regarding the energy dependence of 147Nd, which is of importance to the weapons program.

In recent years, a new instrument has been developed by members of Nuclear Science (LANSCE-NS) to measure fission-fragment yields as a function of the incoming neutron energy, the fragment mass and charge, and the total kinetic energy of the fragments. The instrument, named SPIDER (SPectrometer for Ion DEtermination in fission Research), aspires to achieve 2-5% accuracy for incoming neutrons between 0.01 eV and 20 MeV. Determination of the masses of the fragments utilizes the "2E-2V" method. In this method, the energy of each fragment is determined by its energy deposition in an ion-chamber, and its velocity by time-of-flight. This method provides a mass resolution of better than 1 amu and approximately 1 charge unit for the light fragment.

An illustration of the spectrometer (without its case) is presented in Fig 1 and the actual spectrometer at the flight

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SPIDER Cont.

path is shown in Fig 2. Time pickoff detectors, which use an electrostatic field to focus electrons from a foil to a microchannel-plate detector, are evident on both sides of the fissile foil in the middle.

Fig 3 shows preliminary results from the measurement performed at the Lujan Center at LANSCE between October and November 2013. The graph shows the yield of fission fragments as a function of their mass. The characteristic asymmetric mass distribution in thermal fission of actinides is evident from the data; a light mass peak is observed around 95 amu and a heavy peak around 140 amu. Further work is needed before drawing conclusions about the agreement between the evaluated data (ENDDF/B-VII.1) and this experiment. An improved calibration of the instrument using radiation sources is planned at the end of the current LANSCE run cycle, and this might still change the experimental results slightly.

Future plans include the construction of 8-10 detector arms to enhance the acquisition rate and allow for the measurement of fast-neutron-induced yields.

The detector design, construction, and analysis was the result of a collaboration between Los Alamos, University of New Mexico, Colorado School of Mines, Slovak Academy of Sciences, Lawrence Livermore National Laboratory, and Lawrence Berkeley Laboratory. Los Alamos participants include Fredrik Tovesson, Krista Meierbachtol, and Dan Shields (LANSCE-NS), Morgan White (Materials and Physical Data, XCP-5), Charles Arnold and Todd Bredeweg (Nuclear and Radiochemistry, C-NR), Justin Jorgenson (Applied Engineering Technology, AET-5), and Arnie Sierk (Nuclear & Particle Physics, Astrophysics and Cosmology, T-2).

Instrument construction and research, which supports the Laboratory's Nuclear Deterrence mission and Nuclear and Particle Futures pillar, was funded by the LDRD program.

Technical contact: Fredrik Tovesson

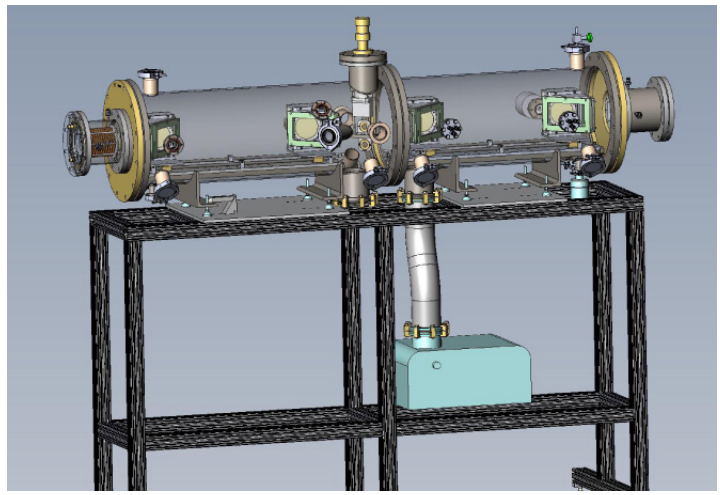

Fig 1. View of SPIDER spectrometer. The source is in the middle and the time pickoff detectors are evident on each side.

