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HEADS UP!

LANSCCE hosts NNSA Academic Alliance Workshop

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



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

Eighteen graduate students and postdoctoral researchers presented talks or posters on their work and attended lectures on defense-related nuclear science at Los Alamos. Two university faculty members also gave talks. Topics presented by the visitors included the potential use of alternate reactions to deduce nuclear reaction cross sections on unstable nuclides that are difficult to measure directly; development of a neutron detector array for use in radioactive beam research; development of a time projection chamber for neutron measurements; nuclear structure studies; and simulations of new experiment designs. Kurt Schoenberg (ADEPS), Bob Haight, (LANSCCE-NS), Shannon Holloway, Patrick Talou, and Takehito Watanabe (T-2); Kevin John

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(SPO-SC); and Chris Morris (P-25) gave lectures that covered the broad nuclear science program at LANL, including neutron-induced capture, fission, and neutron and charged particle emission reactions, level density studies, nucleosynthesis, isotope production, and proton radiography. A tour of LANSCE facilities capped the visit.

Technical contact: Robert Haight (LANSCE-NS)

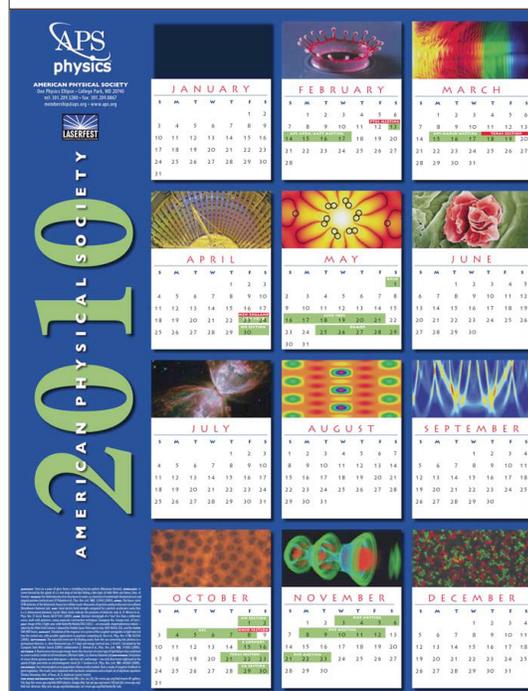
Neutron reflectometry studies of nanostructural phenomena at the fuel cell interface

Polymer electrolyte fuel cells (PEFCs) hold promise for energy production due to their high energy density, high efficiency, and zero emissions. The active power-producing center of a PEFC is the catalyst-coated membrane, which consists of anode and cathode catalyst layers coated onto either side of an ion-exchange polymer (or ionomer) membrane. The triple-phase interface of a PEFC electrode is comprised of three co-mingled two-dimensional interfaces—a platinum/carbon interface (for electron transport and catalyst particle dispersion), a platinum/ionomer interface (for proton transport to reaction sites), and an ionomer/carbon interface (for high dispersion of catalyst-support aggregates, electrode structural integrity, and high porosity for oxygen/hydrogen diffusion). Understanding the basic structure of ionomers across length scales, from molecular to nanostructural to bulk, is important to comprehend water transport, proton transport, and the oxygen reduction reaction mechanism occurring at the triplephase interface. This information will assist in improving the efficiency of PEFCs.

Jerzy Chlistunoff and Rod Borup (MPA-11), Jarek Majewski (LANSCE-LC), and D. Wood (Oak Ridge National Laboratory) used neutron reflectometry at the Lujan Center to examine the interactions of PEFC materials comprising the triple-phase interface. They studied a commercially available ionomer, Nafion. The scientists used smooth, idealized layers of Nafion on glassy carbon and platinum surfaces as an experimental model for the PEFC electrode interfaces. Separate hydrophobic and hydrophilic domains formed within the Nafion layer when equilibrated with saturated deuterated water vapor. The thicknesses of the hydrophobic and hydrophilic domains changed to the same magnitude when a platinum oxide layer was present compared to a thin hydrophobic domain in contact with platinum. The findings are direct experimental evidence that both the interfacial and long-range structural properties of Nafion are affected by the material with which it is in contact. Evidence of physical changes of aged Nafion films show a permanent increase in the thickness of the Nafion

film and a decrease in scattering length density. The researchers attribute these results to irreversible swelling of the Nafion film. Reference: "Exploration of nanostructural phenomena of the platinum/Nafion interface using neutron reflectometry," *Journal of the American Chemical Society* (in press). The DOE Fuel Cell Technologies Program and the DOE Office of Basic Energy funded the work.

