





# ALS ACTIVITY REPORT



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#### INTRODUCTION Janoz Kirz, Acting ALS Division Director

It has been an honor and a privilege to be Acting ALS Division Director while Daniel Chemla is recuperating from brain surgery. I am immensely grateful to the division staff, especially the division deputies—Ben Feinberg, Jim Krupnick, and Neville Smith for their dedication and enthusiastic support during this challenging time.

I bring unique qualifications to the job: I have been, and continue to be, an ALS user. I have gone through the proposal process, set up an account, stayed in the ALS apartments, and enjoyed the help and support of the staff at every level. Having worked at all four of the DOE light sources, I know from experience what a remarkable facility the ALS is. To move it to even greater levels of excellence is my goal.

2004 was indeed another outstanding year for the ALS:

- The number of users hit another all-time record of 1898.
- The number of refereed publications based on work at the ALS also reached a new record.
- The number of new structures deposited in the Protein Data Bank reached a new record as well.
- The Users' Meeting had record attendance and an outstanding set of ten workshops.
- Preparations for top-off operation made excellent progress, and we received funding from DOE BES to move ahead with the project.
- We prepared a new strategic plan, designed to keep the ALS at the forefront of synchrotron-radiation-based science for the coming decade and beyond.
- We put much effort into maintaining a safe environment, and with the excellent cooperation of the user community, we were able to maintain an outstanding safety record.



The latter part of the year was taken up in part by the Division's preparations for our three-year review by DOE BES and by UC's preparations to make a bid for the continued management of the Laboratory, both scheduled for February 2005.

I want to thank the members of the ALS's Scientific Advisory Committee and especially the chair, Sam Bader, for their hard work and excellent counsel. It has been a pleasure to work with the Users' Executive Committee, chaired in 2004 by Dennis Lindle. In 2005, I am looking forward to working with the UEC chaired by Greg Denbeaux. The ALS is here to support users in doing outstanding science in a safe environment. The input of the user community is critical to our ability to fulfill this mission!

### NOTE FROM THE UEC CHAIR

Dennis Lindle, UEC Chair for 2004

It was my pleasure to serve the ALS user community as Chair of the Users' Executive Committee for 2004. The UEC represents the ever-growing ALS user community in a variety of venues, including discussions with ALS management, the wider scientific and lay communities, DOE officials, and members of Congress. Issues addressed by the UEC range from the global, such as strategic planning and congressional support of DOE user facilities, to the local, such as ALS upgrades, facility access, and, yes, user housing. All of these issues, and more, were addressed in regular meetings and informal discussions with ALS management and staff.

The topic upon which the UEC spent the most time during the past year was strategic planning for the future of the ALS. To aid in the planning process, Neville Smith and I organized a joint ALS/UEC workshop where users and ALS staff were asked to imagine breakthroughs in their areas of expertise five or ten years from now and identify the scientific or technical enhancements of ALS facilities or operations needed to achieve them. Along with related workshops, this meeting helped inform the strategic planning effort led by Janos; many of the new ideas contained in the current plans came directly from discussions at these workshops.

Other developments at the ALS over the past year are particularly promising. Work continues on upgrading the ALS. When completed, the upgrades will allow continuous injection of the ring and provide enhanced beamline capabilities, maintaining the ALS as a cutting-edge research facility. A planned new user support building will replace the current Building 10 adjacent to the ALS and provide much-needed experimental and office space as well as seminar and meeting rooms. Availability of housing for visiting



users will receive a big boost in the near future now that plans are in the works for a new on-site facility to provide low-cost shortand medium-term housing. These projects are the outcome of hard work by the management and staff of the ALS, together with user input and financial support from the DOE and UC. Many thanks to everyone involved!

As we look to the future, users will continue to be called upon to work closely with ALS management to develop and implement a shared vision for the ALS as a world-class research facility. It is essential we, as a community, take time to communicate our needs and our achievements to the public and our representatives in Washington. Thank you for your support of the ALS, and please contact me or any other UEC member with your ideas and suggestions.

### Science Highlights





### Ultrafast X-Ray Science

Only a moment's reflection is enough to confirm that the world around us is a work in progress. Change is everywhere and ever present. Applying this insight to the physical, chemical, and biological systems investigated at synchrotron light sources like the ALS yields the conclusion that extracting the full story requires time-resolved experiments in which one can trace in detail the pathways (possibly through transient intermediate states) by which matter changes from one form to another.

At the ALS, a developing program of ultrafast time-resolved x-ray studies, which is itself undergoing a growth spurt, bases itself on the notion that understanding the behavior of condensed matter at the most fundamental level requires measurements on the time scale on which atoms move. For example, the making and breaking of chemical bonds and the rearrangement of atoms, which occur on the fundamental time scale of a vibrational period (about 100 femtoseconds), ultimately determine the course of phase transitions in solids, the kinetic pathways of chemical reactions, and even the efficiency and function of biological processes. A thorough understanding of such dynamic behavior, both atomic and electronic, is a first step toward control of structural evolution and eventual applications.

In this section, Andrea Cavalleri (Materials Sciences Division, Berkeley Lab) traces the past, present, and future of ultrafast x-ray studies at the ALS by examining a general question—how do electronic properties relate to the geometrical rearrangement of the atoms—in the context of the metal-insulator transition in vanadium dioxide  $(VO_2)$ . Two sidebars provide additional insight into the ways of making ultrashort x-ray pulses down to the femtosecond level and plans for ALS beamlines to use such pulses.



#### Time-Resolved X-Ray Absorption with Femtosecond Synchrotron Pulses

Andrea Cavalleri, Materials Sciences Division, Berkeley Lab

An important frontier lies at the convergence of the fields of static x-ray science and femtosecond laser studies of phase-transition and chemical-reaction dynamics. The grand goal that drives this new area of science is no less than the direct measurement of the structural pathways that connect different crystallographic, electronic, and magnetic phases of solids. Similarly, one would also like to directly investigate the short-lived transition states between reactants and products in chemical and biochemical reactions. As a case example, consider the phase transition in vanadium dioxide (VO<sub>2</sub>) in which an insulator with a monoclinic crystal lattice becomes a metal with a rutile structure when heated above the transition temperature  $T_c = 340$  K. The controversial nature of the low-temperature insulating phase, as well as substantial uncertainty over the roles of structural motion and electronic correlations in driving the phase transition, have fueled an enduring debate over the past several decades.

