ALS SPECTRUM

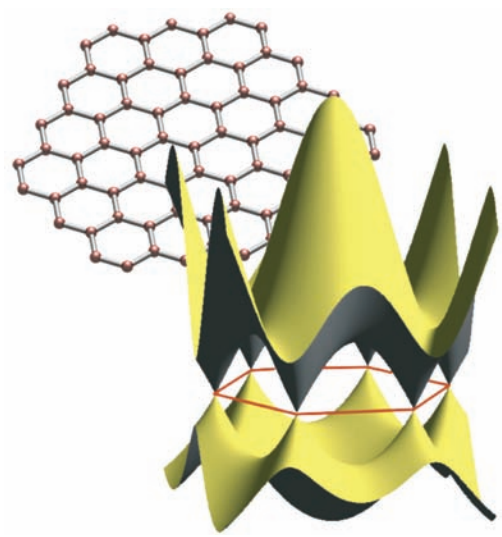
Advanced Light Source :: Facility Report :: 2007

PUBLISHED BY THE ADVANCED LIGHT SOURCE COMMUNICATIONS GROUP

What's Inside:

The ALS Graphene Scene

Like an "unrolled" carbon nanotube, graphene is a densely packed single layer of carbon atoms arranged in a hexagonal pattern like a honeycomb.



The atomic arrangement of graphene (background) is a honeycomb lattice of carbon atoms arranged in a two-dimensional plane. Its electronic band structure consists of two bands (yellow) that intersect only at a few points at the corners of a hexagonal Brillouin zone (red).

Although derived from graphite, the form of carbon in pencils, these two-dimensional graphene sheets may hold the promise of a new generation of faster, smaller, cheaper, and more durable computer chips than today's silicon-based devices. Consequently, interest in the electronic properties of this form of carbon has surged worldwide. At the ALS, two research groups, led by Alessandra Lanzara of UC Berkeley and Eli Rotenberg of the ALS, continue to be very active in this field. In 2007, the groups separately published two high-profile papers exploring graphene's fundamentally interesting and potentially valuable properties.

Before graphene can be engineered into transistors or other electronic devices,

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Top-Off Gets a Boost

The ALS took a big step towards the successful completion of the top-off upgrade late in 2007. The recommissioning of the injector complex was successfully completed and user operation was moved from injection at 1.5 GeV to full-energy injection at 1.9 GeV. Furthermore, there was further steady progress over the last year in studying all relevant radiation safety aspects, culminating in a successful outside review of the radiation safety tracking studies and controls.

The transition to top-off mode is motivated by the possibility of increasing brightness and improving thermal stability, keeping the ALS competitive with newer light sources for the next decade. In top-off mode, beam is injected into the storage ring approximately every minute to replenish lost electrons, as opposed to every eight hours, doubling the average beam current, allowing a reduction in vertical beam size, and eliminating the large swings in temperature that can adversely affect storage-ring and beamline components. The plan is before the end of 2008 to operate with top-off injection at 500 mA, which will result in brightness gains

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Science Roundup

Breaking H_2 Symmetry

Martín et al., *Science* **315**, 629 (2007)
http://www-als.lbl.gov/als/science/sci_archive/150symmetry-break.html

A single hydrogen (or deuterium) molecule consists of only two protons (deuterons) and two electrons and is perfectly symmetric. Linearly polarized photons are similarly symmetric. So one might think that the angular distribution of photoelectrons resulting from photoionization of the molecule by the photon accompanied by dissociation into a hydrogen atom and a hydrogen ion would itself be symmetric. However, an international team of researchers from Germany, Spain, and the U.S. has now shown that this need not be the case. When there are multiple quantum paths for the process, interference between waves in the coherent superposition of electron states (which exists when the molecular fragments are still close together) skews the distribution by breaking the molecular symmetry.

Coherently Condensing Polarons

Mannella et al., *Phys. Rev. B* **76**, 233102 (2007)
http://www-als.lbl.gov/als/science/sci_archive/169manganites.html

Novel quantum phenomena, such as high-temperature superconductivity (HTSC) and colossal magnetoresistance (CMR), arise in certain materials where the interactions between electrons are very strong, but the mechanism driving their appearance remains a major puzzle. Now, angle-resolved photoemission findings from an international team led by researchers from Stanford University and the ALS provide the first direct spectroscopic evidence that the transition from insulator to metal in CMR manganese oxides (manganites) results from coherent "polaron condensation." The new findings also suggest that coherence-driven transitions are a generic controlling factor for novel quantum phenomena in doped transition-metal oxides.

Pt_3 Revs Up Fuel Cells

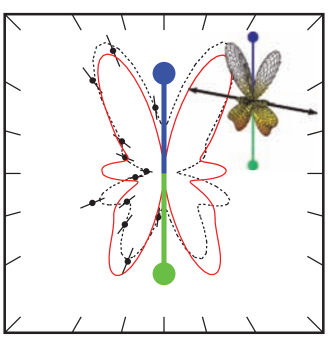
Stamenkovic et al., *Science* **315**, 493 (2007)
http://www-als.lbl.gov/als/science/sci_archive/139cathode.html

Two out of three of the kinetic barriers to the practical use of polymer electrolyte membrane (PEM) hydrogen fuel cells in automobiles have been breached: the impractically high amount of extra energy needed for the oxidation reduction reaction (ORR) on the catalyst and the loss of catalytic surface areas available for ORR. Using a combination of probes and calculations, a group of scientists has demonstrated that the $Pt_3Ni(111)$ alloy is ten times more active for ORR than the corresponding Pt(111) surface and ninety times more active than the current state-of-the-art Pt/C catalysts used in existing PEM fuel cells. This new variation of the platinum–nickel alloy is the most active oxygen-reducing catalyst ever reported.

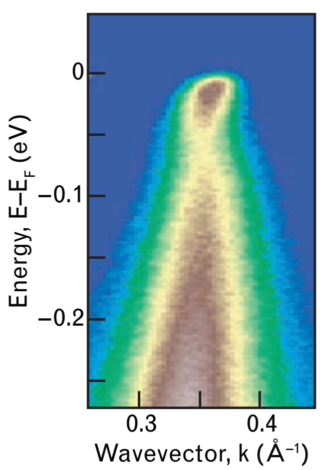
Detangling DNA

Dong and Berger, *Nature* **450**, 1201 (2007)
http://www-als.lbl.gov/als/science/sci_archive/160topoII.html

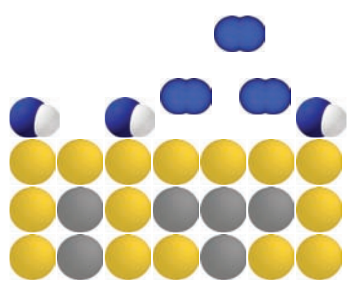
The veil has finally been lifted on an enzyme that is critical to the process of DNA transcription and replication and is a prime target of antibacterial and anticancer drugs. Researchers at Berkeley Lab and the University of California, Berkeley, have produced the first three-dimensional structural images of a DNA-bound type II topoisomerase (topo II) that is responsible for untangling coiled strands of the chromosome during cell division. Preventing topo II from disentangling a cell's DNA is fatal to the cell, which is why drugs that target topo II serve as agents against bac-



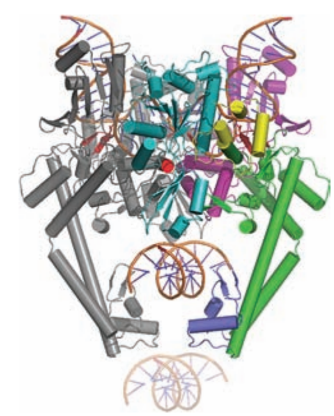
Sample plot of electron angular distribution for ionization of deuterium. The molecule axis is indicated by the blue and green circles. The curves represent theory (solid red line), experiment (circles), and fit of the experimental data (dotted line). The three-dimensional plots are also theoretical results.



ARPES data plots photoelectron intensity variation with energy (relative to the Fermi level) and momentum in the nodal direction. Color represents photoelectron intensity.



With Ni (gray) in the subsurface layers, the topmost Pt atoms (yellow) have a modified electronic structure, which alters different adsorption properties of Pt. Consequently, interaction between OH^- ions (blue/white) and the Pt skin is weakened, leaving more Pt sites active for adsorption of O_2 (blue).



High-resolution three-dimensional crystallography images of the binding and cleavage core of type II topoisomerase (topo II) as it interacts with DNA.

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Read more about these and other science highlights at http://www-als.lbl.gov/als/science/

terial infections and some forms of cancer. This first ever structural image of topo II should help in the development of future antibacterial and anticancer drugs that are even more effective and carry fewer potential side effects.

Diamondoids Display Potential

Yang et al., *Science* **316**, 1460 (2007)

http://www-als.lbl.gov/als/science/sci_archive/155diamondoids.html

Diamondoids are nanometer-sized molecules that feature diamond-crystal cage structures. Adamantane, the smallest member in the family, consists of one cage structure, diamantane two, triamantane three, tetramantane four, and so on. On all of these, the dangling bonds on the outer surfaces are terminated by hydrogen atoms. Because of their potential to possess novel properties of both diamond and nanomaterial, intensive efforts have been made to synthesize the larger diamondoid molecules, but to no avail. This situation was finally changed in 2003 when significant quantities of higher diamondoids were found in petroleum by researchers in Molecular Diamond Technologies. Now, scientists from Berkeley Lab, Stanford University, Lawrence Livermore National Laboratory, and Germany have used photoelectron spectroscopy at the ALS to reveal an intriguing feature: monochromatized electron emission from a self-assembled monolayer of diamondoids. This has caught the attention of people who are searching for materials for next-generation electron emitters.

Magnetic Carbon

Ohldag et al., *Phys. Rev. Lett.* **98**, 187204 (2007)

http://www-als.lbl.gov/als/science/sci_archive/147carbon.html

Although it has long been suspected that carbon belongs on the short list of materials that can be magnetic at room temperature, attempts to prove that pure carbon can be magnetized have remained unconvincing. However, using a proton beam and an advanced x-ray microscope at the Advanced Light Source, a multinational team of researchers from the SSRL, the University of Leipzig, and the ALS finally put to rest doubts about the existence of magnetic carbon.

Pushing the Wall

Meier et al., *Phys. Rev. Lett.* **98**, 187202 (2007)

http://www-als.lbl.gov/als/science/sci_archive/153domainwall.html

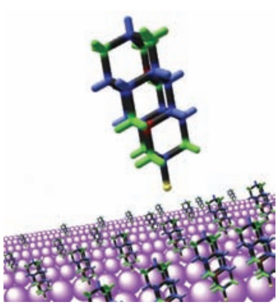
The quest to increase both computer data-storage density and the speed at which one can read and write the information remains unconsummated. One novel concept is based on the use of a local electric current to push magnetic domain walls along a thin nanowire. A German, Korean, Berkeley Lab team has used the x-ray microscope XM-1 at the ALS to demonstrate that magnetic domain walls in curved permalloy nanowires can be moved at high speed by injecting nanosecond pulses of spin-polarized currents into the wires, but the motion is largely stochastic. This result will have an impact on the current development of magnetic storage devices in which data is moved electronically rather than mechanically as in computer disk drives.