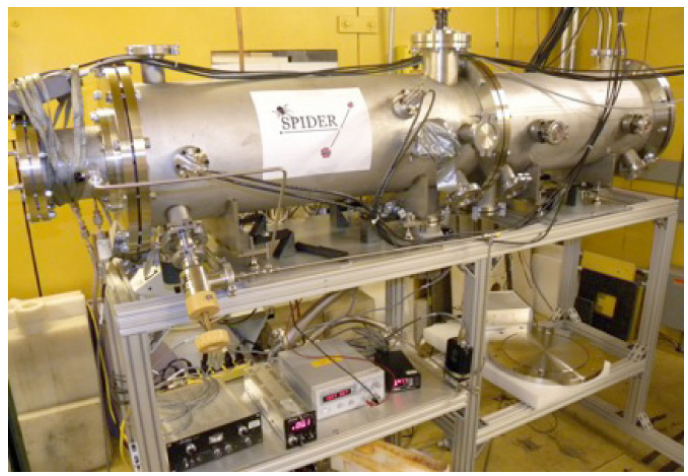

Fig 2. SPIDER at flight path 12 at the Lujan Center

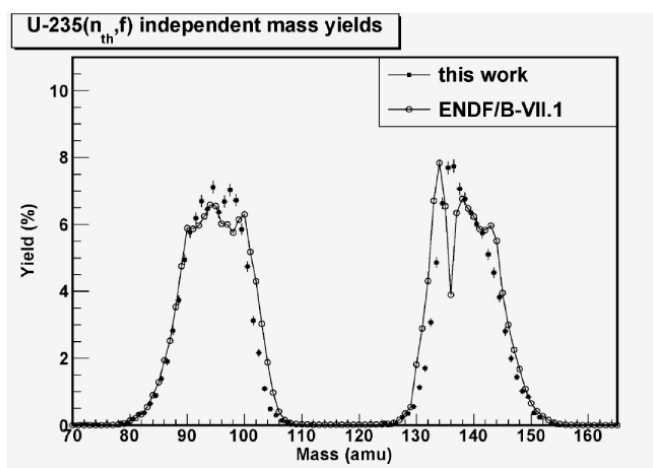

Fig 3.Mass yield results obtained with the SPIDER spectrometer to evaluated data taken from ENDF/B-VII.1

Mike Fitzsimmons Elected NSSA Fellow

Michael Fitzsimmons of the Lujan Center (LANSCE-LC) is a 2014 Neutron Scattering Society of America (NSSA) Fellow. Through the NSSA Fellowship Program, the NSSA recognizes members who have made significant contributions to the neutron scattering community in North America through original research and publication, innovative contributions in the application of neutron scattering, contributions to the promotion or development of neutron scattering, or techniques service and participation in the activities of the NSSA or neutron community.

Achievements

The Society recognized Fitzsimmons "for many important contributions to the study of interfacial and thin-film magnetism using polarized neutron reflectometry."

Fitzsimmons is the Asterix instrument scientist at the Lujan Neutron Scattering Center. In 2001 he garnered a Distinguished Performance Award for single-handedly designing and building Asterix, a polarized neutron reflectometer/diffractometer. The instrument incorporates novel neutron optical concepts to polarize a large, pulsed neutron beam, something the neutron-scattering community had considered difficult to accomplish. Asterix supports studies of the magnetism of thin films and magnetic nanostructures and has produced interesting results related to the magnetic structure of new spintronics devices.

After receiving his doctorate in materials science and engineering from Cornell University, Fitzsimmons performed research in München, Germany as a Fulbright Jr. Research Fellow. He later joined Los Alamos as a Postdoctoral Fellow and became a staff member in 1993. In 2006, Fitzsimmons was named an American Physical Society Fellow for achievements using polarized neutron reflectometry. He also serves on the Board of Directors for the Materials Research Society as Treasurer.

About the NSSA

Formed in 1992, the Neutron Scattering Society of America has more than 1,000 members from 26 countries. No more than one-half of one percent of members are honored as fellows annually through election by the Fellowship Committee.