Up to now, x rays have revolutionized modern science by providing access to the microscopic structural properties of matter, which are these days measured at synchrotron light sources by means of diffraction and spec-



troscopy. These studies have had dramatic success in revealing the static properties of materials near equilibrium. Yet, many questions remain open about the microscopic dynamics of phase transitions and chemical reactions, which are generally mediated by rapid fluctuations that are averaged out and hence invisible in time-integrated experiments. Although ultrafast lasers can access the femtosecond time scale of atomic motion, they provide limited structural insight at the near-visible wavelengths where most experiments are performed.

To date, scientific applications of femtosecond x rays have concentrated almost exclusively on time-resolved diffraction, driven by the availability of ultrafast monochromatic xray pulses from laser-heated plasma sources that fit on a tabletop, from the interaction of femtosecond lasers with relativistic electron beams, and, recently, from the SPPS project-an undulator in the linac at SLAC [A.M. Lindenberg et al., Science 308, 392 (2005)]. However, the lack of femtosecond x-ray sources that emit or are tunable over a broad spectral range has hindered the complementary development of femtosecond x-ray spectroscopy. The technique of "laser slicing" now in use at the ALS is currently the only proven method to generate broadband x-ray pulses of femtosecond duration (see sidebar, "A Long Journey to Short X-Ray Pulses").

One of the areas of research in which femtosecond x rays are opening new horizons is the physics of phase transitions in correlated electron systems (i.e., those in which interactions between electrons cannot be ignored). These materials are characterized by strong interplay between their various degrees of freedom (atomic, electronic, orbital, magnetic), which results in rich, complex phase diagrams with many competing states that exhibit extreme sensitivity to external stimuli. Rather than varying external parameters (e.g. temperature, pressure, magnetic field), in our time-resolved experiments, we seek to study the nonequilibrium pathway of these phase transitions after the

material is impulsively excited with light. Typically, the phase transition is initiated by charge excitations within a particular phase of a correlated solid (e.g. an insulator). Such "photodoping" can, in analogy with chemical substitution, favor relaxation of the system into a competing state of the solid (e.g. a metal).

We have been exploring the photoinduced insulator-to-metal transition in VO<sub>2</sub>. Figure 1 summarizes the atomic structures of VO<sub>2</sub> in both the insulating (low-T or undoped) and metallic (high-T or photodoped) phases, and Figure 2 summarizes the electronic structures. The electronic states that are relevant for the phase transition are the lowest-lying,  $t_{2g}$ -like states that derive from vanadium 3d states split in energy by crystal-field effects, doubling of the periodicity of the crystal unit cell (dimerization) in the low-T insulator, and electron-electron correlations.



Atomic arrangements in the insulating monoclinic phase of  $VO_2$  (T < 340 K) and in the metallic rutile phase (T > 340 K). Top: Each vanadium cation is surrounded by six oxygen atoms, as visualized in this top view of the unit cell. Bottom: The side view shows only the V<sup>4+</sup> lattice to emphasize the pairing and tilting along the c axis it undergoes in the period-doubled, insulating structure.



Diagram of the vanadium 3d states in  $VO_2$ . The degeneracy of the 3d levels, found in isolated atoms, is lifted by the crystal field, as well as by period doubling in the unit cell and electron-electron repulsion. The Fermi level lies within the  $t_{2g}$ -like states, which form valence and conduction bands.

In our experiments, prompt photodoping by exciting electrons out of (and hence holes into) the valence band (formed from 3d<sub>II</sub> states) of the low-T insulator and delocalization of the charge carriers in the spatially extended conduction band cause an ultrafast transition to the metallic state as the valence and conduction bands, once separated by an energy gap, now overlap (Figure 3). This effect is clearly evident in the ultrafast increase in optical reflectivity (and decrease in transmission) at near-visible wavelengths (Figure 4), as the sample becomes opaque to visible radiation when doped. During this process, the structural dimerization of the low-T insulator is coherently relaxed, and the metallic phase is formed, both processes occurring on the 100-fs time scale.

As a first application of tunable femtosecond x rays, we set out to probe the phase-transition dynamics in VO<sub>2</sub> with soft x-ray NEXAFS. The electronic states near the Fermi level that participate in the insulator-to-metal phase transition, which are difficult to probe separately by means of optical spectroscopy, can be distinguished by measuring absorption from symmetry-selective core levels (Figure 5). The photodoped valence band, which has primarily vanadium 3d character, is best probed by measuring x-ray absorption from the vanadium 2p core levels near 516 eV. On the other hand, the conduction band, which originates from stronger mixing between vanadium 3d and oxygen 2p orbitals, is most visible at the 531-eV oxygen 1s resonance.



Schematic diagram of the photoinduced insulatorto-metal transition in  $VO_2$ . Following hole photodoping into the  $3d_{\parallel}$  band, the band gap collapses and a metallic phase is formed.

In our experiments at Beamline 5.3.1, we probed the photoinduced phase transition with picosecond pulses of synchrotron radiation. These experiments were performed along the same lines explored by previous time-resolved x-ray absorption spectroscopy measurements at the ALS by S.L. Johnson et al. [*Phys. Rev. Lett.* **91**, 157403 (2003) and *Phys. Rev. Lett.* **94**, 057407 (2005)]. In these "pump-probe" experiments, a flat-field imaging spectrometer was used to spectrally



4 Optical measurement of the photoinduced insulator-to-metal transition in VO<sub>2</sub>. This effect is clearly evident in the increasing reflectivity (and decreasing transmission) with time at near-visible wavelengths.

disperse the soft x rays transmitted through the sample, thereby capturing the entire absorption spectrum at once for each time delay between the laser excitation and the measurement. Figure 6 depicts the experimental setup.

