AOT & LANSCE The Pulse

August 2010

INSIDE

Katharine Page

Finding reward in physical and mental strength

By Francisco Ojeda
ADEPS Communications

Katharine Page finds several similarities between the two passions in her life—Olympic-style weightlifting and materials science. While one is more physically grueling and the other more mentally demanding, Page enjoys the benefits of both.

"They both take mental discipline and attention to detail," Page said. "Putting the hard work in definitely pays off with results. They both have definitely given me confidence and the ability to perform under pressure situations. Both are rewarding."

Page, who has a PhD in materials from the University of California, Santa Barbara, is a Director's Postdoctoral Fellow at the Lujan Neutron Scattering Center (LANSCE-LC), where she is a member of the Total Scattering Team. A chemical engineer turned materials scientist, she has expertise in synchrotron x-ray and neutron scattering methods for powders, nanoparticles, and thin films, and modeling tools for disordered, complex, and nanostructured materials. Page was a student in the NASA Undergraduate Student Research Program at Los Alamos in 2003 and 2004 and has been a frequent visiting scientist at the Lujan Center.

"She has an intuitive understanding of materials science," said Page's mentor Thomas Proffen (LANSCE-LC). "Her knowledge and experience is more at the level of a staff member than a postdoc."

For her research on probing atomic structure in functional thin films and nanoparticles, Page was 1 of 6 postdoctoral researchers out of 68 to win an award at the recent Postdoc Research Day, which was sponsored by the Laboratory's Postdoctoral Association. A portion of the research presented, "Probing Local Dipoles and Ligand Structure in $BaTiO_3$ Nanoparticles," was published in *Chemistry of Materials.*

Page was the postdoctoral association's president last year and is the vice president this year.

"She has been very influential," said Los Alamos National Laboratory Postdoctoral Association President Shadi Dayeh of the Center for Integrated Nanotechnologies. "She has leadership skills that have helped take the association to new heights."

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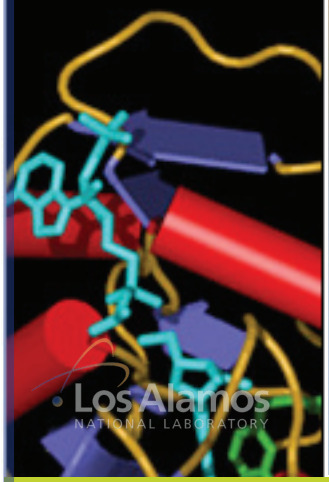


From Kevin's Desk

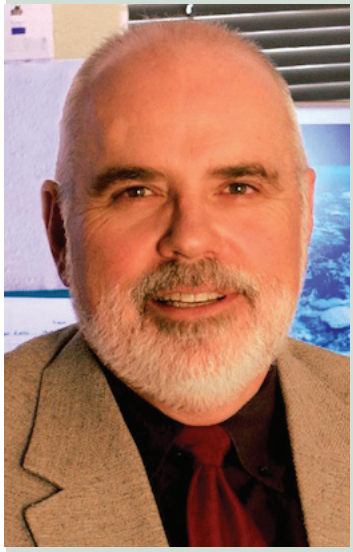
AOT & LANSCE The Pulse

Some 30 years ago as a graduate student I arrived at what was then LAMPF as a user to do my thesis experiments. I knew a little about proton and heavy ion sources, electrostatic accelerators, and low-energy nuclear physics detection techniques, but none of that prepared me for the scale of either the LAMPF accelerator or the High Resolution Spectrometer (HRS) in Area C where proton radiography experiments are now performed. What an opportunity to learn!

Of course, as the student responsible for the experiments I worked mostly nights and weekends, and on the Sunday afternoon of the first weekend of the experiment this kindly older gentleman walked into the HRS counting house and engaged me in conversation about the experiment. I was the only person there at the time and we had a delightful chat about the physics we were pursuing and the progress made to date. I didn't know who Louis Rosen was then, but I quickly learned that he treated everyone with the same consideration and gentility regardless of position. His Sunday afternoon visits were often the highlight of the week, and his commitment to the success of the LAMPF User Program remains the foundation for our ongoing commitment to the success of LANSCE today.

Over the years I learned more about the LANSCE accelerator in order to improve the beam performance for challenging experiments in the nucleon and nuclear physics programs in Areas B and C. This led me to move to the operations organization of what was then MP Division to learn more about the accelerator and beam delivery systems that are the backbone of today's LANSCE facility.