Neutrons used to study model vascular systems

In what may be the first use of neutron scattering to study complex bio-medical systems under dynamic conditions, Los Alamos researchers and collaborators mimicked blood flow by engineering a layer of human endothelial cells (the cells that cover the inner surface of blood vessels) and subjecting them to shear stress. Simultaneously, the team used neutrons at the Lujan Neutron Scattering Center's Surface Profile Analysis Reflectometer (SPEAR) to understand changes in the cell's properties. The technique, which relies on neutron reflectometry to reveal the behavior and composition of the cells, provides a new means to explore conditions that affect human vascular health. The American Journal of Physiology-Lung Cellular and Molecular Physiology has published the research.

Because the vascular system is under constant fluid mechanical stress as a fluid conduction system, mechanical forces influence endothelial cell function and response. The endothelial cells are key in controlling the resistance of blood flow in arteries and veins, as well as blood coagulation. These cells are involved at nearly every level of vascular function as well as pathology. For example, endothelial cells and fluid mechanical shear stress are involved in atherosclerosis, a pathologic buildup of lipids in arterial walls that causes hundreds of thousands of deaths each year from heart attacks and strokes.

Most studies in endothelial mechano-biology have focused on single cells and even single molecules and protein complexes. However, the collective behavior of the monolayer of cells has been less well explored. It is clear that endothelial cells make strong lateral connections between each other and that these connections change as a function of mechanical stress.

In this work, the team examined the structure and composition of the boundary layer between the endothelial cells and the supporting substrate. The thickness of such a layer — its composition (protein rich vs. fluid rich) and how its composition and structure changes as a function of shear stress — has never been explored. By shining a beam of neutrons on the monolayer of cells and measuring the reflected radiation, the researchers revealed these long-awaited details.

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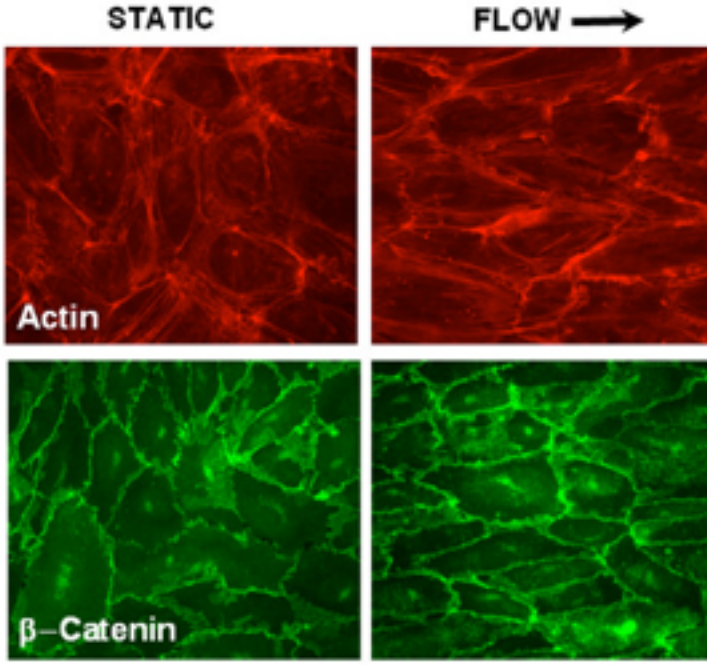
VASCULAR SYSTEMS CONT.

The research measured living tissue adhesion strength under dynamic conditions. The study is the first to provide a direct measure of endothelial monolayer adhesion under physiologic shear stress conditions. The strength of neutron reflectometry is its non-perturbative nature and ability to probe large surface areas with nanometer resolution. Using endothelial monolayers, the team showed that physical models of soft-adhesion could describe large-scale tissue adhesion, which broadens their scope of application far beyond the single cell realm.



Comparison of endothelial monolayers under static conditions (left panels) and laminar shear stress (right panels). Shear stress induces remodeling of endothelial proteins.