Figure 7 summarizes the results of the picosecond x-ray absorption measurement in  $VO_2$ , where the phase transition is evidenced by a red shift of the L<sub>3</sub> edge to lower energy, cor-



5 Static NEXAFS spectrum of VO<sub>2</sub>, as measured with 100-meV (dashed line) and 4-eV (solid line) resolution. The blue part of the spectrum refers to transitions from core vanadium  $2p_{3/2}$  and  $2p_{1/2}$  states and gives information on the density of unoccupied electronic states with 3d symmetry. The red part of the spectrum refers to transitions from the oxygen 1s core levels into oxygen 2p orbitals of the valence band. Even in the formative planning stage of the ALS a decade before operation began in 1993, prospective users envisaged timeresolved experiments made possible by the brightness and the "short" 70-picosecond length of the ALS light pulses. But the focus soon shifted to the femtosecond time scale. There are two general approaches to ultrafast time resolution: producing ultrashort pulses or extracting time-resolved information from a longer pulse with an ultrafast detector.

Taking the first approach, Berkeley Lab's R. Schoenlein (Materials Sciences Division), W. Leemans (Center for Beam Physics), and their co-workers first breached the femtosecond x-ray frontier at the ALS with a 1996 experiment. They aimed 100-femtosecond laser pulses at right angles to the focused beam from the ALS linear accelerator to generate x-ray pulses just 300 femtoseconds long at a fixed photon energy determined by the linac energy, a technique known as 90-degree Thomson scattering [Science 274, 236 (1996)]. Later, in 1999, the group applied the technique to x-ray diffraction, when they probed femtosecond structural dynamics in indium antimonide irradiated by a high-power, ultrafast laser [Phys. Rev. Lett. 83, 336 (1999)].

Despite the experimental success, the flux and brightness of the 90-degree Thomson scattering technique was too low to be widely useful, and attention had already turned to an early 1996 concept developed by Berkeley Lab's A. Zholents and M. Zolotorev (Center for Beam Physics). They proposed "laser slicing" as a way to achieve effective bunch lengths in the femtosecond range over a broad range of photon energies [*Phys. Rev. Lett.* **76**, 912 (1996)]. At the heart of the proposal was the use of a high-power, femtosecond laser synchronized with the electron bunches. As a pulse of laser light passes collinearly with an electron bunch through an undulator or wiggler, it gives kicks of approximately 10 MeV to a 100-femtosecond "slice" of the 70-pslong electron bunches. When each energymodulated electron bunch reaches a bend magnet (or other section of the storage ring with a nonzero dispersion), the energy-modulated electrons are displaced radially onto different orbits. A collimator or aperture selects the femtosecond pulses from the displaced bunch slices. The demonstration of laser slicing by Schoenlein and several co-workers in 2000 [Science 287, 2237 (2000)] established laser slicing as currently the only proven method to generate broadband x-ray pulses of femtosecond duration.

In parallel with the source development, progress with the complementary detector approach came from R. Falcone (UC Berkeley) and his co-workers. After putting aside an earlier program to develop ultrashort-pulse x-ray sources from laser-produced plasmas generated by ultrafast lasers, Falcone's group came up from the UC Berkeley campus to the ALS in the mid-1990s to do time-resolved x-ray measurements via an ultrafast x-ray streak-camera detector that the group had developed earlier [Appl. Phys. Lett. 56, 1948 (1990)]. With their streak-camera technology, they were able to extract information with a time resolution that is now nearing one picosecond, which is well below the normal ALS pulse width if not guite at the femtosecond level [Opt. Lett. 22, 1012 (1997)]. The technique initially was applied to x-ray diffraction [e.g., Phys. Rev. Lett. 84, 111 (2000)].



Schematic diagram outlining the laser-slicing technique for generating femtosecond pulses of synchrotron radiation at either a bend-magnet or undulator beamline. The undulator-based Ultrafast X-Ray Facility (Beamline 6.0.1) now under construction will make femtosecond spectroscopy a readily available technique at the ALS (see sidebar, "The Ultrafast X-Ray Facility").

responding to a collapse of the unoccupied states of 3d symmetry. The "coarse" picosecond time resolution did not allow access to microscopic rearrangements and relaxation, but it could follow the quasi-equilibrium kinetics of the transition as a progressively thicker metallic layer grows into the materials.

For femtosecond x-ray absorption measurements by the same pump-probe approach, we used Beamline 5.3.1 in the laser-slicing mode. The ultrashort x-ray pulses radiated by the femtosecond electron slices traversing a bending magnet were focused onto the  $VO_2$  sample by a toroidally bent silicon mirror and spatially selected using an off-axis slit. Figure 8 depicts the experimental setup.

The results of our optical pump x-ray probe experiment can be seen in Figure 9 for two wavelengths at the vanadium  $2p_{3/2}$  edge and oxygen 1s resonance, respectively. At the vanadium  $2p_{3/2}$  edge, a prompt increase in absorption was observed immediately after photoexcitation, recovering within a few picoseconds. At the oxygen 1s resonance, the absorption coefficient was also initially observed to increase, synchronously with that at the vanadium  $2p_{3/2}$  resonance. Enhanced oxygen 1s absorption at 530 eV was followed



Picosecond NEXAFS experiments performed in transmission geometry at the ALS.

by a decrease (bleaching) and by relaxation on the same few-picosecond time scale as the signal at the 516-eV vanadium  $2p_{3/2}$  edge.

The observed behavior likely results from a combination of hole and electron photodoping, band-structure rearrangement, and dynamic shift of the core levels. This complicated interplay is not discussed here in further detail, and it is difficult to clarify fully with our present measurements. Yet, the data reported in Figure 9 are the first successful measurement of x-ray absorption on the fundamental time scale where the phase transition occurs, a feat that will nucleate deeper studies once

full, high-resolution x-ray absorption spectra can be measured with femtosecond resolution.