Technical contact: Jarek Majewski



LANSCE research featured in American Physical Society calendar

The American Physical Society (APS) features graphics of physics research for its calendars, which the APS distributes to its approximately 47,000 members. For the month of October in the 2010 calendar, the APS chose an image of a polymer supported lipid membrane from a paper by LANSCE-LC researchers Hillary Smith, Michael Jablin, Jessica Saiz, Erik Watkins (also University of California, Davis), Alan Hurd, and Jaroslaw Majewski; and University of South Florida collaborators. The polymer gel layer provides a realistic, controlled environment to study biomembranes. As the polymer swells, it promotes both in- and out-of-plane fluctuations of the supported membrane that mimic the properties of living cellular membranes. The promotion of membrane fluctuations offers far-reaching applications as a surrogate biomembrane. This polymer-membrane system may facilitate otherwise difficult studies of lipid-protein interactions, transmembrane ionic transport, membrane structure, and membrane-based biosensors that

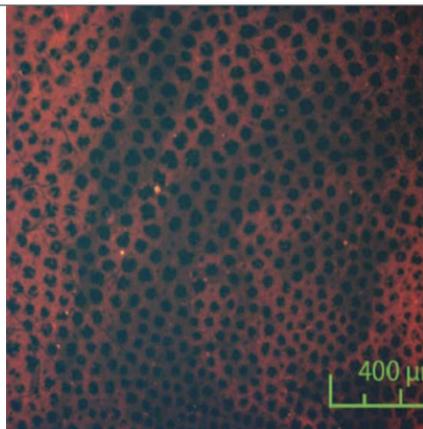
continued on page 3

previously have not been possible because of the limitations of existing models to in-plane studies.

Reference: "Model lipid membranes on a tunable polymer cushion," *Physical Review Letters* **102**, 228102 (2009). The American Physical Society also selected the research to appear in the *Virtual Journal of Biological Physics Research*. This work benefited from the use of the Lujan Neutron Scattering Center at LANSCE, which the DOE Office of Basic Energy Science funds.

Fluorescence microscopy
image of a polymer
supported lipid bilayer

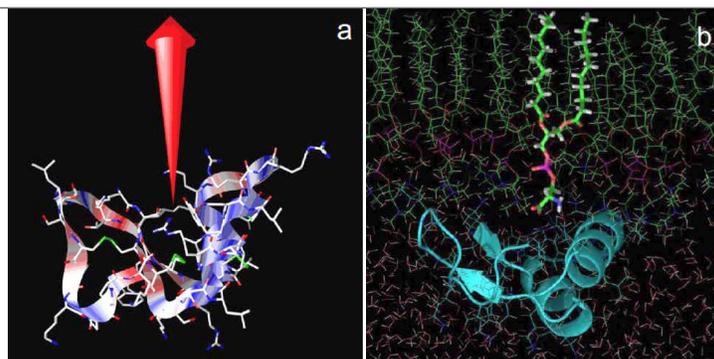
(Image for October in APS
2010 calendar).



X-ray studies reveal how plants defend against bacterial invaders

Purothionins are low molecular weight plant polypeptides that appear to have an important role in defense against bacterial invaders. Their toxic effect may arise from lysis (disruption) of the membranes of the attacking cells. To clarify how purothionins lyse the bacterial phospholipid membranes, Jarek Majewski (LANSCE-LC) and Boguslaw Stec (Burnham Institute for Medical Research, Calif.) used synchrotron x-ray scattering methods (x-ray reflectivity and grazing incidence x-ray diffraction) to investigate the interactions of purothionins with a model lipid membrane. The results suggest that purothionin transiently binds to the surface of phospholipid membranes in the liquid phase and withdraws some of the membrane's components. Information gained from research into the mechanism of bacterial cell lysis could give insight into how antibiotics function and the development of new classes of antibiotics from plants. Reference: "X-ray scattering studies of model lipid membrane interacting with purothionin provide support for one of the previously proposed mechanisms of membrane lysis," *European Biophysics Journal* (in press).

The DOE Office of Science, Office of Basic Energy Sciences (Alan Hurd, LANL program manager) supported the work. Majewski is the principal investigator.



(a) The ribbon representation of beta-purothionin superposed onto bond-stick model showing the distribution of positively charged amino acids. The vector of the electric field originating at the site of binding of a small molecule entity (glycerol, serine, phosphate, etc.) detected in each crystal structure of thionins that is proposed to be the phospholipid binding suite is depicted by the red arrow. (b) Snapshot of a molecular dynamics simulation illustrating the possible attachment of the charged phospholipid to the purothionin.

HIPPO's very high-temperature neutron diffraction capability solves materials question