The team made neutron reflectometry measurements at 25 °C and 37 °C (physiologic temperature) of endothelial cells growing on quartz. At 25 °C, most active biology is suppressed, and the endothelial monolayer responds as a soft matter physical system. However, at physiologic temperature, the full richness of cell biology is available to the system. Shear stress causes major redistribution of proteins involved in cell-cell and cell-substrate adhesion. Even on the relatively short biologic time scales (four hours) relevant to the time scale of the neutron experiments, the scientists observed cell-cell and focal adhesions on endothelial cells. This localization of adhesion proteins may promote linkage between the internal framework of the cell and extracellular matrix, forming enhanced adhesion zones. The researchers concluded that shear stress at 37 oC causes localization of specific proteins, which may alter the adhesion potential in favor of overall increased adhesion.

The scientific team included Ann Junghans and Jaroslaw Majewski of the Los Alamos LANSCE Lujan Center (LANSCE-LC), Luka Pocivavsek of the University of Pittsburgh Medical Center, Noureddine Zebda and Konstantin Birukov of the University of Chicago. Mary Jo Waltman of Bioenergy and Biome Sciences (B-11) helped in preparing monolayers of endothelial cells. This work benefited from the use of the SPEAR at the Lujan Neutron Scattering Center, funded by DOE Office of Basic Energy Sciences. The research supports the Lab's Global Security mission area and Science.

Reference: *The American Journal of Physiology-Lung Cellular and Molecular Physiology*. 2014 ;306(1):L1-9. doi: 10.1152/ajplung.00160.2013

Pressure tuning: a new approach for making zero thermal expansion materials

Materials with zero or near zero thermal expansion coefficients are technologically important for applications in thermal management and engineering. Materials with zero thermal expansion do not undergo thermal shock or fatigue during rapid or repeated heating and cooling cycles, which make them excellent candidates for applications in optics, electronics, and heat-engine components. To date, this class of materials can be produced by chemical routes only, either by changing chemical compositions or by composting materials with positive and negative thermal expansion. In research published in *Scientific Reports* , Los Alamos scientists and collaborators give the first description of a physical route to achieve near zero thermal expansion through the application of pressure.

The team performed neutron diffraction experiments of $PbTiO_3$ up to 700 K and 1.2 GPa. The researchers observed crossover points in pressure dependence of unit-cell volumes at different temperatures. In the negative thermal expansion (NTE) region, the lengths of two Pb-O chemical bonds become closer with increasing pressure or temperature. In the stability field of tetragonal $PbTiO_3$, the scientists detected an unusual phenomenon: pressure-induced reversals between thermal contraction and expansion between ambient pressure and 0.9 GPa.

This hybrid behavior leads to a mathematically infinite number of crossover points in the pressurevolume- temperature space and near-zero thermal expansion coefficients comparable with or even smaller than those attained by chemical routes. The observed pressures for this unusual phenomenon are within a small range of 0.1-0.9 GPa that is potentially feasible for designing stress-engineered materials, such as thin films and nano-crystals, for thermal management applications.

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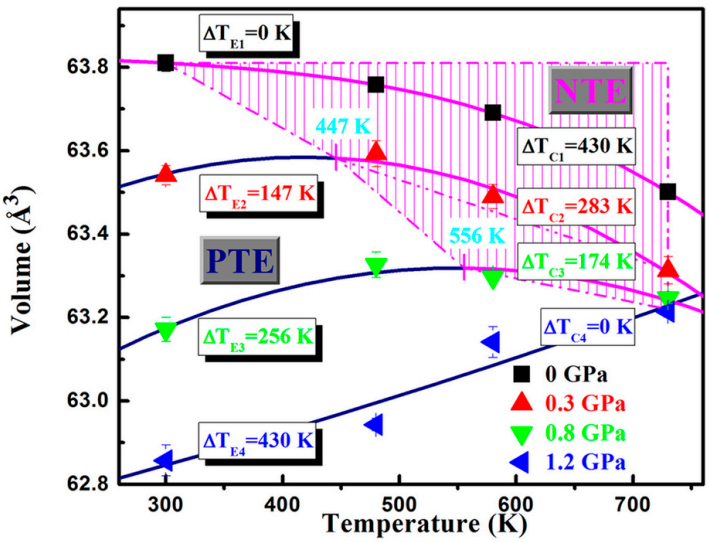
PRESSURE TUNING CONT.