Extensions of the current experiment at the higher-flux Beamline 6.0.1 (see sidebar, "The Ultrafast X-Ray Facility"), will make such improvements possible by taking advantage of the higher x-ray flux from a dedicated undulator source. A number of new experiments will also become possible with such improvements, opening new scientific frontiers in the study of electronic and short-range structural dynamics at surfaces and in the liquid state, as well as femtosecond magnetic dynamics in solids.



Left: Picosecond NEXAFS experiments probe the rising edge of the  $2p_{3/2}$  resonance, which undergoes a red shift to lower energy as the  $3d_{\parallel}$  band gap collapses. Right: The cross correlation between visible synchrotron light and the excitation laser is used to validate the 70-ps time resolution of the measurement.

Designed for x-ray diffraction and spectroscopy with 200-femtosecond temporal resolution, the Ultrafast X-Ray Facility (Beamline 6.0.1) will fill a critical need for the growing ultrafast x-ray research community at the ALS. Funded by DOE BES, this beamline increases the availability of femtosecond x rays at the ALS a thousandfold over bend-magnet Beamline 5.3.1. Moreover, many of the techniques to be developed on this beamline will find direct applications in the experimental program at the LCLS, an x-ray free-electron laser now under development at SLAC with a projected 2009 startup.

Beamline 5.3.1 now serves several groups conducting diffraction and spectroscopy experiments in the picosecond regime with spectrographs and streak-camera detectors. However, in the femtosecond regime, the laser-slicing techniques (see sidebar, "A Long Journey to Short X-Ray Pulses") carries a significant flux penalty of about 10<sup>-10</sup> relative to normal operation because only a small portion of the electron bunch is sliced and the low laser repetition rate means only a small fraction of the bunches are sliced. As a result, the use of Beamline 5.3.1 for femtosecond experiments has been limited. At Beamline 6.0.1, the use of an undulator rather than a bend magnet as the x-ray source and the addition of a new laser with a higher repetition rate combine to result in the thousandfold flux increase for femtosecond x rays.

Based on a proposal with R. Schoenlein (Materials Sciences Division, Berkeley Lab) and R. Falcone (UC Berkeley) as principal investigators, the facility is the fruit of many years of effort by H. Padmore, P. Heimann, E. Glover, and others in the ALS Experimental Systems Group as well as C. Steier and many collaborators in the Accelerator Physics and Engineering Groups and the Center for Beam Physics. An in-vacuum, permanentmagnet dual-mode undulator/wiggler will radiate both soft and hard x rays from 120 eV to 10 keV in both the normal and laserslicing modes. The device has 50 30-mm periods and a peak magnetic field of 1.5 T. Constructed by a vendor from a design developed at the ALS, the undulator awaited installation in the April 2005 shutdown.

For generating femtosecond pulses via laser slicing, the ultrafast facility will use the recently installed W11 wiggler (designed specifically to enable laser slicing without disturbing the protein crystallography beamlines that it also serves), a 20-kHz femtosecond laser system, and the in-vacuum undulator. The laser will be located at the end of the beamline and will serve the dual purposes of providing laser pulses for slicing the synchrotron beam and providing tunable "pump" pulses for sample excitation. Based on the present storage-ring parameters, x-ray pulses of 200-femtosecond duration are expected.

Among two planned branchlines, a soft x-ray branch with a VLS grating spectrograph will come online by the end of 2005. The spectrograph will allow a complete spectrum to be recorded at once. A streak camera will serve as the detector for measurements on picosecond time scales. A hard x-ray branch with a Ge(111) or Si(111) double-crystal monochromator will be ready a year later. In the future, it is hoped to add a half-length small-gap EPU to the chicaned straight section 6, resulting in a doubling of capacity and the use of polarized x rays. The plan is to time-share the EPU between a new dedicated program in ultrafast magnetism and the soft x-ray branch of the slicing source.



Beamline 6.0.1 will increase the flux (photons/second) by 1000 relative to Beamline 5.3.1, thereby making laser slicing a widely applicable technique for the production of femtosecond x rays for spectroscopy as well as diffraction.



Femtosecond x-ray experiments performed with laser-sliced x-ray pulses. Femtosecond laser pulses from the same titanium:sapphire (Ti:Sa) oscillator are used for sample excitation and for slicing of the electron beam after separate amplification, ensuring absolute synchronization between pump and probe. An off-axis slit placed in the image plane of the storage ring (before the sample) blocks the main picosecond pulses and transmits the off-axis femtosecond x rays. A flat-field imaging spectrometer placed after the sample measures the spectra as a function of the pump-probe time delay.



Femtosecond dynamics of photodoping and of the ultrafast phase transition, as performed separately at the vanadium 2p<sub>3/2</sub> and oxygen 1s resonances.

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### CONDENSED MATTER PHYSICS

#### Unusual Isotope Effect in Bi2212 High-Temperature Superconductor

When they burst upon the scene in late 1986, "high-temperature" superconductors spawned an outpouring of enthusiasm among those who foresaw massive new intrusions of superconductivity (the resistanceless flow of electricity) into the workaday world. While work on applications continues, a theory to explain how these wondrous ceramic compounds (called cuprates) performed their magic is turning out to be elusive. The earlier Nobel-Prize-winning Bardeen-Cooper-Schrieffer (BCS) theory of superconductivity in metallic materials relies on the formation of pairs of normally mutually repelling electrons by means of an attractive force due to interaction of the electrons with atomic vibrations (phonons). But it is not directly applicable to the more complex cuprates, and the focus of attention has been on the magnetic characteristics of these materials. Lanzara et al. have produced new evidence that phonons are in fact involved in high-temperature superconductors but in a novel way that also retains a place for magnetic interactions. How this evidence will affect the theory logjam remains to be seen.

Magnetism or lattice vibrations? After almost 18 years of intense experimental and theoretical effort since the discovery of the first cuprate high-temperature superconductor (HTSC), physicists still do not know the origin of this most intriguing of solid-state phenomena. A team of Berkeley Lab, UC Berkeley, and University of Tokyo researchers has come up with evidence from ARPES that strongly implicates lattice vibrations, but in an unconventional way that leaves room for magnetism as well.