Nano Gold

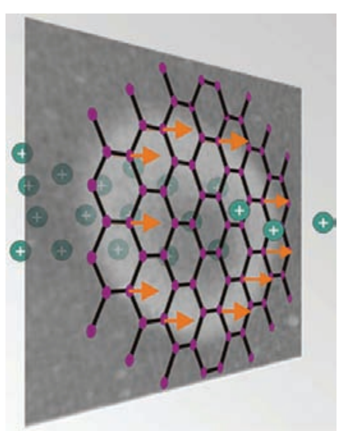
Jadzinsky et al., *Science* **318**, 430 (2007)

http://www-als.lbl.gov/als/science/sci_archive/164gold.html

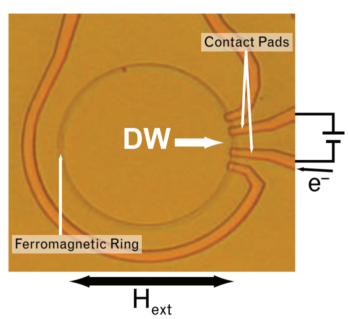
For the first time, a team of scientists led by Roger Kornberg has synthesized thiol-covered gold nanoparticles and, using ALS Beamlines 5.0.2 and 8.2.2 and SSRL Beamlines 11-1 and 11-3, conclusively ascertained their atomic structure (at 1.1 Å resolution). The gold–thiol nanoparticle consists



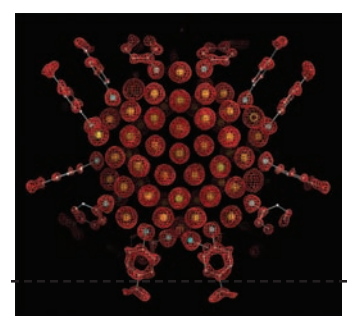
Tetramantane (inset) consists of four diamond cages fused together and terminated with hydrogen. After being functionalized by the replacement of one of the hydrogen atoms by a thiol group (yellow tip), the molecules will self-assemble into large-area monolayers on metal surfaces (purple).



A carbon film is hit by a high-energy proton beam, creating a ring-shaped magnetic pattern that can be imaged with a magnetic-force microscope. The x-ray microscope can then be used to "scan" the sample for magnetism associated with other elements.



A magnetic domain wall (DW) is created between contact pads in a permalloy ring 20 nm thick and 1000 nm wide by applying and releasing an external magnetic field (H_{ext}). A fast electronic pulser then launches short 1-ns current pulses with a current density < 10^{12} A/m^2 into the ferromagnetic wire.



X-ray crystal structure determination of the Au_{102}(p-MBA)$_{44}$ nanoparticle.

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Graphene

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an energy gap must be introduced into graphene's electronic band structure. While there are several promising efforts underway to induce such a gap, by adding impurities (doping) or fabricating geometrically confined structures with one or more dimensions measured in nanometers, the Lanzara group has demonstrated that growing graphene epitaxially on a silicon carbide substrate so that the atoms on each side of the interface maintain their registry could be a more reliable approach for generating a band gap [Zhou et al., *Nature Materials* **6**, 770 (2007)].

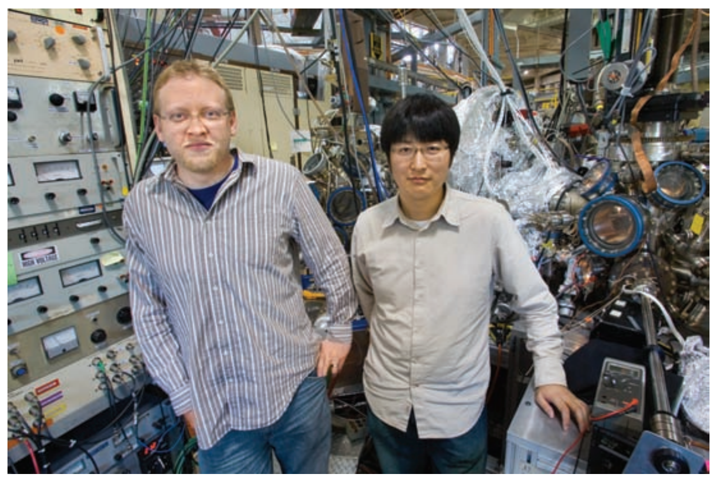
Working at ALS Beamlines 12.0.1 and 7.0.1, the group used angle-resolved photoemission spectroscopy (ARPES) to investigate the electronic structure of epitaxial graphene. The measurements yielded a map of the band structure (energy vs. momentum) with a sizable energy gap of 0.26 eV. However, the Fermi energy (maximum energy occupied by electrons) was well into the conduction band, above where it would be for a normal semiconductor.

In additional experiments with increasing numbers of graphene layers, the team found that the size of the energy gap decreased with thickness and all but disappeared at four layers. Next on the group's agenda are finding ways to control the width of the band gap, perhaps by using a different substrate material with a different graphene–substrate interaction strength, and to lower the Fermi energy from the conduction band into the band gap to allow transistor action.

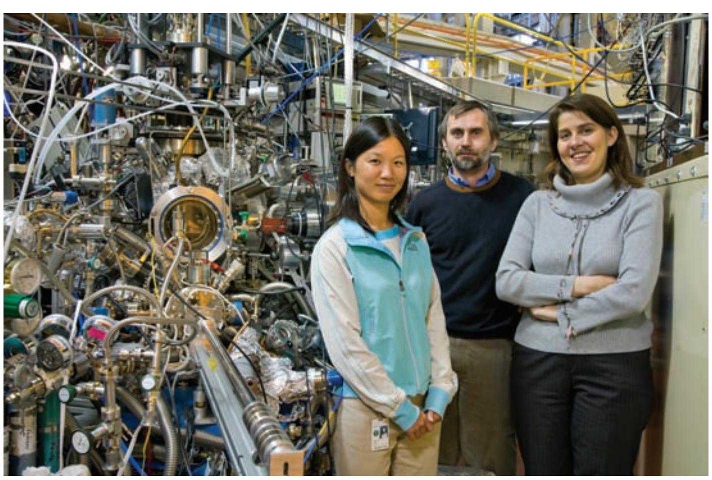
On a more fundamental level, graphene is an ideal playground for exploring "quasiparticle" interactions in a solid system. Electrons in solids hardly travel independently but rather interact with a sea of many quasiparticles—collective excitations that are responsible for exotic phenomena such as superconductivity. While other materials have shown signatures of electrons interacting with phonons (vibrational excitations) or magnons (magnetic excitations), the electrons in graphene show clear signatures of scattering from phonons, plasmons (collective oscillations of the electron "gas"), and electron–hole pairs over a much wider energy scale than usual. Because the interactions have similar energy scales, ARPES measurements are crucial to determining which scattering events are most important.

At ALS Beamline 7.0.1, the Rotenberg group succeeded in making the first ARPES measurement of electron lifetime in graphene over a wide energy scale [Bostwick et al., *Nature Physics* **3**, 36 (2007)]. In the absence of scattering, the ARPES energy band of a single layer of graphene would be smooth. However, the data clearly showed kinks in the band's shape and variations in its sharpness that can only be explained by electron scattering from collective modes, including a strong electron–plasmon interaction.

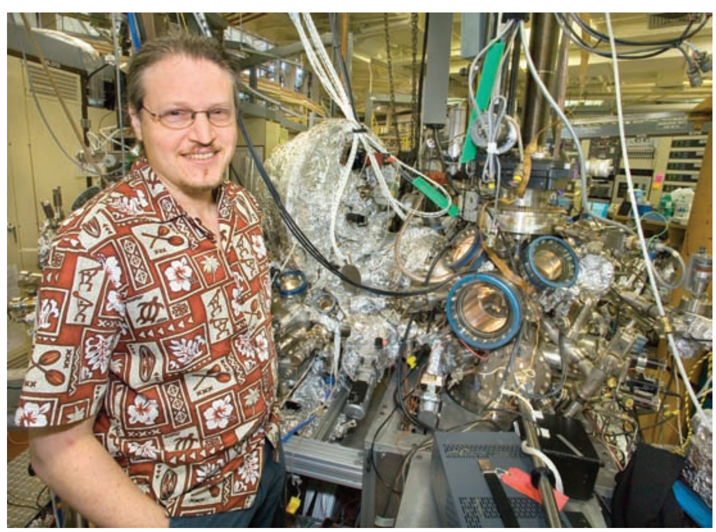
Understanding these interactions is not just an academic exercise; it is important because although various forms of carbon are known to be superconducting, the mechanisms are still unclear. Furthermore, since plasmons can also couple to light, the demonstration of strong electron–plasmon coupling shows that novel carbon-based devices with both electronic and photonic functions might be possible. ■



Aaron Bostwick and Taisuke Ohta at ALS Beamline 7.0.1.



Shuyun Zhou, Alexei Fedorov, and Alessandra Lanzara at ALS Beamline 12.0.1.



Eli Rotenberg at ALS Beamline 7.0.1.

Experimental Systems Group: Focus on Optics

by Howard Padmore

Some of the most exciting frontiers in materials science occur at the nanoscale, where self-organization in energy, space, and time often lead to complex material properties. Soft x-ray light has the right wavelength to access the relevant spatial scale and core levels of the most important elements. Combined with sophisticated spectroscopic and scattering probes, soft x rays give us a uniquely powerful tool in modern materials science. The goal of our optics research is to transport, focus, and condition the very high brightness x-ray sources we have and to utilize them in ways that enable new science at the ALS.

Brightness preservation at the levels needed—close to the diffraction limit—is extremely difficult. Very small perturbations from a theoretically perfect optical surface can lead to catastrophic reductions in performance. While this is important for our current beamlines, where factors of 10–100 may be lost by use of earlier-generation and nonoptimum optics, it's especially important for new beamlines such as the ultrahigh-resolution MERLIN beamline and the proposed MAESTRO and COSMIC beamlines. In the case of MERLIN, surface slope distortions at the level of 0.2 microradians will have noticeable effect, and new beamlines drive this value down even further, to a range challenging to measure and manufacture. Because this problem is not unique to the ALS, we recently held a workshop with leading experts to discuss the issues. The workshop helped confirm our multi-pronged strategy: pushing ex situ optical lab-based measurements as far as possible while developing in situ measurement tools within beamlines.

At the ALS Optical Metrology Laboratory (OML), led by Valeriy Yashchuk, we collaborate internationally on next-generation metrology with target sensitivity and accuracy well below the 100-nanoradian level. Already, the ALS Long-Trace Profiler II, recently upgraded, and the new slope-measuring instrument, the Developmental Long-Trace Profiler, have performances of 0.25 microradian (rms), comparable to the world's best instruments of this type. A universal test mirror calibration method under development is now our strategic direction for further improvement toward 50-nanoradian accuracy. We have also developed an original method to calibrate the modulation transfer function of microscopes. The method is based on use of binary pseudo-random gratings and arrays as surface standards, allowing reliable power spectral density data to be obtained for 3D scattering simulations of the beamline performance of x-ray optics that are also under development at the OML.