Unit-cell volumes of tetragonal $PbTiO_3$ as a function of temperature at constant pressures. The pink shadow area denotes the region of thermal contraction, and the remaining area is the region of thermal expansion.

Reference: "Pressure-induced Reversal Between Thermal Contraction and Expansion in Ferroelectric $PbTiO_3$," Scientific Reports 4, 3700 (2014); doi: 10.1038/srep03700. Authors include Jinlong Zhu (Lujan Center, LANSCE-LC and Institute of Physics, China), Jianzhong Zhang and Sven Vogel (LANSCE-LC), Hongwu Xu (Earth System Observations, EES-14), Changqing Jin (Institute of Physics, China), Johannes Frantti (Aalto University in Finland), and Yusheng Zhao (Institute of Physics, China and University of Nevada).

LANL's Laboratory-Directed Research and Development (LDRD) program funded the Los Alamos research. The experimental work benefited from the use of the High-Pressure Preferred Orientation Diffractometer (HIPPO) at the Lujan Neutron Scattering Center at LANSCE, which is funded by the DOE Office of Basic Energy Sciences. The work supports the Laboratory's Energy Security mission area and Materials for the Future science pillar.

Technical Contact: Hongwu Xu

Neutron scattering enables structural characterization of multifunctional materials

Researchers have discovered a new structure type in a transition metal oxide at the Lujan NeutronScattering Center. The material has potential applications as a solid oxide fuel cell for clean energy production and as a multiferroic material for computer memory applications. The paper, co-authored by Graham King and Anna Llobet (Lujan Center, LANSCE-LC) and collaborators, was published online in journal *Advanced Functional Materials.*

The team used neutron powder diffraction with the Lujan Center's high-intensity powder diffractometer (HIPD) instrument as well as electron diffraction to identify a new pattern of charge ordering in $TbBaMn_2O_{5.75}$ and $GdBaMn_2O_{5.75}$. This charge ordering, combined with the layered ordering of the Tb and Ba cations, results in a polar crystal structure. The combination of a non-centrosymmetric space group and magnetic ions makes this a potential multiferroic material. Because the polarization of the material is directly related to the charge ordering of the magnetic ions, strong magnetoelectric coupling can also be expected. Such materials are rare but greatly sought after by the computer industry.

This material has potential as an ionic conductor for solid oxide fuel cells. Exit wave reconstruction imaging directly imaged the vacancies in the TbO layer. Direct imaging of light atoms, such as oxygen, in the presence of much heavier atoms is very difficult and has only been achieved in a few prior cases. Such imaging can reveal the locations of the vacancies and the mechanism of ionic conduction. Neutron pair distribution function analysis confirmed the ordering of vacancies within the TbO layer. The complementary analytical techniques provided information that enabled the researchers to propose a new model of charge ordering and anion vacancies ordering in these manganites.

Reference: "Structural Determination and Imaging of Charge Ordering and Oxygen Vacancies of the Multifunctional Oxides $REBaMn_2O_{6-\delta}$ (RE = Gd, Tb)," *Advanced Functional Materials* , doi: 10.1002/adfm.201303564. Researchers include G. King and A. Llobet (LANSCE-LC), D. Avila-Brande, E. Urones-Garrote, Subakti, and S. Garcia-Martin (Universidad Complutense de Madrid, Spain).

This work benefited from the use of HIPD at Lujan Center at LANSCE funded by the DOE Office of Basic Energy Sciences.