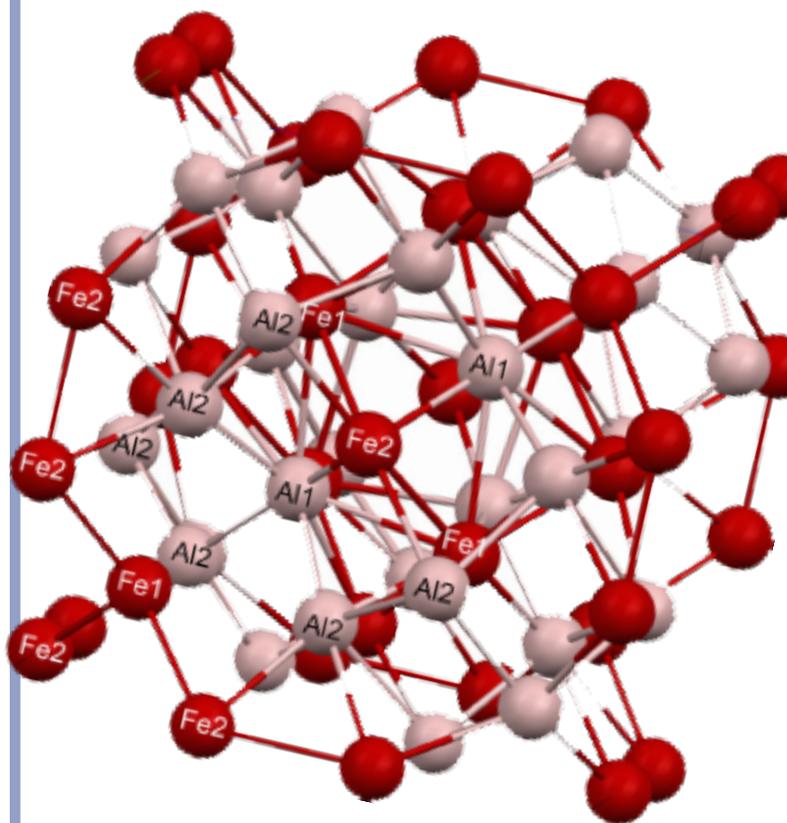
The High-Pressure Preferred Orientation Neutron Diffractometer (HIPPO) is a third-generation neutron time-of-flight powder diffractometer that achieves very high neutron count rates. Besides general-purpose neutron powder diffraction, HIPPO supports studies of crystal orientation distribution (texture), amorphous solids, liquids, magnetic diffraction, small crystalline samples, and samples subjected to non-ambient environments such as temperature, pressure, or uniaxial stress. HIPPO has unique high-pressure anvil cells capable of achieving pressures of 15 GPa at ambient and high temperatures (2000 K). Therefore Los Alamos scientists and external users utilize HIPPO as a powerful tool for materials research.

Recent neutron diffraction measurements performed on HIPPO to temperatures up to 1120°C played a crucial role making the first observation of the existence of the high temperature ϵ phase in the iron-aluminum (Fe-Al) system. These results come about one hundred years after A.C.G. Gwyer made the first observation of some indications for the existence of the high-temperature ϵ phase in the Fe-Al system. Sven Vogel (LANSCE-LC) and collaborators (Max-Planck-Institut für Eisenforschung GmbH, Germany) used HIPPO's high-temperature neutron diffraction capability to show, for the first time, that the crystal structure of the ϵ phase is the body-centered cubic Cu^5Zn^8 -type (g_1 brass structure). Thus, the formula Fe^5Al^8 , as shown in the figure, is the appropriate designation of the ϵ phase.

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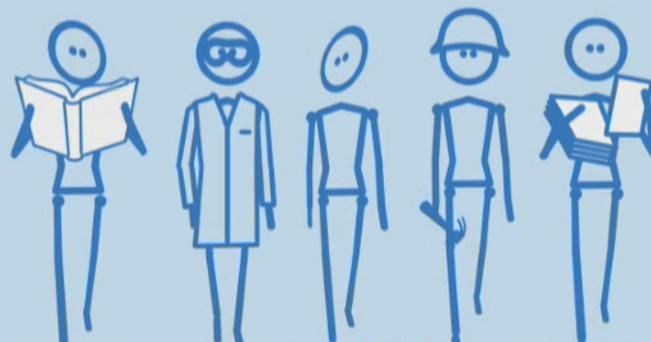
How alloys behave at very high temperatures is of fundamental importance to their application. Therefore, the ability to map and characterize the complete phase diagram is a crucial part of predicting how a material will perform in the real world. One of the central issues for predicting the performance and potential applications of the Fe-Al alloys is to understand the very high temperature ϵ phase. If a material is to perform under extremes of pressure, electromagnetic fields, stress and or very high temperatures, modeling alone is not enough. Experimental data are needed, which this work provides.

Reference, "Determination of the Crystal Structure of the ϵ Phase in the Fe-Al System by High-temperature Neutron Diffraction," *Intermetallics* **18**, 150 (2010). The research benefited from the use of the Lujan Neutron Scattering Center at LANSCE, which the DOE Office of Basic Energy Sciences funds.



Structure model of the atom arrangement in the Fe₅Al₈ unit cell. For clarity, the partial occupation of the Al₂ sites by 5% Fe atoms is not shown in the figure.

HeadsUP!



BEING HUMAN

TRYING TO DO THINGS RIGHT

Being human - What happens before mistakes?

A look at the causes of split focus and workplace stress which can cause mistakes. Power Point and MPG video available at LANL:Safety, <http://int.lanl.gov/safety/index.shtml>

Celebrating Service

Congratulations to Gregg Chaparro, LANSCE-NS, celebrating his 30-year service anniversary this month.

AOT & The Pulse

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