An LDRD project, led by Dmitri Voronov, explores a highly promising technology for ultrahigh-resolution resonant inelastic soft x-ray scattering (RIXS): fabrication of a superhigh-density diffraction grating for soft x-ray energies. An x-ray reflecting multilayer is deposited on an echellette substrate with a relatively low groove density; the blazed multilayer grating is then polished to reveal an oblique cut of the multilayer. The resulting sliced multilayer structure has a potential line density of up to 100,000 lines per mm. We (in close collaboration with a Ukrainian research team) have succeeded in fabricating and testing a Sc/Si sliced grating with 270-nm pitch size (groove density of ~3700 grooves per mm and total number of grooves of ~40,000), the first prototype of a superdense soft x-ray grating. Measurements performed at Beamline 6.3.2 have demonstrated a high efficiency and dispersive ability in the 41- to 49-nm wavelength range. We are working to extend the technology to fabrication of an ultrahigh-density grating for soft x rays,

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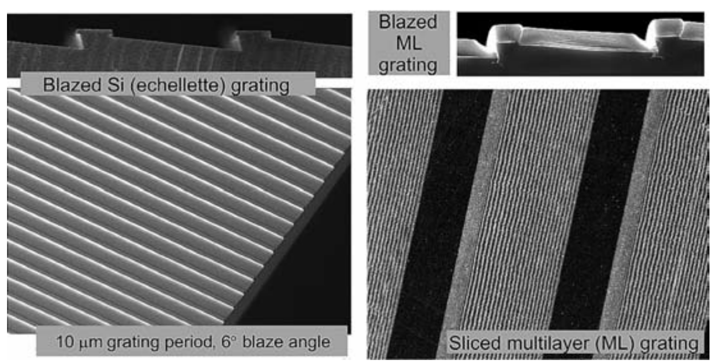
The Advanced X-Ray Optics Metrology for Nanofocusing and Coherence Preservation workshop at the 2007 ALS Users' Meeting, organized by Kenneth Goldberg and Valeriy Yashchuk. Featuring 11 invited talks, the workshop brought together industry representatives and researchers from Japan, Europe, and the US to discuss the state of the art and outline the optics requirements of new light sources.



Fabrication of Sc/Si sliced grating with 270-nm pitch size, first prototype of a superdense soft x-ray grating suitable for the EUV photon energy range.

ESG

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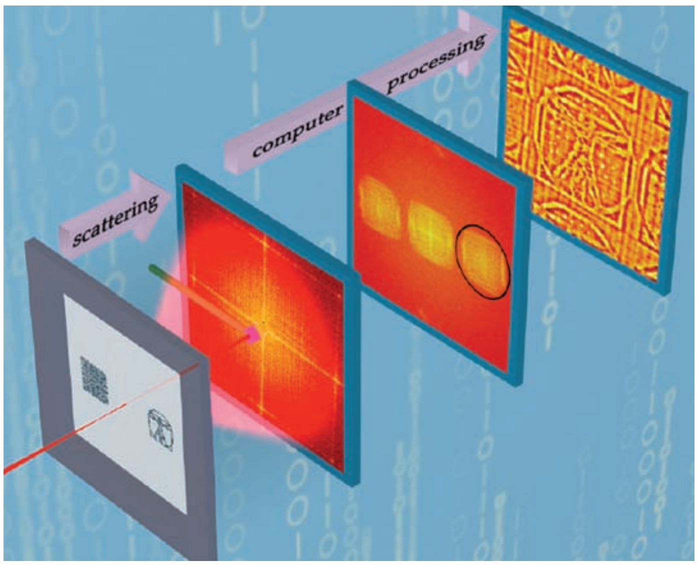

Illustration of FTXH using a URA as a reference object.

where we anticipate spectrograph systems of high efficiency and throughput up to 1 keV, for resolving powers above 105.

Zone-plate lenses are the core component of x-ray imaging systems but have a resolution limited by nanolithography and an intrinsic limit set by sample thickness and the depth of field of the lens. Within the last ten years, led by the pioneering work of Janos Kirz and colleagues, a new form of imaging based on scattering a coherent x-ray beam has become popular because its resolution is, in principle, limited only by the wavelength of the light. Phase information is lost, but can be reconstructed numerically, using prior knowledge of the area containing the sample. This reconstruction can now be done relatively routinely, but the use of constraint information is experimentally limiting and is computationally challenging for reasonably sized images.

Fourier-transform x-ray holography (FTXH) avoids these limitations by "phasing" the scattered beam directly with a reference beam, usually provided by a hole in the object. The disadvantage is that the interference provided by the reference beam is weak. An international, multilab team led by Stefano Marchesini has developed a technique that produces x-ray holograms three orders of magnitude more intense than previously possible. The technique is a variant of normal FTXH but uses a uniformly redundant array (URA) as the reference object, greatly increasing brightness at the maximum resolution. The Marchesini team has used the technique at Beamline 9.0.1 to record a hologram of a nanofabricated test object at 2.3 nm and images of bacterial cells with a resolution of 45 nm in 15 fs using the FLASH free-electron laser. This technique allows direct inversion of the scattering patterns to images without any iterations, overcomes the tradeoff between signal-to-noise ratio and resolution, and provides phase and amplitude contrast information simultaneously. Existing lithographic methods could push the resolution to ~15 nm. Diffractive imaging reconstruction methods could push the resolution beyond the nanofabrication limit to a few nanometers. ■

Scientific Support Group: State-of-the-Art Instrumentation for World-Class Science

by Eli Rotenberg

MAESTRO, the Microscopic and Electronics Structure Observatory, is the new facility planned to replace the existing photoemission branchlines at Beamline 7.0.1 and features a new dedicated "half" insertion device capable of full polarization control above 60 eV and a new entrance-slitless monochromator capable of 3-meV resolution from 20 to 100 eV and extended operation up to 1000 eV. The new beamline's design effort, together with plans for decommissioning the existing beamline, were begun this year to support an application to DOE to fund a new facility dedicated to nanoARPES: angle-resolved photoemission spectroscopy with 50-nm probe size.

A new infrared beamline, dedicated to environmental and biological studies with near-infrared light, is now being developed. The new beamline, to be situated at Sector 5, will accept double the light of the existing IR beamline and is expected to have superior stability.

The MERLIN beamline, planned to achieve the ultimate resolution for ARPES at the ALS, has been designed, and assembly on the ALS floor has begun. The beamline features the

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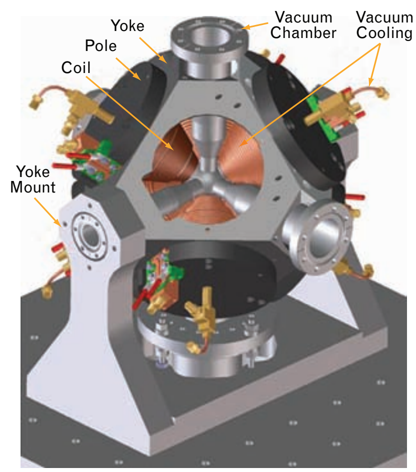


Eight-pole electromagnet installed at ALS Beamline 4.0.2 provides magnetic fields of up to 0.8 T in arbitrary directions, crucial for the study of the XMLD angular dependence.

Macromolecular Crystallography Improves Brightness, Automation

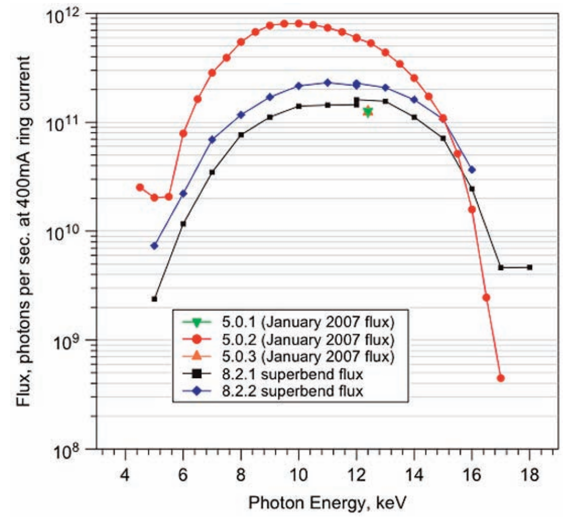
by Paul Adams

Beamlines 5.0.1, 5.0.2, and 5.0.3. An upgrade of the x-ray optical elements in all Sector 5.0 beamlines was completed in early 2007. The performance of Beamline 5.0.2 was improved by a factor of 3 to 4 and now surpasses the performance of the macromolecular superbend beamlines at the ALS, generating 8 × 10^{11} photons per second at 10 keV and 400-mA ring current. This has had a tangible impact on the ability of users to perform experiments. User groups working on membrane protein systems have been able to solve structures that otherwise were not tractable. Other users working with crystals of a large macromolecular complex were able to collect diffraction images with 15-second exposures instead of the 120 seconds required on other beamlines at the ALS.

Replacement of the M101 and M301 mirrors significantly improved the performance of the side-station beamlines (5.0.1 and 5.0.3). A 5- to 10-fold improvement in available flux was achieved, now generating 1.5 × 10^{11} photons per second at 12.4 keV. In February 2007, the 5.0.1 monochromator was replaced with crystals that improve beam focusing and also select x rays slightly above the selenium peak in order to enable single-wavelength anomalous diffraction experiments with selenium-derivatized proteins.

Beamlines 8.2.1 and 8.2.2. In early 2007, the Berkeley Center for Structural Biology (BCSB) received a $4.8 million award from the Howard Hughes Medical Institute (HHMI) to upgrade Beamlines 8.2.1 and 8.2.2 (which are operated for HHMI). The upgrades include the installation of robot equipment for sample mounting, high-precision instrumentation for crystal handling, a larger CCD detector for data collection, and improved x-ray optics to generate a 30-micron beam once the top-off upgrade is complete.

In June 2007, BCSB staff completed the installation of a Rigaku ACTOR robotic sample automounter on Beamline 8.2.2. This robot is able to automatically transfer user samples from a liquid nitrogen dewar into the experimental data collection area without any manual intervention. This permits users to operate the beamline without the need to open the experimental hutch. In the near future it will be possible for users to run their experiment remotely after sending the samples to the BCSB staff for loading into the dewar. ■



Performance of the Sector 5.0 beamlines after the 2007 x-ray optics upgrade.

Rigaku ACTOR crystal automounter robot installed on Beamline 8.2.2.

Imaging, Metrology, and EUV Lithography at CXRO

by Erik Anderson

The Center for X-Ray Optics (CXRO) has made significant progress both scientifically and technologically in its imaging, metrology, and industry-funded EUV lithography research programs. The leading research performed at the Center's nanofabrication and coating facilities enables it to provide high-resolution diffractive optics, coatings, and other nanostructures, for its own activities and for the support of other ALS activities.