The BCS model explains "conventional" or "low-temperature" superconductivity in metallic solids. At a sufficiently low temperature (the critical temperature), electrons near the Fermi energy join with relatively distant electrons with opposite momentum and spin to form Cooper pairs with no net momentum or spin. The pairing is due to a weakly attractive force between the electrons that arises as they interact with phonons. As bosons with identical quantum numbers, the pairs condense into the coherent superconducting state. The story is quite different in the cuprate HTSCs.

Here the underlying or parent material is an antiferromagnetic insulator that is made into a poorly conducting metal by adding small amounts of "doping" elements. Doping usually removes electrons from the electrically active crystal planes containing copper and oxygen atoms, although sometimes doping adds electrons to the planes (Figure 1). It



Crystal structure of Bi2212 showing the copper (purple)-oxygen (black) layer responsible for superconductivity.

also turns out that for all compositions other than the so-called "optimally doped" HTSC with the maximum critical temperature  $(T_c)$ , the pairing occurs at a higher temperature than the formation of the coherent superconducting state.

As a result, the antiferromagnetic character has dominated the thinking of those seeking an explanation for the superconductivity, an inclination reinforced by the absence of a strong shift in  $T_c$  when a heavier or lighter isotope was substituted into the crystal lattice. Such an isotope effect was one of the key pieces of evidence leading to the BCS theory. Nonetheless, evidence supporting a role for electron–phonon interactions in HTSCs exists, some of it from earlier ARPES data gathered at the ALS [A. Lanzara et al., *Nature* **412**, 510 (2001)].

The Berkeley-Tokyo collaboration looked more closely at the electron dynamics revealed by the very high resolution ARPES data that it was possible to obtain at ALS Beamline 10.0.1. They studied an optimally doped bismuth cuprate (Bi2Sr2CaCu2O8+8/ or Bi2212) at three stages of an isotope-substitution loop comprising <sup>16</sup>O (the normal oxygen isotope), <sup>18</sup>O (heavy oxygen), and a return to <sup>16</sup>O. In brief, relative to those for samples containing <sup>16</sup>O, the energy-momentum dispersion curves for samples containing <sup>18</sup>O obtained for several directions in the Brillouin zone reproducibly show a significant shift at energies well away from the Fermi energy, as well as a shift in the energy of the universally observed "kink" that separates the low- and high-energy regions of the curves (Figure 2). The magnitude of the shift correlates well with the values of the anisotropic superconducting energy gap in those directions (Figure 3). This isotope effect also decreases above the critical temperature (Figure 4).

Taken together, these observations confirm that phonons play a role in HTSCs but one in which electron pairing and electron– phonon interactions reinforce each other.



2 Energy-momentum (E-k) dispersion curves for different directions in the Brillouin zone (inset) show a distinct shift when <sup>18</sup>O substitutes for <sup>16</sup>O. In addition, there is a shift in energy of the "kink" that separates the low- and high-energy regions of the curves. The origins of the curves are shown displaced to avoid overlap.



The smaller isotope effects in the E-k curves for the same directions in the Brillouin zone (inset) above  $T_c$  relative to those below  $T_c$  suggest that pairing enhances the coupling to the lattice.

30 30 10 20 Δ (meV)

The isotope shifts measured at a binding energy of 220 meV correlate with the values of the anisotropic superconducting gap  $\Delta k$ .





The researchers suggest a model in which the spins of missing electrons (holes) or extra electrons on nearby lattice sites alternate in orientation, similar to the antiferromagnetic lattice of the HTSCs, but form electron pairs (spin singlets) in the process. The motion of the pairs then perturbs the crystal lattice (dynamic spin Peierls distortion), which leads to an enhanced interaction between the pairs and phonons and further stabilizes the pairs against the strong Coulomb repulsion between the closely spaced members of each pair (Figure 5). INVESTIGATORS G.H. Gweon and J. Graf (Berkeley Lab), T. Sasagawa (University of Tokyo and Japan Science and Technology Agency), S.Y. Zhou (UC Berkeley), H. Takagi (University of Tokyo, Japan Science and Technology Agency, and RIKEN, Japan), and D.H. Lee and A. Lanzara (Berkeley Lab and UC Berkeley). **FUNDING** U.S. Department of Energy, Office of Basic Energy Sciences.

PUBLICATIONS G.H. Gweon, T. Sasagawa, S.Y. Zhou, J. Graf, H. Takagi, D.H. Lee, and A. Lanzara, "An unusual isotope effect in a high-transition-temperature superconductor," *Nature* **430**, 187 (2004).

#### Influence of Topological Spin Fluctuations on Charge Transport in Na<sub>0.7</sub>CoO<sub>2</sub>

For almost two decades, physicists have been asking: What gives ceramic cuprate compounds (so-called because they are copper-based) their miraculous ability to conduct electricity without resistance at much higher temperatures than superconducting metals and alloys? Now they are attacking the problem by studying other materials that are like but not exactly the same as the cuprates. A case in point is the family of materials called cobaltites (because they are cobalt-based), which have many similarities to cuprates, including superconductivity (but at a relatively low temperature) and electronic activity confined to 2D layers. But there are also important differences, such as the symmetry of the atomic arrangement of the cobalt atoms in the layers, which is triangular rather than square, as for copper atoms in the cuprates. Hasan et al. are the first to use an x-ray photoemission technique to demonstrate both the strongly correlated nature of the electrons (the property that makes the problem so difficult) and the influence of magnetic effects (spin fluctuations).

Layered transition-metal oxides are the focus of intense research efforts because they might clarify the superconducting mechanism of cuprate high-temperature superconductors (HTSCs). A case in point is  $Na_xCoO_2$  with x = 0.7, which is a parent compound for a family of cobaltites that exhibits superconductivity. This class of materials is also thought to be ideal for detecting the long-sought resonating valence bond state of matter proposed by Philip Anderson of Princeton University in 1973. Researchers from Princeton and the ALS are the first to use ARPES to demonstrate the strongly electron-correlated nature of this material and to provide evidence that charge transport is strongly influenced by topological spin frustration.