Technical contact: Graham King

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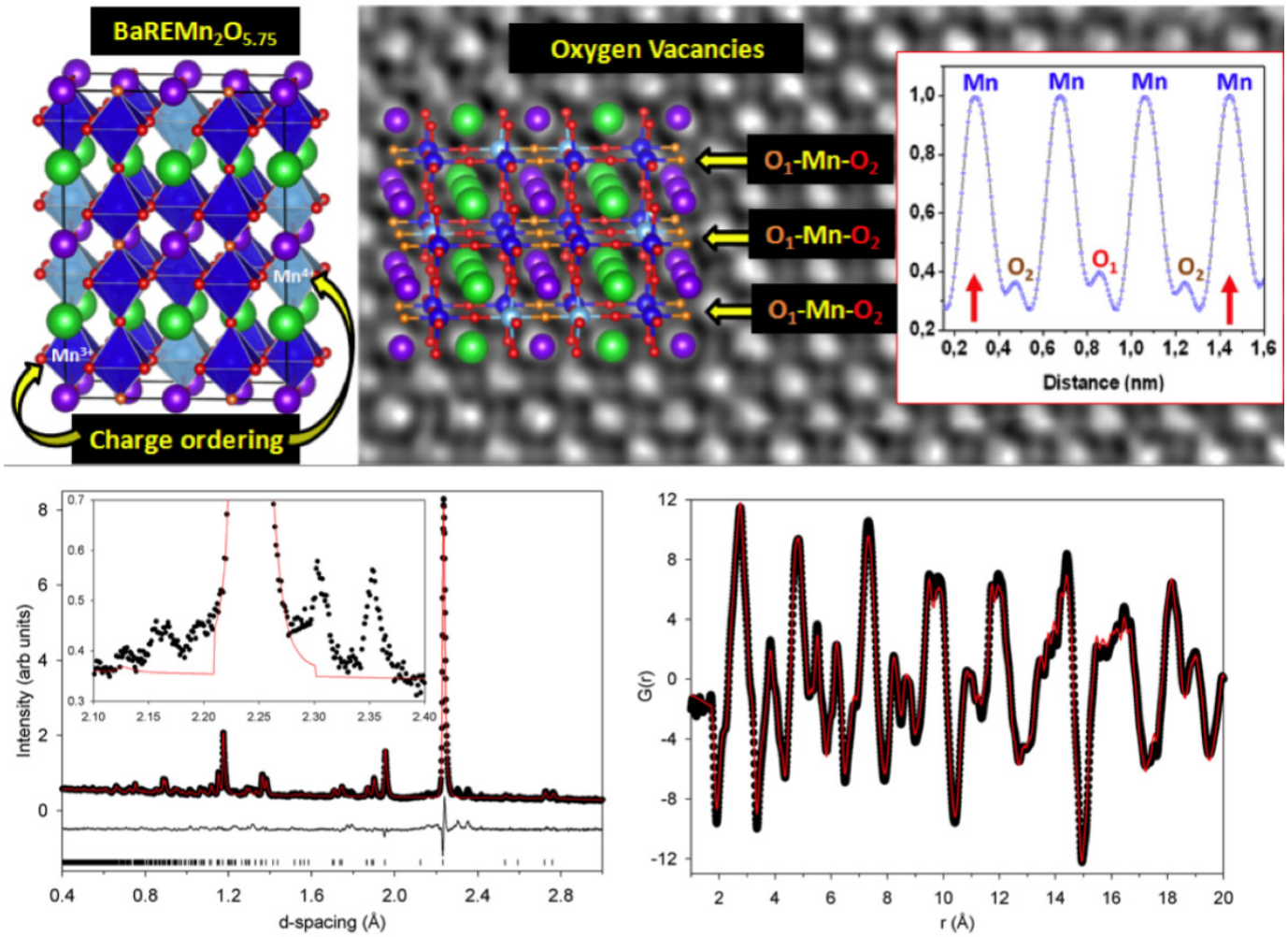
MULTIFUNCTIONAL MATERIALS CONT.