The full-field soft x-ray microscope at Beamline 6.1.2 is a unique tool for nanoscience, combining high spatial resolution (15 nm) and temporal resolution (70 ps) with a rich set of contrast mechanisms: elemental, chemical, topological, and magnetic. Magnetism research using this microscope is important to the development of high-density and high-speed magnetic storage media. Time-resolved x-ray images of the vortex core motion revealed for the first time the degree of spin polarization of conduction electrons, and magnetic domain structure analysis of nanogranular CoCrPt thin alloy films confirmed a stochastic behavior in the domain nucleation process.

Specialized zone plates are extending imaging capabilities at the microscope. Depth of field extension with the cubic zone plate and wavefront coding technique, performed at Beamline 6.1.2, provides a method for

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CXRO

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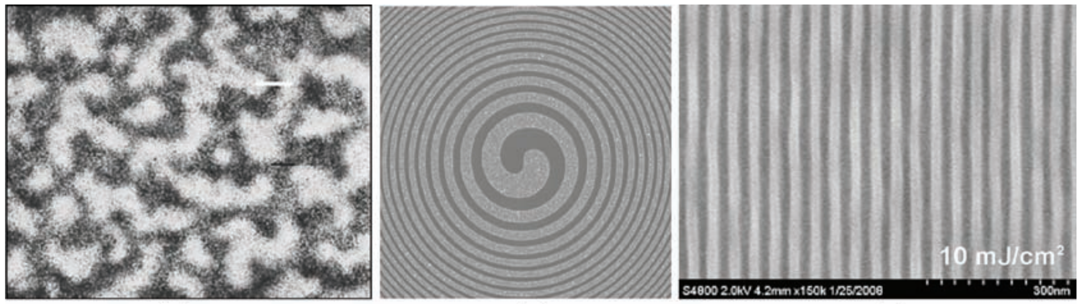
overcoming the depth-of-field–limited resolution for soft x-ray tomography. Spiral and Zernike zone-plate imaging, demonstrated at the coherent optics Beamline 12.0.2.1, enhances contrast through phase sensitivity.

The Micro Exposure Tool (MET) on Beamline 12.0.1.3 provides the world's highest-resolution EUV printing for resist and mask research. Resist innovations are pushing the envelope of resolution (22-nm half-pitch lines), sensitivity, and line-edge roughness. Collaborative efforts at the MET and the metrology Beamline 6.3.2 unraveled a systematic underestimation of the sensitivity of resists. Fortunately, this reduced the required source power, which invoked a collective sigh of relief from the industry. The EUV zone-plate microscope on Beamline 11.3.2 emulates the optical parameters of EUV lithography tools and is dedicated to photolithography mask research. As the highest-performing tool of its kind, it serves a broad group of semiconductor company researchers by finding and classifying mask defects as small as 20 nm wide and 1 nm tall and by validating the effectiveness of repair and cleaning strategies. ■



(a) (b) (c)

(a) Magnetic domains in a CoCrPt nanogranular alloy thin film imaged at the Co L_3 edge with 15-nm spatial resolution. Scale bar is 120 nm. (b) SEM image of the spiral zone plate. (c) 22-nm spatial resolution patterning with a high-sensitivity EUV resist.

Molecular Environmental Science Under Realistic Conditions

by Hendrik Bluhm, Mary K. Gilles, Tolek Tyliszczak, and David K. Shuh

Scientific investigations at Beamline 11.0.2 are split between two experimental capabilities: a scanning transmission x-ray microscope (STXM) and an ambient-pressure photoelectron spectrometer (APPES). Spectroscopy and microscopy in the soft x-ray region are excellent tools for probing environmentally relevant samples under realistic conditions, i.e., with water or water vapor present at ambient temperature.

While other microscopies provide exquisite images or elemental content, none offers the chemical specificity of STXM with comparable spatial resolution. The spatially resolved chemical information, with resolutions of 25–35 nm, is unique. Investigations include studies of magnetic materials, actinide, atmospheric and cometary particulates, synthesized or naturally occurring nanoparticles, biofilms, mineral–bacteria suspensions, and polymers. Experiments on magnetic materials probe changes in the magnetization vector during exposure to magnetic or spin polarized electric fields. This relaxation, reversal, or precession of the magnetization vector is examined in time-resolved experiments (70 ps) and addresses scientific issues related to information storage in magnetic materials. The discovery at the STXM of low-field switching of magnetic vortex cores may lead to a new type of magnetic memory. Linear dichroism microscopy studies include naturally occurring materials and organic nanomaterials. The magnetic and linear dichroism experiments are uniquely feasible due to the combination of the insertion device (EPU) and

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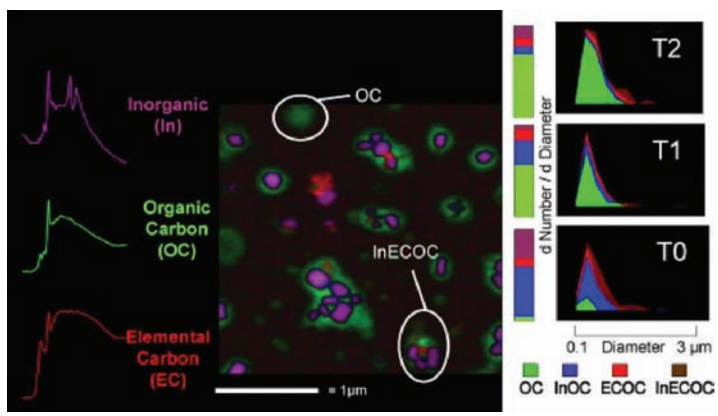

Figure 1. Left: Carbon K-edge NEXAFS spectral components. Center: Size and composition of collected particles determined by STXM: organic particles (OC, green), inorganic particles surrounded by annular organic shell (InOC, blue), mixed organic inorganic elemental carbon particles (ECOC, red) and mixed inorganic, elemental and organic carbon (InECOC). Right: Number fraction and number size distribution indicate a systematic increase in number of particles with organic composition as a function of distance downwind from central Mexico City (T0) to T1 to T2. (R.C. Moffet et al., in preparation)

SSG

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first quasiperiodic undulator at the ALS—designed to minimize the contaminating higher harmonics that plague the existing ARPES experiments—and is expected to achieve sub-1-meV resolution for the first time at a beamline for condensed matter studies at the ALS. Operation is expected in early FY09.

At the Electronic Structure Factory endstation, we have commissioned a new liquid-helium-cooled goniometer, capable of temperatures from 11 to 2000 K and compatible with the previous sample holder design.

HARP, the Beamline 12 photoemission endstation, will be completely replaced with a new chamber featuring an upgraded analyzer: the SES-R3000. This analyzer features about 1.8 times the throughput for a given resolution, and almost three times the maximum angular acceptance, of the previous analyzer, and will achieve around five times improved throughput over the old analyzer. Together with a recent upgrade to the x-ray optics, the new capabilities will enhance the effectiveness and alleviate crowding at one of the most oversubscribed endstations at the ALS.

The SSG group strives to create state-of-the-art instrumentation to enable new science. The following selected highlights reflect not only world-class science but illustrate the unique capabilities created in the ALS by the SSG.

The x-ray magnetic linear dichroism (XMLD) spectrum of transition-metal ions in magnetic materials is a very complicated function of the relative angles between photon polarization and crystalline and magnetic polarization directions, and from this function we can derive rich information about the coupling of spins in magnetic systems. SSG's Elke Arenholz, in collaboration with Y. Suzuki's group (UC Berkeley) and G. van der Laan (Daresbury), have shown that the full double angular dependence of the Ni XLMD in a NiO/Co interface can be modeled by two functions that depend only the atomic multiplets involved in the Ni 2p level probed, together with the detailed symmetry of the materials [Arenholz et al., *Phys. Rev. Lett.* **98,** 197201 (2007)]. In fact, these results can be applied generally to Ni in any similar cubic environment, even in situations previously approximated by only one angular function. Consequently, previous results will have to be reexamined to derive a true understanding of the magnetic states.

A study led by J. Banfield (UC Berkeley) used infrared spectroscopy as well as other techniques to analyze dense aggregates of bacterially formed

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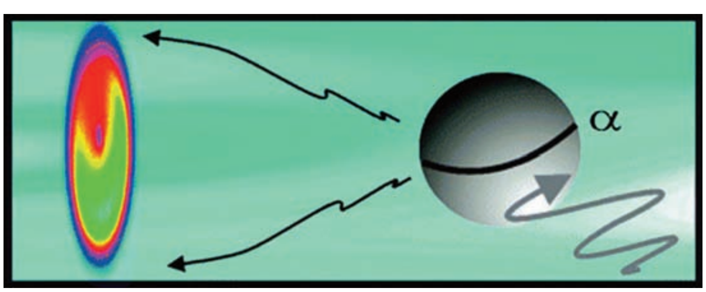
Chemical Dynamics from Table Salt to Titan

by Musa Ahmed

The Chemical Dynamics Beamline 9.0.2 provides state-of-the-art experimental resources to undertake studies of fundamental chemical processes using VUV radiation. Projects undertaken at the beamline in 2007 included chemical reactions on model particle surfaces reflective of atmospheric aerosols and diesel exhaust, molecular growth mechanisms relevant to combustion chemistry and astrochemistry, details of hydrogen bonding and structure of small water and alcohol clusters, gas phase microhydration studies of DNA bases, flame chemistry of biofuel surrogates, elementary reaction kinetics of hydrocarbon radical reactions with relevance to combustion and the atmosphere of Titan, and the photoionization of dopants in ultracold helium droplets. Of the many interesting results obtained, four are of particular interest: Angle-resolved threshold photoelectron spectra recorded for size-selected beams of sodium chloride nanoparticles (radius = 25–250 nm) exhibit a size-dependent asymmetry that is inversely proportional to particle radius. The internal electric field amplitude and the photoelectron escape probability inside the particles were modeled and accounts for the observed asymmetry (Wilson et al., *Nano Lett*. **7,** 2014 (2007)]. A novel multiplexed time-resolved photoionization mass spectrometer technique has been employed to investigate the ionization behavior of two 1-alkenyl peroxy radicals, which play key roles in low-temperature oxidation and photo-oxidation of hydrocarbons (Meloni et al., *JACS* **129,** 14019 (2007)]. An experimental study that provides information about the photoionization energies of small carbon clusters was undertaken. Coupled with elaborate electronic structure calculations, insight was provided into the structure and composition of these species in a laser-ablated supersonic molecular beam (Belau et al., *JACS* **129,** 10229 (2007)]. Photodissociation and photoionization experiments suggest that, in Titan's upper atmosphere, VUV radiation may play an important role in the formation of complex organic molecules through photoionization of N_2 (Imanaka and Smith, *GRL* **34,** L02204 (2007)]. ■



Photoelectron imaging of size-selected nanoparticles exhibit a size-dependent asymmetry that is inversely proportional to particle radius.

