AOT & LANSCE The Pulse

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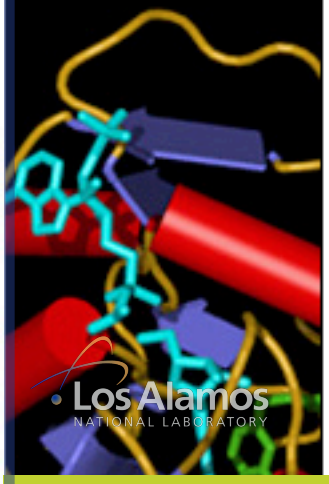

Students learn about neutron scattering at world's most powerful neutron source

More than 30 graduate students, postdoctoral researchers, and researchers from across the nation came to Los Alamos recently to participate in the LANSCE School on Neutron Scattering. This year's focus was on structural materials and classes described how neutron scattering methods can provide unique insights in diverse areas such as shape memory alloys, intermetallics, super-alloys, and bulk metallic glass composites. Lecturers provided overviews, discussed a series of case studies, and described exciting opportunities deriving from new DOE-funded instruments and the next generation spallation neutron source. Don Brown (Structure/Property Relations Group, MST-8) was the chair of the Neutron School Organizing Committee, and Jim Rhyne (LANSCE-Lujan Center, LANSCE-LC) was the school director. Los Alamos lecturers included Don Brown and Carlos Tome (MST-8); Bjørn Clausen, Thomas Proffen, and Sven Vogel (LANSCE-LC).

Don Brown shows students the SMARTS diffractometer for in-situ strain measurements.

Neutron scattering makes a critical impact on a multitude of science-related fields. Every year, organizers select one focus area of Los Alamos technical expertise from a list that was developed by a Lab-external advisory committee. Organizers then invite leading researchers to present the latest breakthroughs in the area, tie them to current events, and provide hands-on applications. Past topics have included phase transformations, magnetism and neutron scattering, structural materials, soft matter and biological structures, and hydrogen in materials.

The schools bring together graduate students and postdoctoral researchers to gain an in-depth knowledge of specific science topics to which neutron scattering makes valuable contributions. Because of its more specific focus, LANSCE's school differs from other neutron scattering schools, such as Argonne National Laboratory's National School on Neutron and X-ray Scattering and the National Institute of Standards and Technology's Center for Neutron Research Summer School. Those schools provide a general overview of scattering or have an instrumentation focus. The LANSCE school includes lectures and an experimental portion that allows each student to conduct hands-on neutron experiments on Lujan Neutron Scattering Center instruments at the Spallation

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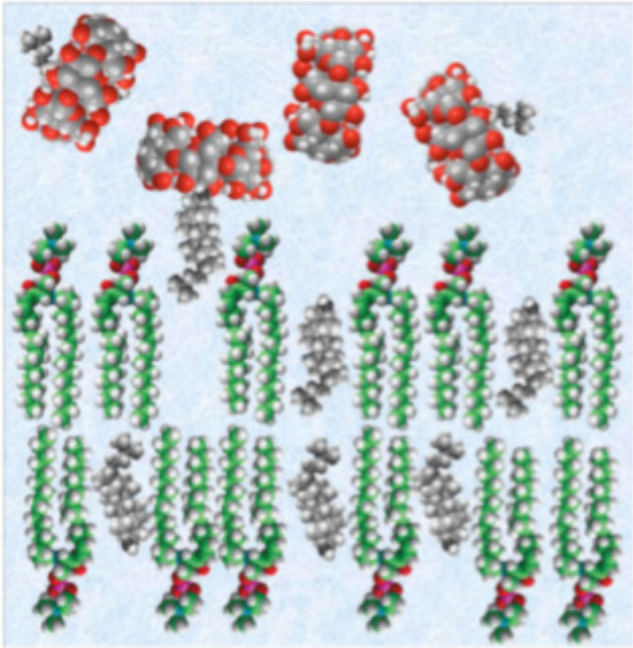
Source… Neutron Source. At the end of the week, students are asked to choose their favorite experiment, team with others who also selected that particular experiment, and give a talk. The National Science Foundation and the DOE Office of Basic Energy Sciences support the tuition-free school. Assistance for travel, lodging, and subsistence is available.

Neutron scattering reveals removal of cholesterol molecules from membranes

Cellular membranes contain ordered microstructures, called "lipid rafts," which display different physicochemical properties from their disordered fluid surroundings. The rafts are vital for a cell's functionality. These small, closely packed domains of 100-2000 Angstroms contain cholesterol (Chol) and sphingolipids in a molar ratio of 2:1. At this composition, they form a stable complex, which is resistant to many disruptor substances that can disturb the less organized, surrounding domains of biomembranes. β-cyclodextrin (β-CD) is a disruptor that modifies the structure and function of cellular membranes. The external surface of the β-CD is hydrophilic, while its nonpolar cavity can form inclusion complexes. β-CD has applications in many scientific and industrial fields, such as pharmaceuticals, food processing, cosmetics, environmental protection, and biochemical production. Because β-CD has been shown to bind to cholesterol molecules, it has been used to probe the stability of lipid rafts. However, the complexity of the previously investigated experimental systems has made it difficult to assess the effect of β-CD on the structure of the membrane.