The hallmark of the organizations that have operated and used LAMPF/LANSCE over the years is the ability to solve complex problems that optimize and maximize the utilization of the uniquely flexible LANSCE accelerator. This began with the Los Alamos design of the side-coupled-cavity linac and the prescient flexibility of accelerating both H+ and H- beams, continuing with the "dial-a-spin" capabilities for polarized proton and neutron experiments



"…I am confident that the success of the past will be repeated yet again. There is no better team of leaders and no better staff at any accelerator facility in the United States than that of AOT Division together with LANSCE and LFO Divisions…"

in Areas B and C, the design and commissioning of the Proton Storage Ring, where we learn new beam physics almost every year, the re-invention of Area C for proton radiography and of Area B for ultra-cold neutron experiments, the reconstitution of isotope production capability at 100 MeV at the Isotope Production Facility and the continuing evolution of neutron science at the Lujan Center and the Weapons Neutron Research facility.

The people of MP, AT, AOT, LANSCE, LFO, P and (again) AOT Divisions are the reason that LAMPF and LANSCE have been so successful. That success was and continues to be built on competence and dedication. I was a relatively young staff member when Don Hagerman, Lew Agnew and Jim Bradbury retired—the entire Division Office leadership! I recall thinking that we would be very challenged to continue our success absent their knowledge, wisdom, and leadership. But what I experienced was that the next generation of leaders stepped up and assumed the burden of sustaining and improving the performance of the facility and expanding its capabilities. The staff responded to this leadership and the transition to the next generation was very successful. Similar changes happen at the team and group level on a more frequent basis, and we always manage to be successful.

As I move on to a new challenge at the Spallation Neutron Source at Oak Ridge National Laboratory I am confident that the success of the past will be repeated yet again. There is no better team of leaders and no better staff at any accelerator facility in the United States than that of AOT Division together with LANSCE and LFO Divisions; you are well equipped to ensure continued successful operation of LANSCE, implement the LANSCE Risk Mitigation Project, make the Material Test Station in Area A successful, and bring the accelerator and beam technology portions of MaRIE to fruition.

I will miss everyone at LANSCE a great deal, and I wish all of you the best for continued growth and success.

AOT Division Leader Kevin Jones

LANL Postdoc Association wins poster award at National Postdoctoral Association meeting

The Los Alamos Postdoc Association (LAPA) earned third place in the National Postdoctoral Association (NPA) Poster Competition for the poster "Combinatorial Strategies Adopted by Los Alamos Postdoc Association (LAPA) for Personal and Professional Growth of Postdocs." NPA presented the award at its annual meeting.

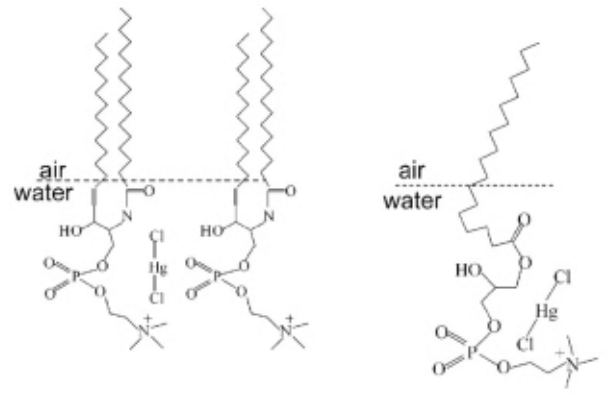
Praveen Sekhar (Sensors and Electrochemical Devices, MPA-11) and Shadi Dayeh (Center for Integrated Nanotechnologies, MPA-CINT) presented the poster, which focused on LAPA's activities for personal and professional growth of postdoctoral associates at LANL. LAPA's Social, Career, Policy, and Communications committees organize the career fair, career development workshops, and informal social sessions. The poster also described LAPAs' latest initiative, the Los Alamos Postdoctoral Associate Research Day. This Lab-wide event provides postdoctoral researchers the opportunity to present a summary of their LANL research to an audience that includes staff scientists and upper management. Sekhar and Dayeh collaborated with Sridhar Balasubramanian (Neutron Science and Technology, P-23), Amanda Klingensmith (Nuclear and Radiochemistry, C-NR), David Kuiper (Materials Chemistry, MPA-MC), Katharine Page (Los Alamos Neutron Scattering Science Center–Lujan Center, LANSCE-LC), and Mary A. With (Science and Technology Base Programs–Education Program Office, STBPO-EPDO) for the poster.