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SSG

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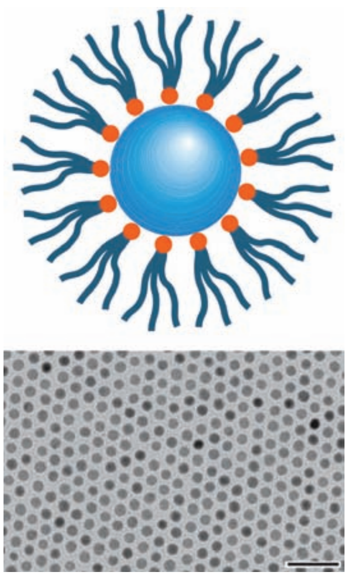

Top: Illustration of a colloidal nanocrystal with a cobalt center surrounded by a ligand layer made up of molecules of an organic surfactant (oleic acid). Bottom: Transmission electron microscope (TEM) image of cobalt nanocrystals. Scale bar = 50 nm.

metal sulfide nanoparticles [Moreau et al., *Science* **316**, 1600 (2007)]. They found that proteins trapped within the nanoparticles may have played a key role in the aggregation process. Sulfate-reducing bacteria can lower the concentrations of metals in anoxic waters by sequestering metals into nanoparticles. The worry is that these very small particles could be highly mobile, redissolving quickly if conditions change. The results presented in the paper, however, suggest that microbially derived extracellular proteins can limit dispersal of nanoparticulate metal-bearing phases, such as the mineral products of bioremediation that may otherwise be transported away from their source by subsurface fluid flow. This work used the high spatial resolution of Beamline 1.4.3 to spectrally identify the presence of proteins within these nanoparticles.

Colloidal nanocrystals (crystalline nanoclusters suspended in liquid) were analyzed using a combination of x-ray absorption and emission spectroscopies at Beamline 7.0.1 [Liu, et al., *Nano Letters* **7**, 1919 (2007)]. Because these techniques normally are conducted on solids in ultrahigh vacuum, application to nanocrystals in liquid required development of a new water cell with sufficiently thin windows to allow the x rays to be absorbed and emitted to the detector. Special care was taken to protect the beamline and the synchrotron from accidental venting. The principle finding was the ability to discriminate the chemical state of Co atoms in the interior of clusters from those on their surface. The distinguishing feature of these atoms is that the surface atoms have a different chemical state due to charge transfer to ligand molecules that were used to functionalize the nanocrystal surfaces. The technique should find wide application to many future studies, since such functionalization can be used to tailor the properties of new materials for a variety of needs, including magnetism, electronics, and energy collection. ■

Molecular Environmental Science

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accessible energy range (130–2000 eV) at this beamline. Due to the minute amounts of material needed for STXM experiments (10 fg for a particle), a variety of radioactive materials can be safely studied.

Particulate studies examine differences in the chemical bonding of a particular element. Atmospheric particles collected at ground sites, successively distant from Mexico City, show an increase in the number of particles containing organic carbon (Figure 1). This increased oxidation results from atmospheric processing and influences the particles' water solubility and atmospheric lifetime. The APPES endstation is excellent for probing liquid/vapor and solid/vapor interfaces at Torr pressures. This is ideal for examining the chemistry of interfaces, the role of water, and for probing changes in the interface arising due to chemical reactions. Under identical relative humidity (5%), water wets Cu(110), but not Cu(111) (Figure 2). However, if the Cu(111) surface is partially covered by oxygen, water does wet Cu(111). The wetting is controlled by the presence of OH groups on the surface, acting as anchors for water adsorption. This behavior results from the difference in the dissociation barrier for the two surfaces: Cu(110) < Cu(111). When Cu(111) is partially covered by atomic oxygen, its dissociation barrier is decreased and hydroxylation and water adsorption are observed.

Experimental capabilities at Beamline 11.0.2 are in a constant state of improvement. The endstation area was substantially rearranged to provide optimal space for experiments. Major STXM developments included improved timing schemes for time-resolved experiments, experiments employing fluorescence or electron yield detection as well as progress in tomography and the development of a mini-STXM. Improvements related to the APPES endstation include the development of a separate droplet train apparatus, new material sources, and the addition of new turbopumps. ■

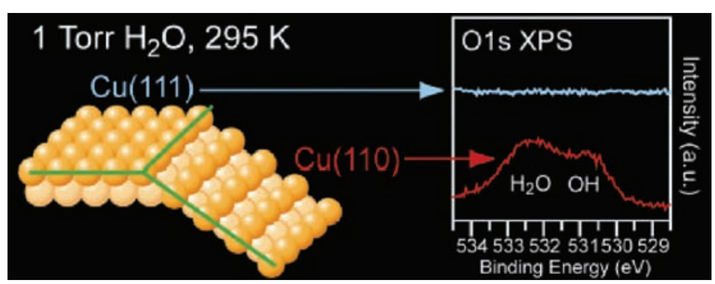


Figure 2. Differences in oxygen bonding between Cu(111) and Cu(110) surfaces (S. Yamamoto et al., *J. Phys. Chem. C* **111,** 7848 (2007)].

PEOPLE AND EVENTS

by Roger Falcone

High Praise for the ALS in BES Triennial Review Report

Pedro Montano, DOE Basic Energy Sciences (BES) Scientific User Facilities Division Director, has sent me a summary of the report from the triennial DOE BES review of the ALS that was held last March, and I am extremely proud of the results. To quote the opening paragraph, "The ALS scientific output continues to excel with an exceptional percentage of publications in the 'high impact' category. This reflects positively on its world-class beamline capabilities and outstanding scientific staff." This is high praise indeed, only made possible by the contributions of all members of the ALS staff and users working together.

I would like to share with you some of the observations. Reviewers noted that the ALS has made significant improvements for the user community, including a web-based proposal system described as being transparent and fair. They also commended ALS Safety Program Manager Jim Floyd's collaborative style of working with users to implement pragmatic safety measures.

There was praise for the progress made toward top-off operation, as well as for several instrument achievements, including the new EPU Beamline 11.0.1 and the steps taken toward the PEEM3 microscope; superbend Beamline 12.3.2, which extended the energy range for white-beam x-ray Laue microdiffraction and provided enhanced strain sensitivity; the progress on Beamline 4.0.3 (MERLIN), including an aperiodic undulator for harmonic rejection; and the move of the ultrafast program to Sector 6.0, which resulted in much improved intensity on the high- and low-energy branch lines.

Finally, reviewers were impressed by the strong interactions between the ALS and both the Scientific Advisory Committee (SAC) and the Users' Executive Committee (UEC). They also commented favorably on the ALS Strategic Plan and pointed out that the ALS has taken the lead in establishing a graduate student and postdoc support program, vital to developing a pipeline for future beamline and accelerator scientists.

Other than our well-known staffing shortages, no major shortcomings were identified in the review. Dr. Montano's letter accompanying the report summary concludes by "commending the ALS on continuing its outstanding scientific output and instrument development," a view I heartily share.

This was a gratifying review, a testament to our collective efforts at the ALS. I thank everyone for a job well done. ■

by Hendrik Ohldag, 2008 UEC Chair

Users' Executive Committee Update

The ALS Users' Executive Committee (UEC) represents more than 2000 scientists worldwide who are using the ALS for their research and it has been my pleasure to serve as the UEC chair this past year. In order to assist ALS users, that is you, we interact very closely with ALS management, represent you during external reviews, and voice your concerns to various groups on Capitol Hill. In all of these capacities, the UEC addresses a large variety of topics and issues, ranging from facility access, safety regulations, user housing, ALS upgrades to congressional support for DOE facilities.

This has been a truly exciting year for the ALS. In March the ALS hosted the triennial facility review by the DOE. The review committee was very impressed with the quality of the research conducted at ALS and by the level of support that scientists, engineers, technical and administrative staff provide to users in order to facilitate their research programs. Congratulations and a big thanks to everybody for a job well done! It will require the continued efforts of all of us to ensure that the ALS will be able to provide top-level support to its users leading to outstanding science in the future in the light of dire current and future budget scenarios.

This has also been a year of visible changes around the ALS building. Already last years Users' Meeting featured the groundbreaking ceremonies for the User Guest House and the User Support Building, and the construction work on the guest house is making good progress. Unfortunately, the start of construction for the USB had to be delayed due to the budget shortfall, but work on the foundation will begin during the fall shutdown. In the past, one of our major concerns was the shortage of lab and office space and the lack of on-site accommodations during beam time. Thanks to the efforts of the ALS User Services Office, ALS management, and previous UECs as well as your continued support, we will soon be able to put these issues behind us.

Finally, I want to thank you for your support and help and would like to ask you to work closely with next year's UEC chair Kenneth Goldberg to ensure that the ALS continues to be an outstanding facility for synchrotron radiation science worldwide. I would also like to thank Wayne Stolte and Phil Heimann, the program chairs of the 2008 Users' Meeting. Together with the help of Sue Bailey and her team at the ALS User Services Office, they put together an outstanding program for the 2008 Users' Meeting with exciting and informative plenary sessions as well as a list of excellent workshops.

I wish all of you an enjoyable, exciting, and productive future at ALS. ■

PEOPLE AND EVENTS

In Memoriam

Daniel Chemla, former director of the ALS and Materials Sciences Divisions and major intellectual driver in the establishment of the Molecular Foundry, died at home on Thursday, March 20, 2008, at the age of 67. He had been battling a series of health problems since suffering a stroke four years ago. Despite those difficulties, he continued to actively lead his research group until very recently.

As ALS Division Director, Daniel's ambitious 20-year roadmap for the ALS laid the groundwork for new beamlines, accelerator upgrades, and expanded scientific programs in materials sciences, ultrafast science, microscopy, and protein crystallography. During his seven-year tenure at the ALS, the number of users grew from 659 to over 2000. He stepped down as director in 2005. Acknowledging Daniel's extraordinary contributions to the ALS, current ALS Director Roger Falcone observed, "He was a visionary and tireless leader. He set the ALS on a path of frontier science that we continue today, as was pointed out explicitly in the recent BES review. As a teacher and researcher, Daniel was inspirational for his students and colleagues. Along with his extensive network of friends, I will greatly mourn his passing, while appreciating his extraordinary life."

Daniel is survived by his wife Berit, two children, Yann, an assistant professor of physics at the University of Illinois, Urbana-Champaign, and Britt Chemla Jones, an art history lecturer in Houston, Texas. To read the full obituary on the ALS Web site, go to *http://www-als. lbl.gov/als/news/chemla.html.*

Gary Krebs, the popular leader of the ALS User Services Group, passed away suddenly on the evening of May 22, 2007, in the midst of travel to Long Island for his annual visit to attend the National Synchrotron Light Source (NSLS) user meeting at Brookhaven National Laboratory.

Since arriving at the ALS in 1993, Gary had major impacts in several important areas: bringing the nascent accelerator survey and alignment system into adulthood as a functioning, productive tool, leading the first User Services Group as it evolved to serve an ever-larger user community, and as the ALS representative to the Lab group that has been formulating plans for the on-site Berkeley Lab Guest House. For the last two years, he also served as Deputy Scientific Director to the late Neville Smith and then as Deputy Science Advisor to Janos Kirz. "Over the past three years I had the privilege to work closely with Gary, and I learned a lot from him," said Janos. "He was devoted to the ALS, and in particular to the users of the ALS. He worked hard to make the Guest House a reality, and his efforts are now bearing fruit. His passing is a great loss to all of us, and to me personally."