The family of sodium cobalt oxides or oxyhydrates (cobaltites) Na<sub>x</sub>CoO<sub>2</sub> (with variable x) is similar to cuprate HTSCs. The parent compounds are Mott insulators, in which a strong electrostatic repulsion blocks charge transport; they have layered crystal structures with electronic two-dimensionality; and they can be chemically doped by altering the sodium concentration, thereby changing the electron concentration in the electronically active cobalt-oxygen layers (Figure 6). There is one very important difference, however. While the electronically active copper-oxygen planes in HTSCs have square symmetry, in cobaltites, the symmetry is triangular, a configuration that geometrically frustrates formation of the antiferromagnetically ordered Néel state present in HTSCs and results in a less well ordered "quantum spin liquid" state.

The interplay of charge and spin degrees of





freedom is indeed exciting in cobaltites and leads to a bouquet of changing electronic properties with doping. With increasing sodium concentration, the material progresses from a paramagnetic metal that is superconducting at low temperature for 1/4 < x < 1/3 to a charge-ordered insulator at x = 1/2, to a Curie-Weiss metal (with the magnetic susceptibility of an insulator) at x = 2/3, and ends as a weakly magnetically ordered spindensity wave metal for x > 3/4.

The Princeton–ALS group performed a detailed investigation of the low-energy electronic structure and charge dynamics of the parent cobaltite compound  $Na_{0.7}CoO_2$  at ALS Beamlines 7.0.1 and 12.0.1. This technique is sensitive to an electron's quantum corre-



**2** Left: Photoemission intensity (bright regions are highest intensity) maps of the valence excitations at T = 10 K along the two symmetry directions ( $\Gamma$ -M and  $\Gamma$ -K) in a 2D hexagonal Brillouin zone. Solid curves are from mean-field calculations [D.J. Singh, *Phys. Rev. B* **61**, 13397 (2000)]. Co  $t_{2g}$  and 0 2p indicate that the origin of the bands is predominantly from these states. Right: The difference (green) between photoemission energy distribution curves taken at T = 18 K in resonance with the cobalt  $3p \rightarrow 3d$  transition (red) and out of resonance (blue) shows a resonance enhancement of the correlation satellite centered near 11 eV.

lations because it directly probes the electron distribution function over a complete Brillouin zone (unit cell in momentum space) with good resolution.

ARPES spectra taken in the energy range of valence (loosely bound) electrons are in good agreement with the results of meanfield (first-principles) calculations and map the dispersion (energy–momentum relationship) of several distinct bands (Figure 7). Most exciting, ARPES spectra also reveal an additional satellite feature centered at a much higher binding energy near 11 eV. Separation of this correlation satellite from the valence band gives an estimate of a strong on-site Coulomb repulsion (Hubbard *U*) between electrons of about 5 eV, which is in the same range as the Hubbard *U* for the cuprates and provides strong evidence for the highly correlated nature of electrons.

In addition, the researchers discovered a tiny feature (quasi-electron) adjacent to the Fermi energy (zero binding energy) that was dwarfed by the presence of the valence band (Figure 8). This feature is essentially flat in momentum space with a dispersion less than 100 meV, which is a factor of 5 smaller than in cuprates and an order of magnitude below the mean-field calculations. Accompanying the small bandwidth is a very weak nearest-neighbor single-particle hopping energy *t* of about 10 meV. That *t* is of the same order of magnitude as the spin exchange coupling *J* for this family implies that the charge dynamics are strongly perturbed by spin fluctuations.

The distribution of quantum coherent quasielectrons in momentum space forms a single







9 Quasi-electron distribution in momentum space. The occupied area (blue) in the Brillouin zone (red line) forms a single large hexagonal pocket around the center of the Brillouin zone. The Fermi surface is the inner edge of the pocket.



10 Quasi-electrons lose their coherence above 150 K (well below room temperature) and a coherent-toincoherent crossover is observed. A combination of very small hopping and magnetic exchange energies causes the low coherence temperature.

large hexagonal pocket around the center of the Brillouin zone (Figure 9). Temperaturedependent ARPES measurements revealed that quantum coherent quasi-electrons exist only at low temperatures and linearly disappear as their motion becomes incoherent beyond 150 K (Figure 10). This value, which is well below the decoherence temperature of tens of thousands of degrees in conventional metals, is of the order of t and J, making geometrical frustration of antiferromagnetic interactions in triangular cobalt lattice planes the leading cause of a quasi-electron's quantum decoherence.

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#### Extracting the Eliashberg Function

Theorists face a huge problem when trying to apply quantum mechanics to the calculation of the properties of solids, most of which are determined by the spectrum of energies characterizing the electrons as they zip around and between the framework (lattice) of vibrating atomic nuclei that make up the skeleton of the solid. Salvation comes from the Born-Oppenheimer approximation (BOA), which allows theorists to consider the slow-moving atoms to be frozen in space while the more energetic electrons do their thing. But it turns out that many of the most interesting behaviors of matter—such as superconductivity (loss of resistance to the flow of electricity at ultracold temperatures) in metals—result from so-called vibronic interactions that are due to coupling of electronic motion and lattice vibrations; that is, from the breakdown of the BOA. Shi et al. have combined a well-known soft x-ray spectroscopy technique with theoretical calculations in a new way to paint the first precise pictures of which vibrational modes couple to which electrons.

A multitude of important chemical, physical, and biological phenomena are driven by violations of the BOA, which decouples electronic from nuclear motion in quantum calculations of solids. Recent advances in experimental techniques combined with ever-growing theoretical capabilities now hold the promise of presenting an unprecedented picture of these violations. By means of high-

resolution angle-resolved photoemission at the ALS and theoretical calculations, a multiinstitutional collaboration that includes researchers from Oak Ridge National Laboratory, University of Tennessee, Stanford University, and the ALS has obtained the first high-resolution spectroscopic images of the specific vibrational modes that couple to a given electronic state. Breakdown in the BOA results from low-energy excitations of the electrons near the Fermi energy coupling with vibrational excitations of the solid. The resulting vibronic interactions are a necessary ingredient in any process that makes or breaks a covalent bond, such as conventional catalysis or enzymatically facilitated biological reactions. Conventional superconductivity, which is driven by the





electron–lattice interaction, is another classic result. And many of the emergent properties of complex materials or artificially nanostructured materials result from coupling of the electronic and lattice motion in systems that are inherently anisotropic.