The NPA is a member-driven organization that provides a unique, national voice for postdoctoral scholars. The NPA issued a call for poster abstracts to approximately 7,000 postdoctoral researchers around the country for its poster competition with the subject regarding how their specific institutions aid postdoctoral researchers. Of those, 23 abstracts were chosen as the subject of poster presentations at the NPA meeting. Three judges chose the top three poster presenters and presentations from criteria such as overall visual appeal, poster content relevant to the NPA's goals, and oral presentation. The LANL Postdoc Program Office funded the research.

Technical contact: Mary Anne With

Studies of the mechanism of mercury neurotoxicity

Mercury (Hg) is one of the most serious environmental pollutants. Although the acute and chronic effects of mercury toxicity are well known, the mechanism of mercury toxicity at the cellular level is less clear. Because of its significant affinity to thiol (-SH) groups, mercury binds non-specifically to proteins, changing and disabling their functions, which, in consequence, can lead to dysfunctions of the cells, and, at a larger scale, to pathological changes in the target organs. Mercury also interacts with other functional groups. When it reaches different target cells, mercury first must penetrate the cellular membrane barrier to gain entry into the cell. Therefore, the interactions with cellular membrane components are of great importance regarding the molecular mechanism of mercury toxicity.



Complexation of inorganic mercury to (left): SM; and (right) lyso-PC.

Jarek Majewski (Lujan Neutron Scattering Center, LANSCE-LC) and collaborators (Jagiellonian University, Poland) report research that sheds new light on the neurotoxic effects of mercury in living organisms. The scientists, with professional advice from the Lujan safety officer, Frances Aull (Industrial Safety and Deployed Services, IHS-IS), performed systematic studies applying synchrotron x-ray scattering methods to model membranes containing phospholipid monolayers. They examined the interactions of inorganic mercury salts dissolved in the aqueous subphase with selected membrane phospholipids: dipalmitoylphosphatidylglicerol (DPPG), dipalmitoyl-phosphatidylcholine (DPPC), 1-octadecyl 2-sn-phosphatidylcholine (lyso-PC), and sphingomyelin (SM).

The results show that the elastic properties of phospholipid monolayers are a key factor regarding the interactions with mercury ions. DPPG and DPPC form well-organized, solid-like monolayers in which dense packing of the headgroups limits the possible contact of the donor atoms with mercury ions and impairs the possibility of complex formation. Significant differences occur for phospholipids that form more compressible films (SM and lyso-PC), which can complex permanently and accumulate mercury ions at the water/air interface. The scientists propose a limiting case model for SM in which two SM molecules complex one $Hg(Cl)_2$. This is an

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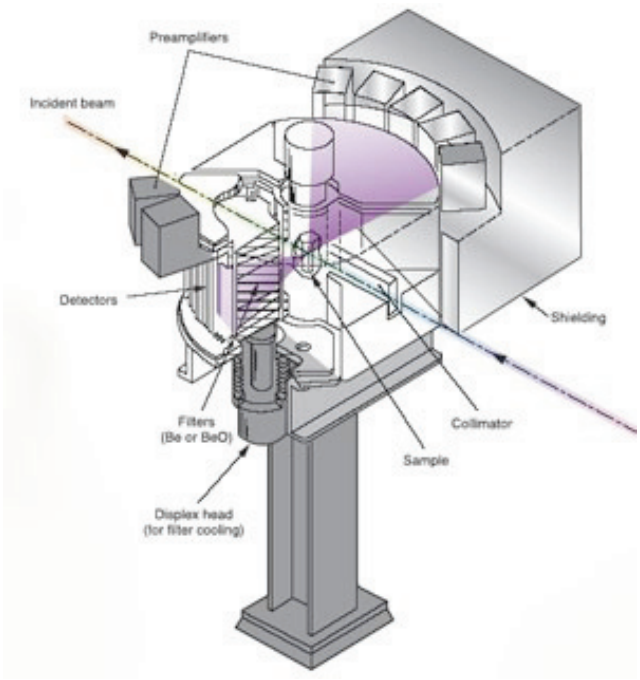
Mercury... important finding taking into account the accumulation of mercury in the central nervous system and its neurotoxic effects. Given that SM is one of the most abundant lipids in neuron sheath, and it is the main lipid component of the myeline shell, SM can be considered as a target lipid to complex mercury ions.