In addition to his wife Kathy, he leaves behind one son, Matthew, and in Vancouver, British Columbia, a brother, Dennis, and his parents. To read the full obituary on the ALS Web site, go to *http://www-als.lbl.gov/als/news/krebs.html.* ■

NIH Director Visits the ALS

On March 31, 2007, the Director of the National Institutes for Health (NIH), Elias Zerhouni, visited Berkeley Lab and the UC Berkeley campus. As part of his visit, he toured the ALS with Graham Fleming (former Berkeley Lab Deputy Director), Roger Falcone (ALS Director), Paul Adams (Head of the Berkeley Center for Structural Biology), and Carolyn Larabell (Director of the National Center for X-Ray Tomography). The BCSB has five beamlines optimized for macromolecular protein crystallography. The NCXT carries out research in biological and biomedical imaging and cell biology.

Director Zerhouni's tour of the BCSB beamlines included a look at Beamline 5.0.3's new 315r CCD detector and the Berkeley Automounter System (developed by Thomas Earnest and colleagues at Berkeley Lab). Adams described the upcoming upgrades to Beamlines 8.2.1 and 8.2.2, and Zerhouni responded enthusiastically about the prospects for increased automation of crystallographic experiments.

As part of his tour, Zerhouni also inspected the NCXT's newly constructed soft x-ray microscope. This is the first such microscope to be designed and built specifically for biological and biomedical imaging. (The NCXT is an NIH National Center for Research Resources that also receives joint funding from the Department of Energy, Office of Biological and Environmental Research.)

Zerhouni, a radiographer with considerable experience in full-body CAT scanning, was enormously enthusiastic about the potential of the new technique and told the assembled group, "I love this stuff!" Nearing the end of the NCXT tour, Mark Le Gros, the Berkeley Lab scientist responsible for the design and construction of the new microscope, showed Zerhouni his latest innovation, an instrument for a technique known as correlated microscopy. At the end of his inspection of the NCXT beamline, Director Zerhouni, with overall responsibility for the NIH's $29 billion budget, beamed and said, "This was money well spent!" ■

NIH Director Elias Zerhouni, NCXT Director Carolyn Larabell, and former Berkeley Lab Deputy Director Graham Fleming at the NCXT.

PEOPLE AND EVENTS

2008 Beam Instrumentation Workshop

The 13th biennial meeting of the Beam Instrumentation Workshop (BIW) took place at Lake Tahoe on May 4–8, 2008. It was sponsored by Berkeley Lab's Accelerator and Fusion Research, Engineering, and ALS divisions. This international conference on beam diagnostics and instrumentation for accelerators is probably the most important gathering in the field of beam instrumentation, together with its European counterpart, the Diagnostics for Particle Accelerators Conference (DIPAC), which alternates with BIW on alternate years. The conference offers formal presentations, a poster session, and informal discussions to promote the exchange of ideas and issues between scientists, engineers, and representatives of companies operating in the field. Approximately 120 people attended, tutorial sessions served as introduction to relevant topics, and a vendor exhibition allowed participants to get updated information on related commercial products.

BIW08 conference attendees pose for a group photo outside the Granlibakken Conference Center and Lodge near Lake Tahoe, California.

The Faraday Cup Award, which recognizes and encourages innovative achievements in the field of particle accelerator beam instrumentation, was presented during the workshop. The award consists of a money prize and a certificate, and the BIW program committee is solely responsible for the selection of the recipient. This year's winner is Suren G. Arutunian, of the Yerevan Physics Institute, Yerevan, Armenia, for the development, publication, and successful testing of the diagnostic system, "Vibrating Wire Scanner."

Fernando Sannibale of the ALS Accelerator Physics Group was the BIW08 chair this year, and the local organizing committee was coordinated by Joy Kono of the ALS. Berkeley Lab's contribution included three invited talks, one contributed talk, and two posters. More information on BIW08 and its program (including PDF files of the presentations) can be found at the conference Web site at *http://www-als.lbl.gov/biw08/*. The proceedings of the conference will be published on the Joint Accelerator Conferences Website (JACoW), the free-access database for particle accelerator conferences, at *http://accelconf.web.cern.ch/AccelConf/*. ■

Left to right: Julien Bergoz (Faraday Cup Award sponsor), Suren Arutunian (2008 Faraday Cup Award recipient), and Fernando Sannibale (BIW08 chair).

Coherence 2007 Workshop Draws Record Attendance

Interest in coherent x-ray science is increasing rapidly, both in the areas of diffraction microscopy and x-ray photon correlation spectroscopy. The first workshop devoted to these topics was held in Berkeley in 2001. This was followed by gatherings in Cairns, Australia (2003), and Porquerolles, France (2005). The most recent workshop took place at the Asilomar Conference Center near Monterey on June 25–28, 2007. It was attended by 150 practitioners (50 more than anticipated) from all parts of the world. In addition to more than 30 talks, 70 posters were presented, showcasing progress on both the experimental and theoretical fronts. In addition to ongoing work and plans for new beamlines at third-generation light sources, new results from FLASH [the x-ray free-electron laser (FEL) in Hamburg] and from laboratory-scale x-ray lasers were discussed, as well as plans for experiments at x-ray FELs under construction on three continents.

The workshop was sponsored by the ALS, the Center for X-Ray Optics, Lawrence Livermore National Laboratory, and the Center for Biophotonics at the University of California, Davis. The poster sessions and banquet were further enlivened by refreshments generously contributed by XRADIA. The program and abstracts can be found on the conference Web site at *http://www-als.lbl.gov/coherence2007/*. ■

Asilomar Conference Center.

PEOPLE AND EVENTS

Honors and Awards

ALS user Franz Himpsel won the 2007 Davisson-Germer Prize "for pioneering investigations of the electronic structure of surfaces, interfaces, adsorbates, and nanostructures."


Himpsel

Himpsel has been a long-time involved and dedicated ALS user. He was part of the group that argued for the establishment of the ALS, was among the team that built one of the first two undulator beamlines, and later took part in the development of a nano-NEXAFS endstation at Beamline 8.0.1. He served on the ALS Science Policy Board and Users' Executive Committee. Himpsel is a pioneer in the field of surface science using synchrotron radiation and is also a long-time user of the Synchrotron Radiation Center (SRC) in Madison and served as its Scientific Director from 1997 to 2002.

Sam Bader, member and past chair of the ALS Scientific Advisory Committee, received the 2007 David Adler Lectureship Award for his "spirited lectures, writing and experimental research in the area of nanomagnetism, magnetic films, multilayers and surfaces of metallic systems, including championing the surface magneto-optic Kerr effect approach." The award was presented at the March meeting of the American Physical Society, where Bader gave an invited talk in the awards session of the Division of Materials Physics. Bader is an Argonne Distinguished Fellow and currently serves as Chief Scientist of the new Center for Nanoscale Materials and as Associate Division Director and group leader in Argonne's Materials Science Division.


Bader

Former ALS postdoc and current user Byron Freelon has been awarded the first Morehouse Prize by the National Society of Black Physicists (NSBP), which recognizes graduates of historically black colleges and universities who have shown considerable promise as physics researchers and teachers. The prize was awarded for his work in x-ray Raman scattering on artificial superconducting materials and his strong support of NSBP student programs. Freelon accepted the award at Morehouse College on April 5 and gave a talk entitled "Probing High-Temperature Superconductors with Layers and Light." Freelon attended Prairie View A&M University and received a Ph.D. in physics from the University of Minnesota in 2001.


Freelon

Chuck Fadley, long-time ALS user, ALS Professor, and a physicist with Berkeley Lab's Materials Sciences Division and at UC Davis, was presented with an award from the Japanese Society for the Promotion of Science for his development of characterization methods based on photoelectron spectroscopy and synchrotron radiation and for his mentoring of young scientists. Fadley received the award while attending the Sixth International Symposium on Atomic-Level Characterization for New Materials and Devices in Kanazawa, Japan. He is one of the world's foremost practitioners of photoelectron spectroscopy.


Fadley

In 2007, ALS Deputy Division Director Ben Feinberg (now retired) was one of five Berkeley Lab scientists selected as a fellow of the American Association for the Advancement of Science (AAAS). AAAS fellows, a tradition that began in 1874, are chosen by their peers for their distinguished contributions to science research, teaching, technology, or administration. Ben was elected "for outstanding contributions to user facilities, especially the Advanced Light Source." Ben and the other new fellows were recognized for their contributions at the Fellows Forum on February 16, 2008, during the AAAS Annual Meeting in Boston.


Feinberg

Howard Padmore, ALS Division Deputy for Experimental Systems, has been elevated to the rank of fellow by the Optical Society of America (OSA) Board of Directors at their meeting in September 2007 in San Jose, California. OSA members who have served with distinction in the advancement of optics are eligible for nomination to the rank of fellow. The number of fellows is limited to ten percent of the total membership. The Society recognizes Howard for his pioneering contributions to the application of x-ray optics to scientific research using synchrotron radiation. ■


Padmore

PEOPLE AND EVENTS

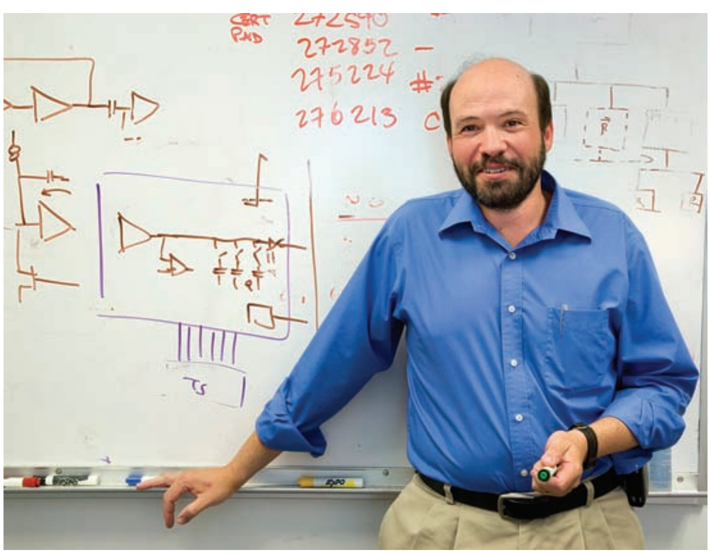
New Faces

Peter Denes of Berkeley Lab's Engineering Division has joined the ALS as our Deputy for Engineering. "Peter has been a leader within Engineering and in detector development at the Lab, and we're now looking forward to his playing a larger role in these efforts for the ALS," said Roger Falcone, ALS Division Director.