The manifestation of this coupling is a distortion in the measured dispersion (energy  $\varepsilon$  vs momentum k) near the Fermi surface relative to that from a first-principles calculation for the electron bands in a solid without vibrational motion (a frozen lattice) or, failing that, a simple parabolic ( $\varepsilon ~ k^2$ ) band. This distortion has been seen in several materials using high-resolution ARPES. The anisotropic nature of this coupling can be seen directly because the ARPES technique allows measurements to be made as a function of the magnitude and direction of the electron's speed.

The researchers chose to study the  $(10\overline{1}0)$  surface of beryllium because it is a light element (Z = 4), is strongly bonded (i.e., has large vibrational energies), and is known to have 2D surface states. Previous measurements on Be(0001) had already revealed a breakdown in the BOA near the Fermi energy. The group has found a similar breakdown in their comparison of the measured and calcu-



By means of the maximum entropy method, the experimental data was used to extract from  $\text{Re}\Sigma(\epsilon)$  (blue) the Eliashberg function (red)  $\alpha^2 F(\omega)$ , allowing identification of the specific vibrational states that couple to a given electronic state.

lated energy vs momentum for a surface state on  $Be(10\overline{1}0)$ .

Physicists call the difference between the first-principles calculation and the measured curve the real part of the self-energy  $\text{Re}\Sigma(\varepsilon)$ , where  $\varepsilon$  is the energy measured in eV with respect to the Fermi energy  $\varepsilon_{\rm F}$  (Figure 11). The breakthrough in this work occurred when the researchers demonstrated that by means of a procedure called the maximum entropy method, the experimental data could be used to extract from  $\text{Re}\Sigma(\epsilon)$  the spectroscopic function  $\alpha^2 F(\omega)$  (Figure 12). Known as the Eliashberg function, this function is the product of the density (F) of vibrational modes with frequency  $\omega$  at the surface and the coupling constant ( $\alpha^2$ ) of the modes to the electrons. Hence, for the first time, one can see which vibrational modes are important and compare them with experimental and theoretical determinations of the energies and character of the vibrational modes.

In the 1960s, the most definitive signature for determining the mechanism in conventional superconductors was the measurement of the electron-tunneling current–voltage characteristic and the concomitant inversion procedure to display the Eliashberg function. The procedure developed in this work can produce in unprecedented detail a spectroscopic picture of the direction-dependent nature of the coupling between the electrons and the lattice vibrations in anisotropic 2D systems. The researchers are now exploring the application of the maximum entropy method to extract the Eliashberg function from photoemission data on other materials, including high-temperature superconductors.

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#### Polaron Behavior in CMR Manganites: A New Spin on Electrons

Spintronics, or spin-based electronics, is a new technology that manipulates an electron's spin (its orientation up or down), in addition to its charge, to store and transmit information. In 1988, "giant magnetoresistance" (GMR) was discovered, a spintronic effect that used a weak magnetic field to align the spin of electrons, inducing up to a 20% change in a magnetic material's electrical resistance. GMR technology is used in modern computer hard drives for dense data storage that can be read quickly. In the mid-1990s, materials were discovered that allowed magnetic resistance changes several orders of magnitude greater than GMR, and this became known as "colossal magnetoresistance" (CMR). Computers with spintronic memory (magnetic RAM) will be able to store more data in a smaller area, access that data faster, and consume less power than today's semiconductor RAM chips. And, once aligned, the electron spins remain that way until changed by a magnetic field, thus creating an "instant-on" computer that won't require booting up to move hard-drive data into memory.

Spintronic devices manipulate electron spin to sense magnetic fields, store information, or perform logical operations. CMR manganites are a class of materials under study for future spintronic applications such as nonvolatile magnetic computer memory (MRAM). Researchers have recently used several soft x-ray spectroscopies at the ALS to study a prototypical CMR manganite as it was heated past its Curie temperature-the point at which the material ceases to be magnetic. They were able to observe the formation of polarons: electrons whose interaction with the lattice creates a deformation (energy well) that traps the electron, as a pocket on a pool table traps a billiard ball. For the first time, this provided a direct look inside polaron formation in a CMR material, indicating that electron localization as polarons is a defining characteristic of all CMR materials.

CMR manganites are important to spintronics for two reasons. First, they exhibit an extremely large drop in electrical resistance (the CMR effect) when a magnetic field is applied. Second, for some cases, CMR materials conduct electricity via electrons of only one spin (half-metallic ferromagnetism). However, a complete understanding of the charge and spin state of the manganese atoms, crucial to determining and engineering the properties of these materials, is still lacking.

To explain the magnetoconductive properties of these manganites, in which the manganese is present in at least two different valence states (Mn<sup>3+</sup> and Mn<sup>4+</sup>), Zener proposed the mechanism of double exchange (DE). According to DE, the alignment of adjacent localized  $t_{2g}$  spins on manganese atoms rules the dynamics of itinerant  $e_g$  carriers, which hop from one atom to the next to yield electrical conductivity. If adjacent  $t_{2g}$ spins are parallel (the ferromagnetic state), conduction is favored; if they are randomly aligned (the paramagnetic high-temperature state), conductivity drops dramatically.

While Zener's DE model provides a qualitatively correct picture of the CMR effect, theoretical calculations have shown that DE alone is insufficient to account for the observed CMR resistance. An additional consideration is the localization of itinerant e<sub>g</sub> electrons by Jahn-Teller distortions of the octahedral cage of oxygen atoms surrounding each manganese atom.