Jarek Majewski, student Michael Jablin, and postdoc Manish Dubey (Lujan Center, LANSCE-LC); and collaborators from the Jagellonian University (Poland) and Clemson University examined the influence of β-CD on the structure, composition, and reorganization of model membranes composed of mixed sphingomyelin (SM)/Chol bilayers. The scientists created and structurally characterized model bilayer membranes at a solid-liquid interface and subjected them to interaction with β-CD. The model membranes consist of controlled molar ratios of SM and Chol above and below the stable complexation ratio (2:1). The researchers used neutron reflectivity at the Lujan Center's Surface Profile Analysis Reflectometer (SPEAR) to assess the amount of material removed from the SM/Chol bilayers. Unlike x-ray scattering, neutron reflectivity does not alter membrane structure. These are the first neutron scattering studies of the interactions between β-CD and SM/Chol bilayers.

The scientists demonstrated the presence and stability of the 2:1 sphingomyelin (SM)/Chol complex. While β-CD has no effect on membranes at or above the stable complexation ratio (2:1), it removes all uncomplexed Chol from membranes below the stable complexation ratio. The removal of Chol from lipid membranes shows that β-CD has the appropriate molecular dimensions to form inclusion complexes with sterol molecules. In contrast, double-chained phospholipids have a cross-sectional area that exceeds the dimensions of the β-CD cavity. Therefore, β-CD cannot complex sphingomyelin. Reference: "Effects of β-Cyclodextrin on the Structure of Sphingomyelin/Cholesterol Model Membranes," *Biophysical Journal* **99** (5) 2010 (in press). The work benefited from the use of the Lujan Neutron Scattering Center, which the DOE Office of Basic Energy Sciences funds.



Schematic of selective cholesterol removal. The researchers investigated the interaction between β-cyclodextrin (β-CD, red cyclic molecules) and model membranes containing sphingomyelin (green molecules)/cholesterol (Chol, gray molecules) complexes.

Workshop on f-electrons highlights expertise of Los Alamos researchers

Several of the Laboratory's scientific leaders in condensed matter physics gave invited presentations at an international workshop in Dresden, Germany aimed at better understanding the dual nature of f-electrons. Tomasz Durakiewicz (Condensed Matter and Magnet Science, MPA-CMMS) and Gedrtrud Zwicknagl (Technische Unversitat Braunschweig, Germany) organized the third international

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Scientists from all over the world attended the third international workshop on the dual nature of f-electrons in Dresden, Germany.

f-electrons… workshop on the Dual Nature of f-Electrons. The four-day workshop drew 36 scientists, including 9 from Los Alamos, who participated in invited talks and roundtable discussions regarding f-electron materials.

Eric Bauer, Krzysztof Gofryk, Filip Ronning, Chuck Mielke (MPA-CMMS); Zachary Fisk (University of California, Irvine and MPA-CMMS); Tomasz Klimczuk (Lujan Center, LANSCE-LC); Jian-Xin Zhu, Cristian Batista, and Matthias Graf (Physics of Condensed Matter and Complex Systems, T-4) gave invited presentations on specific topics. Two highlights of the workshop included Fisk's and Graf's presentations. Fisk's talk, "Electronic Inhomogeneity Near Quantum Criticality," included a thermodynamic analysis of alloyed $CeCoIn_5$. The research provided evidence for an inhomogeneous electronic state at low temperatures. Graf's talk, "Uncovering the Hidden Order in URu_2Si_2," presented a new theoretical interpretation of the nature of the hidden order developed in collaboration with Alexander Balatsky and Jonatan Dubi (T-4). The theory is based on nuclear magnetic resonance (NMR) and scanning tunneling microscopy (STM) experiments performed by collaborators Nicholas Curro (University of California, Davis) and Kei Davis (Cornell University). The NMR analysis revealed that the coupling between antiferro-magnetism and the hidden order parameter in the strongly correlated f-electron metal URu_2Si_2 is not a competing order, but rather a parasitic effect. This result is contrary to conventional scenarios. Similarly, the STM analysis inspired the Los Alamos group to postulate a hybridization density wave between d and f electrons as the relevant interaction for the hidden order. Although the exact character of this order parameter has eluded researchers for more than two decades, a series of new NMR and STM experiments demonstrated that the hidden order transition at 17.5 K above absolute zero temperature is accompanied by a partial gap in the single particle density of states. Moreover, the NMR spectra showed that impurities in the hidden order phase generate local patches of antiferromagnetism. The emergence of the hybridization gap as seen in STM experiments is consistent with this novel scenario of a hybridization density wave.