In the Engineering Division, Denes was responsible for electronics, software, and instrumentation engineering and brings this expertise to his new position. Peter's dedicated and on-site presence will provide tighter coupling between the Engineering Division and the ALS, more integrated management of engineering resources within the ALS, and a long-range focus as the ALS looks to its future as well as to the next-generation light source. A primary component of his job will be the ALS detector program. "This program is a virtual umbrella that brings together talent from the ALS, Engineering, and Physics to focus on the detector needs of the ALS," stated Peter. "Detectors can be purchased from manufacturers, but the unique requirements of the ALS beamlines often require unique detectors which are not available commercially." This new program aims to help users with existing detectors as well as to develop novel detectors that will improve ALS science. As the detector program gets off the ground, Peter also anticipates incorporating a postdoc program where new engineers can be mentored and trained. This detector program anticipates the Department of Energy's Office of Basic Energy Sciences (BES) detector and accelerator R&D initiative that is slated for FY 2008 and will enhance Berkeley Lab's ability to do research in this area.

Sue Bailey recently joined the ALS as leader of the User Services Group, which includes the User Services Office, Communications Section, and Experimental Setup Coordination. She brings to her new position over 20 years of scientific, software, and managerial experience. Sue also has the perspective of working at two synchrotron facilities, Daresbury Synchrotron Radiation Source in the United Kingdom and the ALS. At Daresbury, she was the group leader and user point of contact in the European community for a protein crystallography computational project and led her own research team on structure-function relationships of bacterial metalloproteins. She also performed research on enzymes in the sulphur cycle and secretion systems of pathogenic bacteria.

In 2003, Sue came to the ALS for a two-year stint as a beamline scientist in the Berkeley Center for Structural Biology. This evolved into a position as the BCSB's user support manager for the ALS protein crystallography beamlines. Sue returned to England and to Daresbury, but was soon lured back to the Bay Area and the ALS. "I'm pleased and honored to again be part of this world-class facility," she stated. "I have an open-door policy, and all users are welcome to drop in." Sue's office is in Building 6, Room 2212D, within the User Services Office. You can also contact her by email at SBailey2@lbl.gov or telephone at 510-486-7727. ■



Peter Denes.

Sue Bailey.

FACILITY UPDATES

Accelerator Availability and Reliability

by David Robin

The ALS operating schedule is divided into user beam shifts, accelerator physics/machine setup shifts, maintenance and installation shifts, and vacation shutdown shifts. In a "typical year," there is usually one long shutdown for major servicing, large installations, and upgrades. This long shutdown and associated startup usually occurs in the spring and lasts about six weeks. Also, in a typical year the ALS schedules and delivers more than 5000 beam hours to users. Below is a summary of events during the previous three fiscal years and the availability and reliability of the facility.

Availability is one of the most important performance parameters of the facility. Availability is defined as the ratio of delivered versus scheduled user time, while reliability is defined as the ratio of the number of actual fills that were completed without interruption versus the number of scheduled fills. Maintaining a high availability as the facility becomes more mature and complex (e.g., the addition of new insertion devices, injector upgrades, feedback and feed forward) is a challenging task.

The number of hours scheduled and delivered is shown in the table. In this review period, there was a deviation from the typical yearly shutdown pattern as described above. In FY06 the ALS ran the entire year without a major shutdown, and in FY07 the ALS had two long-term shutdowns—one in the fall of 2006 and the other in the spring of 2007. Therefore, the number of scheduled and delivered user hours were rather different in those two years. Because of this anomaly, it is convenient to look at the availability over the entire three years. Of the 16,001 scheduled hours, the ALS delivered 15,253 hours, which averages to 5083 hours per year, with a total availability of 95.3% delivered in schedule.

There was a drop in availability in FY07. This was because of two cascading effects that arose from the injector upgrade. In the fall of 2006, the ALS underwent a major shutdown to install and commission components necessary for full-energy injection. At the end of the shutdown, there was a major failure in one of the components (the booster bend power supply), which resulted in a loss of nine user days. The second effect was that this failure resulted in longer fill times for the remainder of FY07.

Reliability is another important performance parameter of the facility, which is distinct from availability. Reliability is defined as the ratio of the number of actual fills that were completed without interruption versus the number of scheduled fills. Providing good availability is necessary but not sufficient to ensure good reliability. For example, a user run with many unscheduled dropouts but fast recovery times would result in good availability but poor reliability. A good measure of reliability is the mean time between failures (MTBF). The MTBF was 40 hours in FY05 and increased to 50 hours in FY06 and 51 hours in FY07. ■

HOURS SCHEDULED AND DELIVERED

	Scheduled hours	Delivered hours*	Availability	Mean time between failures (hours)
FY05	5600	5344	95.4%	40
FY06	6201	6045	97.5%	50
FY07	4200	3864	92.0%	51

*Does not include unscheduled hours delivered to users.

User Demographics and Publications

As a national user facility, the ALS is required to report user demographics and publication information annually to the U.S. Department of Energy. Figure 1 shows the growth in particular scientific fields and the overall user growth from 1998–2007. The drop-off in 2007 is attributable to the fact that there were two long shutdowns in FY07 as opposed to just one, as in a typical year. The breakdown of different types of institutions that make up our user base is shown in Figure 2. The growth of the user community over the past 10 years is mirrored by the growth in beamlines and publications, as shown in Figure 3. As the number of beamlines approaches the capacity of the storage ring, new beamlines will be created by chicaning straight sections and revamping some of the older bend-magnet beamlines. ■

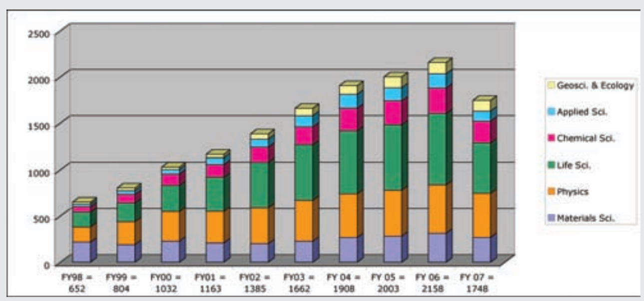


Figure 1. Bar graph showing growth in areas of science. The 2007 numbers reflect the two shutdowns that occurred in FY07.

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FACILITY UPDATES

Construction Projects Update

The User Support Building project team has been working to minimize the impacts of the directed funding change for the project this fiscal year ($5M instead of the planned $17M). We are moving forward with a phased-construction model and plan to break ground during the September 2008 shutdown to install the foundations, underground utilities, and major vertical steel columns. The six-week shutdown, beginning on September 2nd, was scheduled to accommodate construction work that is not compatible with ALS user operations due to vibrations. Work on this phase should be completed around the end of the calendar year. The next phase will begin in spring/summer 2009 and will include the remainder of the structural steel and exterior skins of the building. This phase be will completed around the end of calendar year 2009. The final project phase will begin in spring/summer 2010 and include the entire interior of the building. Depending on how early the funding for the 2010 fiscal year arrives, the project will be completed in either late 2010 or early 2011. We are thrilled that we are moving moving forward on this critical facility, which will improve our support for our users.

Design work on the 57-room Berkeley Lab Guest House is substantially complete. Construction on the site began with mass excavation activities to ready the building pad. Foundations are currently being installed. We anticipate construction of the relatively simple wood-framed structure to be completed in June 2009 and the Guest House to be open for guests shortly thereafter. We are currently working with the UC Berkeley Residential and Student Service Program to finalize an agreement to operate the Guest House. Once this agreement is in place we will be able to determine the final room rates. ■

User Support Building.

Berkeley Lab Guest House.

User Demographics and Publications *continued from page 16*

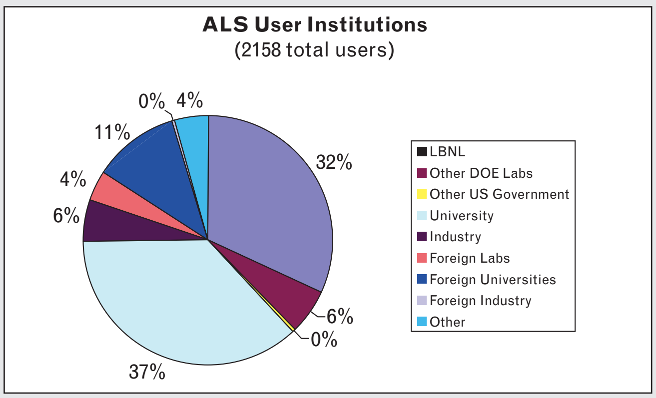

Figure 2. Pie chart showing percentages of different types of user institutions.

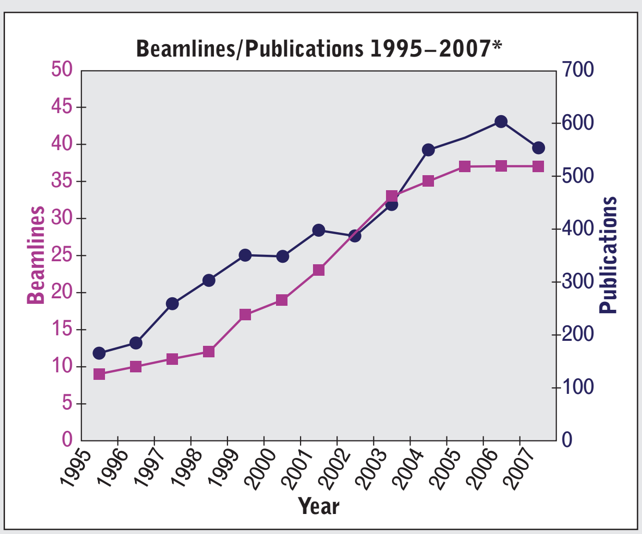

Figure 3. Graph of growth in beamlines (pink) and publications (blue). *Note that publications for 2007 were still being collected at the time this section was being written.

FACILITY UPDATES — The ALS Moves Forward: New Initiatives

We are in the process of submitting a variety of funding requests to DOE, ranging from a theory program, to detector development, to research on energy problems, to the rebuilding of Sector 7, and more, all in anticipation of new programs that Congress and the President seem poised to support in the next fiscal year. For example, a recent DOE call for proposals spans a wide range of activities, extending from single-investigator and small-group research (SISGR) to Energy Frontier Research Centers (EFRCs). Funding for new awards under these programs should be available in FY09, pending appropriations. The research and instrumentation areas covered include those outlined in the Grand Science Challenges Report of the Basic Energy Sciences Advisory Committee, and Use-Inspired Discovery Science, as described in The 10 Basic Research Needs Workshop Reports.

The EFRCs will focus on the scientific breakthroughs needed for advanced energy technologies. Examples of research areas include the direct conversion of solar energy to electricity and chemical fuels, biological feedstock conversion into portable fuel, and new radiation-tolerant materials. The SISGR grants cover areas such as ultrafast science, chemical imaging, complex materials research, and instrumentation.

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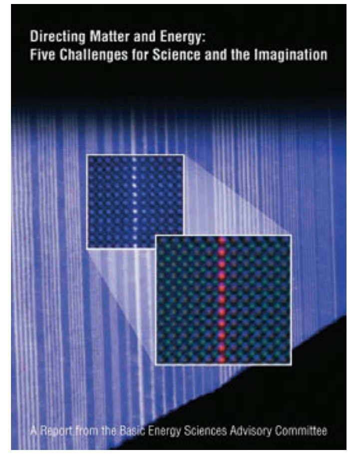


BES Grand Challenges Report.

