AOT & LANSCE The Pulse

March 2009

INSIDE

Don Brown completes fellowship at the Japan Atomic Energy Agency

Don Brown (MST-8) recently completed a 5-week fellowship at the Japan Atomic Energy Agency, sponsored by the Japanese Society for the Promotion of Science. Brown performed experiments on a high resolution x-ray diffractometer at the SPring-8, a synchrotron facility in Himeji Prefecture.

The purpose of the experiment was to deconvolute the diffraction line profile contributions from dislocations and twins in magnesium samples deformed in situ to varying levels of strain.

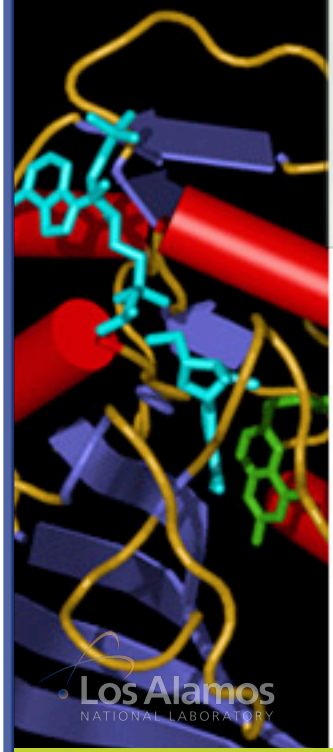
Brown also gave educational lectures at six different facilities, including the National Institute of Materials Science and the Japan Atomic Energy Agency on the use of spallation neutron sources (such as LANSCE) to study the micro-mechanics of the deformation of materials.

The new Japan Proton Accelerator Research Complex and the TOKAMI diffractometer will begin user operation in the coming calendar year.

◀ Don Brown (MST-8) recently returned from Japan where he performed x-ray diffraction experiments and gave educational lectures.

The lecture series was particularly relevant to the Japanese community because the new Japan Proton Accelerator Research Complex and the TOKAMI diffractometer, which is similar to SMARTS (Spectrometer for Materials Research at Temperature and Stress) at LANSCE, are in commissioning mode and will begin user operation in the coming calendar year.

Brown's host in Japan, Hiroshi Suzuki of the Japan Atomic Energy Agency, will visit Los Alamos and perform experiments on SMARTS at LANSCE.



Los Alamos NATIONAL LABORATORY

Enzyme study at the Lujan Center explains nerve agent detoxification

Organophosphorus molecules such as Tabun, Sarin, Soman, VX, and diisopropylfluorophosphate have the potential for devastating use as highly toxic chemical warfare agents. Scientists from Germany and Los Alamos are collaborating to develop a biologically inspired defense against these deadly nerve agents. Diisopropyl fluorophosphatase (DFP ase), an enzyme found in squid, can detoxify these agents by breaking a chemical bond in their phosphate groups.

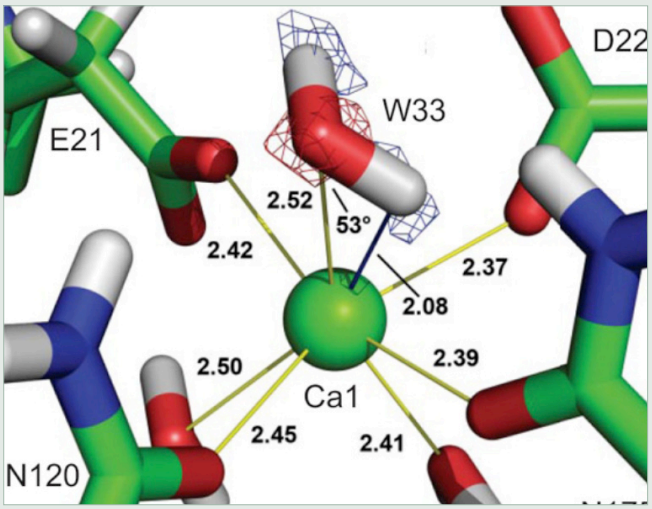
DFPase is a prime candidate for development as a decontaminant because large amounts can be produced cheaply using bacterial expression systems, and it is stable under a wide variety of environmental conditions. However, before DFPase can be used in the field, its efficiency and specificity against different nerve agents must be improved.

Engineering DFPase with improved performance against nerve agents requires understanding how DFPase binds the agents. Researchers Marat Mustyakimov, Benno Schoenborn, and Paul Langan (all in B-8) and collaborators used a new computational approach and software developed at Los Alamos to combine neutron diffraction data collected on the Lujan Protein Crystallography Station with x-ray data collected elsewhere. The resulting joint x-ray/neutron structure of the DFPase active binding site is more accurate and complete than structures obtained by either technique alone.

DFPase binds in an unexpected configuration, which rules out current ideas about its catalytic mechanism. It is the first protein for which neutron diffraction data report an extended network of internal water molecules, connected by hydrogen bonds in the form of a water tunnel in the center of a propeller-like structure. The protonation states of DFPase side groups and solvent molecules in the active site support a newly proposed catalytic mechanism (figure above right) involving a water molecule coordinating the catalytic calcium ion in a highly strained environment. This mechanistic insight enabled engineering improvements in DFPase for enhanced performance against nerve agents.

Reference: "Rapid Determination of Hydrogen Positions and Protonation States of Diisopropyl Fluorophosphatase by Joint Neutron and X-ray Diffraction Refinement," *Proceedings of the National Academy of Sciences USA* **106**, 713-718 (2009). Zoe Fisher, Andrey Kovalevskyi, Marat Mustyakimov, Mary Jo Waltman, Benno Schoenborn and Paul Langan (all in B-8) run the Protein Crystallography Station as a user facility at LANSCE.