The Max Planck Institute for Complex Systems, Germany funds the conference, which Max Planck Institute Director Peter Fulde co-hosts.

Technical contact: Tomasz Durakiewicz

Study of high-speed surface dynamics using a pulsed proton beam

Los Alamos is developing and implementing ejecta source and transport models for integration into the Laboratory's hydrodynamic computer codes. The underlying postulate for ejecta formation is that ejecta are produced by a special limiting case of a Richtmyer-Meshkov (RM) instability. Therefore, a key element of source modeling and transport centers on high-explosive shocked-tin proton radiography RM experiments at LANSCE.

The tin targets were machined with sine-wave patterns in the surface to seed the growth of the RM instability. The researchers examined growth of the RM instability into three environments: vacuum, neon (Ne), and xenon (Xe).

The vacuum data in Figure A show that the short-wavelength, large-amplitude RM spikes travel the fastest, with the short-wavelength and small-amplitude traveling at a similar yet lower velocity as the long-wavelength and large amplitude. Bubbles are also evident and distinguishable from the free-surface velocity that is determined by the flat regions between the sinusoidal perturbations.

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Proton beam. . . A comparison of the RM instability growth in the three environments shows that the RM spikes in the Ne gas behave much more like the vacuum series than do the spikes in the Xe gas (Figure B). This is interesting because the viscosity of Ne is about twice the Xe viscosity. Moreover, the density of Xe is about five times the density of Ne, so the kinematic viscosity of Ne is about ten times the kinematic viscosity of Xe. This result implies that the Weber number (ratio between the inertial force and the surface tension force) dominates the spike-breakup.

Particle breakup is important to particle transport in gases. Hydrodynamic models predict that the RM spike tips will not continue to grow thinner with time, but they will become blunted due to surface tension. This effect is nominally seen at around 11.6 microseconds in the vacuum series, which implies that the effect happens in the Ne and Xe series as well. Drag may be stripping liquid tin off the blunted tips, streaming the material toward adjacent neighbors. This assumption is supported by the fact that the RM spikes appear to breakup in the middle of the spikes in the Ne gas at time 15.1 microseconds, and at time 12.1 microseconds in the Xe gas. Close inspection reveals evidence of the mass streaming from the fastest Ne spike tips, in the shape of a mach-stem, to their nearby neighbors at time 11.4 microseconds.

These observations can be used for code validation and verification studies. The collection of results will be used to inform FY10 experimental packages and test the Laboratory's working ejecta model. William Buttler and David Oro (Neutron Science and Technology, P-23), Guy Dimonte (Materials and Physical Data, XCP-5), Chris Morris (Subatomic Physics, P-25), Guillermo Terrones (Safety and Surety, XTD-1), Patrick Reardon and Felix Garcia (Polymers and Coatings, MST-7), and the proton radiography core team performed the work. NNSA Campaign 1 (Bob Reinovsky, LANL campaign manager) funded the research.

Technical contact: William Buttler

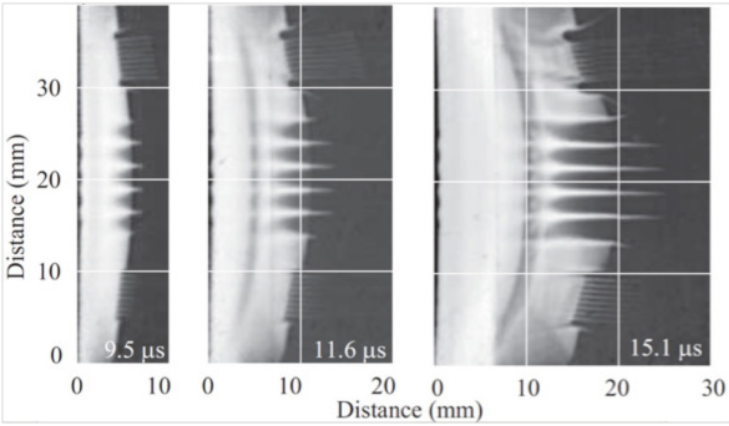

Figure A (above right): Three of 19 FY09 proton radiography RM images with image times. The instabilities are not fully resolved at this scale and contrast level. Salient features, including bubble and spike positions relative to the flat regions, are evident.