Science Roundup

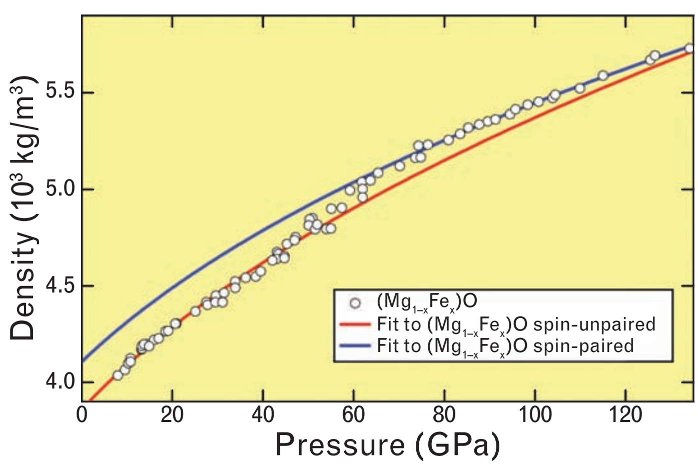
continued from page 3

of 102 gold atoms surrounded by 44 molecules of a thiol compound (para-mercaptobenzoic acid, or p-MBA). The central gold atoms are grouped in a fivefold symmetric packing arrangement known as a Marks decahedron, which is surrounded by additional layers of gold atoms in unanticipated geometries. The protective p-MBAs interact not only with the gold but with one another, forming a rigid surface layer. This research is a success on several levels. The group developed a technique that solves a previously unsolvable nanostructure. They delivered a very detailed atomic map of this structure, which itself reveals an unusual discovery: the discrete nature of the nanoparticle, which can be explained by the closing of a 58-electron shell.

Squeezing Iron

Speziale et al., *J. Geophys. Res.* **112**, B10212 (2007)
http://www-als.lbl.gov/als/science/sci_archive/166iron.html

It is now known that the iron present in minerals of the lower mantle of the Earth undergoes a pressure-induced transition with pairing of the spins of its 3d electrons. A team from the University of California, Berkeley, Tel Aviv University, and Lawrence Livermore National Laboratory has used x-ray diffraction at very high pressure to investigate the effects of this transition on the elastic properties of magnesiowüstite ($(Mg_{1-x}Fe_x)O$), the second most abundant mineral in the Earth's lower mantle. The new results suggest that the effect of the spin-pairing transition on magnesiowüstite can be large enough to require a partial revision of the most accepted model of the lower mantle composition.



Pressure dependence of the density of $(Mg_{1-x}Fe_x)O$ ($x = 0.17$ and 0.2) shows an anomalous change in slope, modeled as a "mixed-state" region where iron with spin-paired and spin-unpaired 3d electron configurations coexist in the structure of magnesiowüstite.

Toward Curing Autism

Araç et al., *Neuron* **56**, 992 (2007)
http://www-als.lbl.gov/als/science/sci_archive/165autism.html

Establishment of neural connections at specialized intercellular junctions called synapses is critical for proper brain function, and errors in the process are thought

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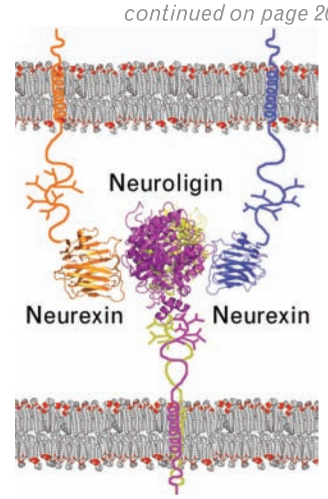

Model for the arrangement of the neuroligin-1/neurexin-1β complex at the synapse. Neurexins are tethered to the pre-synaptic cell membrane (top) and neuroligins are tethered to the post-synaptic cell membrane (bottom) by their stalk regions. Their interaction provides trans-synaptic connectivity.

New Initiatives

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Together with users, the ALS is proposing a collaboration involving the Berkeley campus and Stanford called the Theory Institute for Photon Sciences (TIPS), which will provide theoretical support to the users of existing and future light source facilities in meeting the Grand Challenges. One of the missions of TIPS will be to initiate stronger interactions between experimentalists and theoreticians.

Proposals for rebuilding Sector 7 of the ALS focus on the MAESTRO and COSMIC instruments; this remains a priority in our strategic plan. The Microscopy and Electronic Structure Observatory (MAESTRO)

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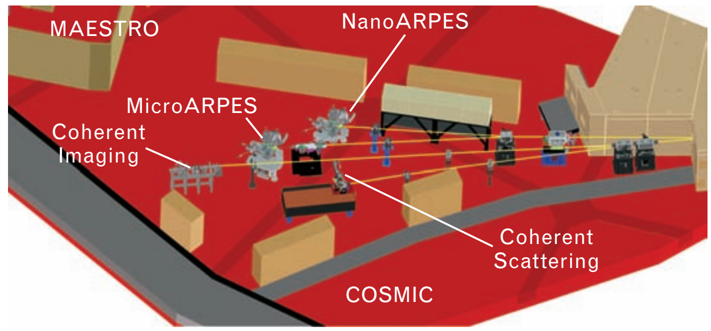


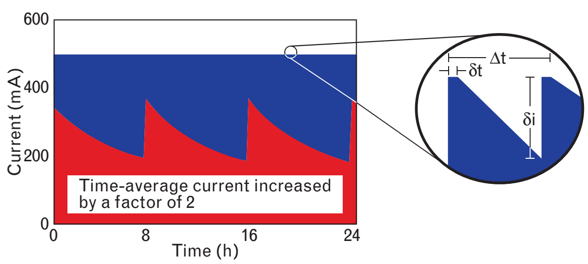
Depiction of the COSMIC and MAESTRO beamlines on the ALS floor at Sector 7.

Top-Off

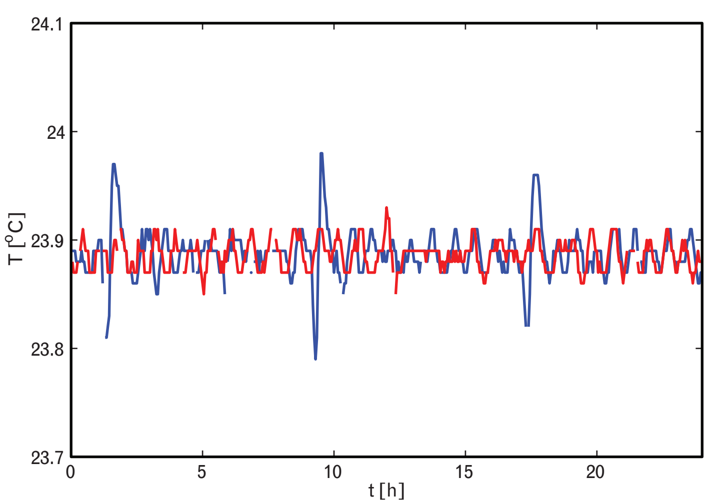
continued from page 1

for all sources—insertion devices as well as bend and superbend magnets. These gains result from the doubling of the average current, smaller vertical beam sizes, and smaller vertical gaps.

For top-off injection to work, the injector energy had to be increased from 1.5 to 1.9 GeV.



Sketch of the beam current history during one day before and after top-off.



Average air temperature in the ALS accelerator tunnel for a typical day with injection at 1.5 GeV (blue) as well as with full energy injection (red), showing the improved thermal stability.

This required an upgrade of parts of the booster synchrotron (particularly rf components, power supplies, diagnostics and controls) as well as an upgrade of the some of the pulsed-injection elements. With the completion of the 2006 shutdown and commissioning period, the major hardware work for the top-off upgrade was complete. However, although all the hardware installations were completed at the end of 2006, the new power supply for the booster dipole chain failed during the final testing conducted by the vendor. This caused several days' delay in user startup in January 2007 and subsequently limited performance. A successful collaborative effort between the vendor and ALS engineers during the Thanksgiving shutdown in November 2007 resolved the problem.

The first beam operation of the booster synchrotron at up to 1.9 GeV occurred on December 3, 2007. During the following week, injection rates into the storage ring were improved, and full-energy injection became standard on December 11. Once full-energy injection was implemented, an immediate benefit became obvious: transients in air and cooling water temperatures—previously caused by the change in magnet currents for injection—disappeared, resulting in better stability of the accelerator. The goal for summer 2008 is to slowly increase the peak stored current to 500 mA. This will result in an increase in average flux and brightness even before full top-off operation.

Also in 2007 and 2008, a set of very extensive radiation safety studies were performed, an important activity to be completed before top-off operation can begin. Top-off operation requires that the beamline shutters remain open during injection. There has been good progress, culminating in an outside peer review of the tracking studies, demonstrating that injection with the safety shutters open is safe, given certain controls involving interlock systems and verification of all necessary apertures. This includes the installation of some new apertures. All additional interlock systems and apertures necessary to ensure safe operation in top-off mode will have been installed by the beginning of 2009. The process that leads to regulatory approval for top-off operation was started in late summer 2007 and we hope to receive approval in August 2008. We anticipate beginning initial top-off operation on most of the beamlines during some accelerator physics shifts in fall 2008 and then begin full top-off operation for all beamlines during user time beginning in early 2009. ■

Science Roundup

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to be associated with autism and other disorders. Researchers from Stanford University and the University of Texas Southwestern Medical Center have reported high-resolution, three-dimensional structures of the proteins, called neuroligin-1 and neurexin-1β, that form this connection. Because mutations in the neurexin and neuroligin genes are among the multiple genetic causes of autism, understanding the molecular mechanism of these proteins in synapse development is a first step towards development of novel therapeutics directed to treat and possibly cure autism. ■

New Initiatives

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will address the need for improvement of spatial and energy resolution for photoemission. Coherent Scattering and Diffraction Microscopy (COSMIC) will provide improved, intense coherent light in the 0.5–3 keV range with full polarization control.

We also see opportunities for advances in how we generate and detect photons. We have submitted two proposals—one for advanced accelerator R&D toward a next-generation light source and one for advanced x-ray detector technology. The detector proposal is specifically tuned to the soft x-ray needs at the ALS, with an initial emphasis on the needs of new beamlines such as MAESTRO and COSMIC.

It is important to note that although growth at the ALS and other national facilities has been limited under recent federal budgetary restraints, new opportunities for funding continue to arise. We strongly encourage our users and staff to bring forward new ideas to take advantage of such opportunities. We can provide important assistance in bringing such proposals to funding agencies, foundations, etc. Partnerships among users and the ALS can be very persuasive. ■

BERKELEY LAB
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Design, layout, photography, and additional writing provided by the Creative Services Office and the Communications Department of Berkeley Lab's Public Affairs Department.

The editors gratefully acknowledge the ALS users and staff for their contributions, advice, and patience.

August 2008
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This work was supported by the Director, Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

OCTOBER 15

2009

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ALS Users' Meeting

OCTOBER 15–17, 2009