Reference: "Grazing Incidence Diffraction and X-ray Reflectivity Studies of the Interactions of Inorganic Mercury Salts with Membrane Lipids in Langmuir Monolayers at the Air/Water Interface", M. Broniatowski, M. Flasinski, P. Dynarowicz-Latka, J. Majewski), *The Journal of Physical Chemistry*, in press. The DOE Office of Basic Energy Sciences funded the Los Alamos work. *Technical contact: Jarek Majewski*

Upgrade to Filter Difference Spectrometer enables more science

The Filter Difference Spectrometer (FDS) at the Lujan Neutron Scattering Center is undergoing an upgrade that will significantly improve its functionality and usefulness for scientific research. In neutron vibrational spectroscopy, FDS exploits the large incoherent scattering cross section of hydrogen to obtain the vibrational spectrum of hydrogenous materials (see illustration). FDS is used mostly to study chemical bond dynamics in materials. The science addressed by the instrument includes heterogeneous catalysis and surface science, hydrogen bonding, organometallics, explosives, water in materials, hydrogen storage materials, hydrous minerals, and numerous other problems involving hydrogen. The instrument is particularly well suited to address scientific challenges relevant



Top view of the FDS filter tank. Samples reside in the 5-inch hole in the middle of the tank.

to the DOE hydrogen initiative, and use of the instrument within this context has increased dramatically over the past five years.

The principle of operation of the instrument is simple. Time-of-flight determines incident energy of the neutron. The final energy of the scattered neutron is set by a filter placed between the sample and the detector. Beryllium (Be) filters set the final neutron energy at 5.22 meV (nominally), and beryllium oxide (BeO) filters impose a final neutron energy of 3.76 meV. These filters do not have a perfectly sharp transmission function, but the difference between the Be and BeO data sets produce a vibrational spectrum with a resolution of the order of 1 meV, hence the name "Filter Difference Spectrometer." Early on, the difference could be computed with a minimum of hardware. When more powerful computers became available, numerical deconvolution methods replaced the filter difference method. Be and BeO data sets could be deconvoluted separately to produce a spectrum with better resolution than the filter difference method. Currently, the typical energy resolution is 2 to 5% depending on the data analysis method. Since BeO filters never lent themselves to reliable numerical deconvolution, users often ignored the corresponding data. Therefore, Lujan is replacing the BeO filters with Be filters.

The FDS filters are located in an evacuated tank and cooled to 100 K to reduce phonon scattering. This tank had not been opened in more than 20 years. The scientists assessed the condition of the various components, including filters, inside the tank. This operation, which took place in February, revealed a perfectly clean system in pristine condition with minor (and inconsequential) oxidation on a few sheets of cadmium. Brush-Wellman (OH, USA) produced the five new Be filters with high purity (> 99%) Be and near theoretical density. Each filter comprises three

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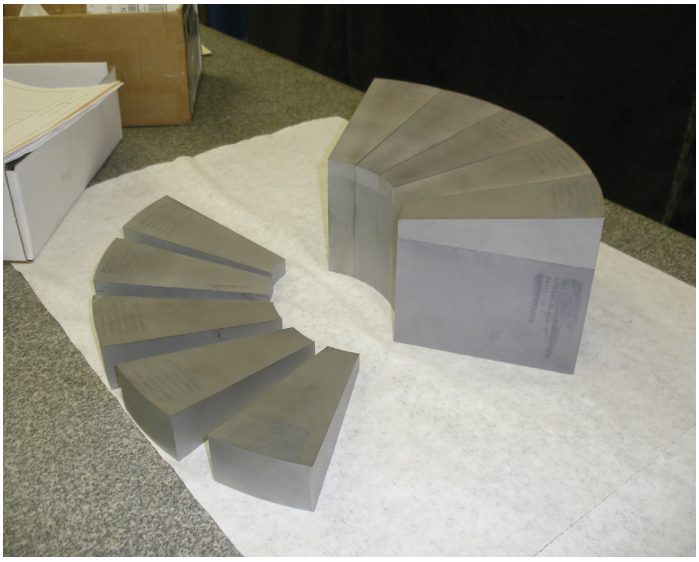
Upgrade . . . parts (see photo below), stacked on top of each other. This low cost upgrade will make the entire FDS detector more useful and will double the count rate of the instrument. The increased decoupling between filters of will also help reduce instrument background.