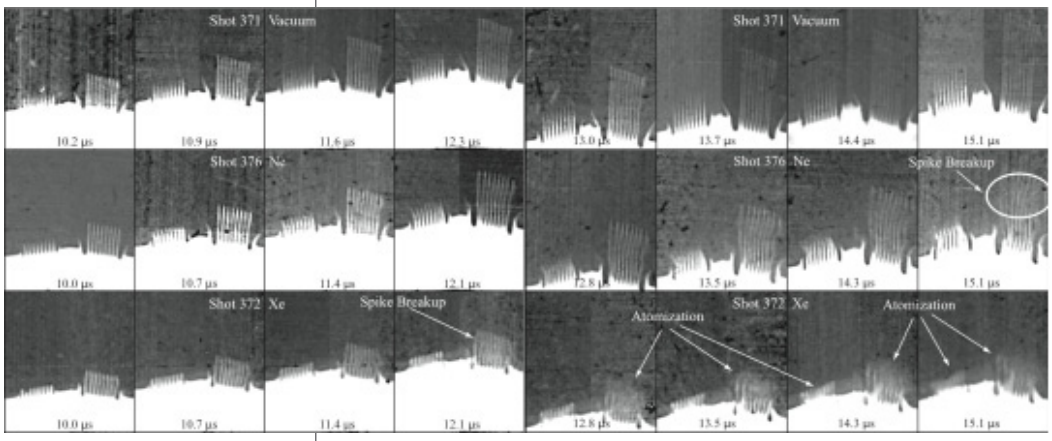

Figure B (right): Vacuum, Ne, and Xe proton radiography RM time-series data, beginning just after shockwave breakout. The tin is fully liquid on release, and the gas pressure was approximately four atmospheres for each pressurized experiment. Image times are closely matched.

Laboratory communicators recognized in international technical publications competition

An international technical publications competition recently recognized the work of several Los Alamos employees. The Society for Technical Communication sponsored the 2010 International Technical Publications Competition to recognize and encourage excellence in communication through printed media. With 14,000 members worldwide, the society is the largest professional organization of technical communicators and is dedicated to advancing the art and science of technical communication. The awards honor technical writers and editors who set the standards for published technical communication. Entries are judged for technical communications by industry experts from multiple disciplines. An award is both peer recognition as well as acknowledgment of quality that stands out among significant corporate and industrial entries.

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Competition… From Los Alamos, the following entries received awards:

LANSCE Activity Report 2006, (Award of Merit), Clay Dillingham, editor/writer; Barbara Maes, desktop publisher; and Brenda DeVargas, graphic artist (Communication Arts and Services, IRM-CAS).

MPA Materials Matter, (Award of Merit), Karen Kippen and Robb Kramer (Experimental Physical Sciences Directorate, ADEPS) and Thomas King (Communication Arts and Services, IRM-CAS).

To compete in the international competition, entries must first win a Distinguished Technical Communication award (the highest level of award) at a regional STC competition. Technical publications are evaluated for writing, graphics, copyediting, and overall integration.

Celebrating service

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

Jean Trujillo, AOT-DO	35 years
Michael Fitzsimmons, LANSCE-LC	20 years
Jonathan Ferris, AOT-MDE	10 years
Cecilia Duenas, AOT-IC	5 years
Dominic Tafoya, AOT-MDE	5 years

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HeadsUP!

Lab goes after worst slip-trip problem areas

Improved lighting, better footing, sidewalk repairs

Rust was removed, sidewalks were leveled, lights were installed, and employees are now safer from the single biggest cause of injury to Los Alamos workers. Remediation of the top slip, trip and fall locations across the Lab has now been completed, resulting in a 16% drop in related injuries.

Some 52 sites across Laboratory property were identified as problem areas and then fixed or remedied by the LANL Utilities and Infrastructure group.

Some of the primary improvements included:

- The parking lot in TA-3 off of Bikini Atoll Road. The lot was recently repaved by the Maintenance and Site Services Division -- Utilities and Infrastructure (MSSUI).
- The sidewalk outside the J. Robert Oppenheimer Study Center. Uneven sections of the walkway were ground down to be level.
- Lighting for the walkway outside of the National Sciences Security Building was installed, along with lighting near the parking garage on Mercury Road.
- Lighting was installed in the covered stairwell leading down into the buildings of TA-59.

It was in October 2009 that the Institutional Worker Safety and Security Team received the word from LANL Deputy Director Ike Richardson that the Lab would fund the remediation.

One of the keys to success was the involvement of the employees, who acted as identifiers for the issues to be remedied. Each directorate helped—giving recommendations about slip-and-trip locations that needed to be fixed. The Utilities and Infrastructure group also gave recommendations, using its professional assessment and rating scale to locate the most unsafe areas. Sites selected to be fixed were spread across Lab property, as the WSST did not want to concentrate the work, but instead hit a balance. Attention was given to high-use areas as well as more remote sites.

On a visit to the Lab, the DOE Voluntary Protection Program's Assessment Team gave the remediation project high praise for its accomplishments and promotion of worker safety. The assessment team is made up of 16 individuals from across the country.