The DOE Office of Science, Office of Biological and Environmental Research, and the National Institutes of Health support this research at the Laboratory.



▲ The active site environment of DFPase around the catalytic calcium ion, showing neutron scattering density from a functionally important solvent molecule (W33) that was expected to be an hydroxyl ion in the previously proposed catalytic mechanism and is demonstrated to be a water molecule in the newly proposed mechanism.

HeadsUP!

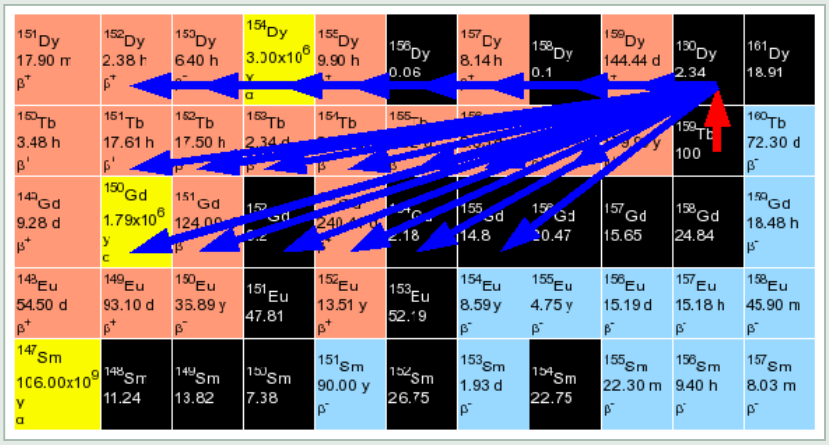
Annual key inventory
The annual key inventory must be completed by March 20. Work with your lock-and-key custodians to verify Laboratory level I, II and III keys issued to you.

Temporary government parking placards
The 2008 placards are no longer valid. Those who continue to use them will be cited for parking illegally. The 2009 temporary government parking placards have been sent to division offices for distribution.

Briefing book metrics updated
See how the Laboratory and your organization are performing against goals. The Laboratory Briefing Book is updated monthly and is available to all employees with a crypto card and yellow network access. Point your web browser here: int.lanl.gov/organization/performance/lanlbriefing/.

Enhanced capability to measure energy-dependent proton-induced isotope production cross sections

Radioisotopes are important for medical therapy, medical diagnostic tests, basic research, and other applications. The high-current LANSCE accelerator provides a unique facility to investigate the production of new radioisotopes over a range of proton beam energies and to produce usable quantities of isotopes at the Isotope Production Facility (IPF). Scientists demonstrated this capability by measuring the energy-dependent reaction probabilities (cross sections) to make gadolinium-153 (^{153}Gd) by proton irradiation of naturally-occurring terbium-159 (^{159}Tb). Gadolinium-153 is a low-energy gamma-ray source for medical imaging and diagnostic scanning and is also needed for basic research in nuclear astrophysics and stockpile stewardship. The experiment demonstrates the measurement of energy-dependent cross sections from 100 to 800 MeV to optimize the beam energy for future gadolinium-153 production and reestablishes the research techniques for development of other radioisotopes.



▲ The region of isotopes near terbium-159 (^{159}Tb). The blue arrows show some of the possible products from proton irradiation of ^{159}Tb.

The IPF produces radioactive isotopes by bombarding material with energetic protons. This process results in a net removal of protons and neutrons from the original nucleus, mostly leaving a distribution of neutron-deficient products (shown above right). Chemical separation is performed to extract the radioisotope of interest. With detailed knowledge of the energy-dependent production cross sections, the irradiation can be designed to enhance the production of the desired isotope and suppress production of undesirable or difficult-to-separate by-products. This present experiment is designed to measure those production cross sections over a wide energy range.

The sample activation was performed at Target 2 (the Blue Room) of the Weapons Neutron Research (WNR) Facility at LANSCE. Irradiations were performed with the LANSCE proton beam energies of 800 MeV and 197 MeV. The accelerator operations team had to reestablish the ability to deliver a lower-energy proton beam (197 MeV). Measurements were performed at six energies between 197 MeV and 100 MeV by further degrading the beam energy in the experiment target assembly. Immediately after irradiation, the targets were transported to a nearby counting room where the abundance of radioactive isotopes with half-lives as short as 15 minutes were measured. The samples were subsequently transferred to the TA-48 Count Room where the radioactive decay will be tracked to follow the isotope populations as they slowly decay back to stability.

This measurement combined the capabilities of the Los Alamos isotope production program, the C-NR Count Room, the AOT accelerator operations group, and the LANSCE-NS expertise in nuclear cross section measurements. Researchers include F. M. Nortier and H. Bach (C-IIAC), R. Gritzo (C-NR), D. M. Smith (SPO-CNP), A. Couture, L. J. Bitteker, J. L. Ullmann, and S. A. Wender (LANSCE-NS); M. Gulley (AOT-IC); and C. Pillai (AOT-ABS). This unique combination of capabilities provides the ability to measure the energy dependence for production of new isotopes and can extend the range of isotopes that could be used for medicine, basic science, and industrial applications both at Los Alamos and throughout the nation. This developmental work is part of the LANSCE user program.

AOT & LANSCE The Pulse

is published by the Experimental Physical Sciences Directorate.
To submit news items or for more information contact Karen Kippen, EPS Communications Team, 606-1822, or kkippen@lanl.gov.

LALP-09-016