These upgrades will enable more science on FDS, such as use of smaller samples, greater sensitivity, the ability to conduct time-dependent experiments, faster measurements of unstable samples, and the capability to run more compositions or conditions. An upgrade of the data reduction software for FDS will provide users with additional graphical features, in addition to the two traditional data analysis methods of direct deconvolution and Maximum Entropy. The capital funding component of the DOE Basic Energy Sciences-Lujan Center Operations supported the work.
Technical contact: Luc Daemen



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HeadsUP!

Your LANSCE and AOT Electrical Safety Officers

LANSCE: Tommy Martinez, 4-0548
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- LANSCE-NS: Chuck Alexander

AOT: Tommy Martinez, 4-0548
- AOT-ABS: Gary Sanchez
- AOT-IC: Danny Olivas
- AOT-MDE: Tsuyoshi Tajima and Joe Raybun
- AOT-OPS: Jim Sturrock
- AOT-RFE: Mark Prokop

IWM Toolbox site features pre- and post-job guidance

Conducting moderate or high hazard/complex work? Then you should check out the Web site devoted to pre-job briefings and post-job reviews.

Pre-job briefs are required by P300, Integrated Work Management, for all moderate and high hazard/complex work activities. Pre-jobs should be conducted preferably right before work starts, and as frequently as necessary when:

- Assignments have changed or new personnel are involved which may be an individual, specific pre-job briefing,
- A change in work scope, R&D boundary/limits, and/or in facility or work area conditions has occurred that may affect safety, security, or the environment, or
- Work activities are resumed after an extended period of inactivity.

Post-job reviews and capturing lessons learned are required by P300 when an activity is terminated or fully completed and the IWD or equivalent work control document is no longer needed. For ongoing activities, post-job reviews, feedback or lessons learned should be obtained during the normal course of the work by completing Part 4 of the IWD.

A good refresher for persons-in-charge (PICs) and a good start for new PICs, the Web site features a 30-minute video, briefing and review guides and checklists. Find it at int.lanl.gov/saftey/iwmc/.

Page . . . Page earned the award for her research using the atomic pair distribution function formalism of neutron and x-ray total scattering to determine the detailed atomic structure of functional nanoparticles and thin films, a first-ever demonstration of this technique on amorphous and polycrystalline thin film samples. She and her colleagues are exploring the atomic structure that promotes reversible amorphous-crystalline transitions and leads to optical and electronic contrast in traditional and new phase-change materials—materials that may be used in the future for new, more robust data storage technologies.

Their recent study of perovskite $BaTiO_3$ nanoparticles was aimed at determining the nature of ferroelectricity at small size, absent the effects of substrate or support. Page described determining the structure of a complete nanoparticle system as "an exciting advancement in neutron scattering," and said she and her fellow researchers "are looking forward to using this method in the future in different fields and materials." In doing so, the researchers hope to gain further understanding of how size affects materials properties, for example, in nanocrytalline quantum dots.

"She has a bright future," Proffen said. "Every project she has been involved in she has made great contributions. She has impressed a lot of people in the materials science field."

Heavy lifting outside the lab

Outside the Laboratory, Page is a nationally competitive Olympic-style weightlifter, a field that includes the snatch and clean and jerk competitions. She developed an interest in the sport when she was an undergraduate and befriended theoretical chemist David Kent (formerly of CCN-8), who was an Olympic-style weightlifter. She began training with him and Joaquin Chavez, a strength and conditioning coach at the University of New Mexico.

Page has earned numerous top-five finishes at USA National and American Open Championships and has won three straight Collegiate National Championships in the 69-kilogram weight class. Page also competed in the 2008 US Olympic Trials, finishing third in her weight class and eighteenth out of 30 competitors in all weight classes. Page said she hopes to recover from a knee injury in time to attempt to make the 2012 Olympic Team.

"I enjoy how fast and explosive the sport is," Page said. "I picked it up pretty quickly and really enjoyed it. Both the science and the weightlifting have given me an outlet from the other, which has made me better in each area."

Celebrating service

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

Sven Vogel, LANSCE-LC	10 years
Terry Madison, AOT-IC	5 years