Above: The crystal structure of these materials with the charge ordering pattern highlighted (left) and the exit wave reconstruction data reveal vacancies only within the TbO layer (right). Below: The neutron powder diffraction pattern (left) showing supercell reflections resulting from the superstructure and the neutron pair distribution function (right) that gives information on the bond lengths indicate where the oxygen vacancies are located.

Julian Chen

Julian Chen, new Protein Crystallography Station lead scientist, carving out elite niche: neutron studies of membrane proteins

Julian Chen, an internationally recognized neutron crystallographer and structural biologist, is the new lead scientist for the Protein Crystallography Station (PCS) at the Lujan Neutron Scattering Center. In addition to performing research as a Bioenergy and Biome Sciences (B-11) staff scientist, he will lead the science program of the PCS instrument and assist scientists from all over the world in crafting crystal samples, running experiments, and turning results into published papers.

Chen holds a PhD in biophysics from the University of California, San Francisco, where he was a postdoctoral fellow focused on membrane protein ion channels and transporters. As an assistant professor of biophysical chemistry at Germany's Goethe University, he visited Los Alamos National Laboratory in 2004 with a colleague to determine the inner workings of a particular enzyme using PCS, the first macromolecular diffractometer built at a spallation neutron source. The result was a landmark paper published in the Proceedings of the National Academy of Sciences.

As a Bioscience Division visiting scientist since 2011, Chen has collaborated with Laboratory researchers to obtain the world's first neutron structures of membrane proteins—an ongoing pursuit. Membrane spanning transport proteins are essential to all aspects of life, yet little is known about how they function largely due to a lack of structural information.

Chen's emphasis has been on ammonia and the bicarbonate transporter, important targets within the Lab's energy security mission and the bioenergy portfolio of the Biological and Environmental Research Division of the Office of Science at the Department of Energy, which funds the PCS. Other applications abound, especially pharmaceuticals, many of which target membrane proteins.

Based on work at PCS, the Lujan Center has reported the highest resolution neutron structure of a protein to date, was the first to report the neutron structure of a clinically used drug bound to its human target and is responsible for about 50% of the reported protein crystal structures obtained using neutrons. PCS program is conceived as an integrated support capability called "gene to structure". It is unique to Los Alamos and includes neutron beam-time, access to deuteration facilities, the expression of proteins and the synthesis of substrates with stable isotopes, and also support for data reduction and structure analysis. As well as access to a Rigaku HighFlux X-ray system to provide access to both room temperature and cryo X-ray to complement the neutron data. The PCS accommodates around 25-40 users (~25 proposals) per year and beam time is allocated through a peer review process by an external committee.

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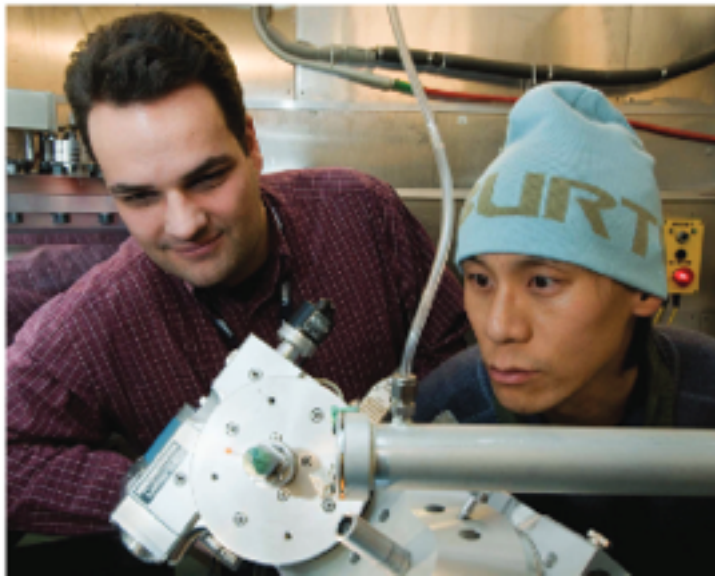

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