A Jahn-Teller distortion can take place when an electron hops into an empty  $e_g$  orbital so that, while hopping from site to site, the electron "drags" the lattice distortions after itself. The electron with its accompanying lattice distortion forms a so-called "lattice polaron" (Figure 13). Since the surrounding oxygen atoms are much more massive than the bare electron, the polaron behaves as a negatively charged particle with a larger mass and lower mobility than an isolated electron.

In this study, the temperature-dependent evolution of the electronic and crystal structure of a prototypical CMR compound,  $La_{0.7}Sr_{0.3}MnO_3$  (LSMO), was investigated. Spectroscopic experiments were performed using the multitechnique spectrometer/diffractometer at ALS Beamline 4.0.2. As the LSMO compound was heated through its Curie temperature (T<sub>c</sub>), core photoelectron spectroscopy data provided direct evidence for charge localization onto the manganese atom via a change in the manganese 3s multiplet splitting and for chemical shifts in the core levels of the other atoms in the sample







Left: Manganese 3s photoelectron spectra. The manganese 3s spectrum exhibits a doublet due to multiplet splitting. The energy separation of this doublet depends on the net spin of the manganese atom, providing a direct and element-specific measure of its magnetic moment. The manganese 3s splitting changes markedly as the temperature increases from  $T_c$  to a saturation temperature  $T_{MAX}$ , indicating an increase in the magnetic moment corresponding to the transfer of about one electron to manganese. Right: Oxygen 1s photoelectron spectra. The "bulk" oxygen 1s binding energy shows an increase consistent with charge transfer to manganese. Similar shifts are also found for lanthanum and strontium.

(Figure 14). Valence photoemission spectra also showed parallel changes with temperature. Additional hard-x-ray EXAFS measurements detected the presence of Jahn-Teller lattice distortions in the oxygen octahedra surrounding the manganese atoms as the temperature rose above  $T_{c}$ .

These experiments permitted the detection of polaron formation via its effects on the manganese and other atoms in the LSMO. This challenges the long-standing belief that LSMO is a simple DE system that can be described without the formation of polarons. Therefore, the presence of polarons above  $T_c$  is a general defining characteristic of all CMR materials, bringing unity to their theoretical description. Beyond spintronic applications, these results could also have implications for the magnetic states of atoms under high pressure, as in the Earth's core.

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#### ARPES Provides Direct Evidence of Spin-Wave Coupling

A crystal lattice at the atomic level is far from a static structure frozen in space: atoms and ions vibrate, and electron spins rotate and flip. Such lattice "excitations" can occur randomly, manifesting on the macroscopic scale as heat. They can also occur in coordinated waves, with the excitations rippling through the lattice like spectators doing "The Wave" at a sporting event. In quantum physics, waves are often quantized as particles. Thus, in the quantum world inside a crystal, vibrational waves can be treated as particles known as phonons, and spin waves (where it's the electron spins that are doing the waving) can be treated as particles dubbed "magnons." If the crystal happens to be a conductor, then mobile conduction electrons are added to the mix, and they can become "dressed" by a cloud of lattice perturbations. An electron coupled with its associated magnon forms a quasiparticle of increased effective mass and reduced Fermi velocity. This type of coupling is thought to underlie unusual phenomena of great practical and theoretical interest, such as high-temperature superconductivity.

The electronic properties of a metal are determined by the dynamical behavior of its conduction electrons. However, coupling to further microscopic degrees of freedom can alter the electron dynamics considerably. For example, "conventional" superconductivity emerges as a result of the electrons' interaction with lattice vibrations (phonons). In magnetic materials, coupling with spin waves (magnons) is also expected. Such interactions may contribute to high-temperature superconductivity in novel materials. Unfortunately, lattice vibrations and spin waves have similar energy scales, hindering detailed study. A research team from Germany, Austria, and the ALS has taken a new approach in analyzing the electron bands of ferromagnetic iron. ARPES provides direct spectroscopic evidence of altered electron mass and energy (quasiparticle formation) in a magnetic solid due to coupling with spin waves.

Conventional band theory accounts for the interaction of the electrons with the static ion lattice. However, when conduction electrons interact with excitations in a solid, the electrons become "dressed" by the excitations, forming quasiparticles of increased effective mass. This is reflected in the electron band by a reduction in the slope of the energy-momentum relationship, the slope being inversely proportional to the electron mass. Beyond a characteristic energy scale  $\omega_{0}$ , determined by the excitation spectrum, the electrons lose their dressing (Figure 15). Spin-wave energies in iron are exceptionally high, making it a good candidate for such studies.





The formation of electronic quasiparticles is best studied by ARPES on sharp surface states. The (110) surface of ferromagnetic iron provides such states with the required metallic character. They overlap in energy with bulk bands of opposite spin, thereby enabling spin-flip scattering processes between them. Samples of high purity were generated by evaporating thick iron films onto a tungsten substrate. ARPES was performed at the Electronic Structure Factory endstation on ALS Beamline 7.0.1.

Band-map data provide the basis of the electron energy analysis. In the raw data of the surface state, the dressed quasiparticle





shows up with high intensity, extending beyond 0.1 eV below the Fermi energy,  $E_F$ (Figure 16). A graph of the dispersion (E vs k<sub>II</sub>) of the surface state exhibits a weak "kink" in the region between 0.1 and 0.2 eV below  $E_F$ . An accurate determination of the peak position and width was obtained from a fit of the momentum spectra. A band corresponding to the noninteracting case (no spin-wave coupling) was obtained by parabolic interpolation between the lowest data points and the Fermi-level crossing, making the kink-like deviation more apparent. This "kink" reflects the interaction experienced by the electrons.



**17** Energy range of the interaction experienced by the electrons, as reflected by a broadening of the photoemission spectra for two different surface states,  $S_1$  and  $S_2$ . The observed 160-meV interaction range corresponds well to that of spin waves.

The width of the momentum spectra, also referred to as the imaginary part of the selfenergy,  $Im\Sigma(\varepsilon)$ , reflects scattering processes that become increasingly dominant with increasing (more negative) binding energy. A pronounced increase in the scattering with binding energy saturates at about 160 meV (Figure 17).

The large energy scale of about 160 meV rules out electron-lattice coupling effects, and we are left to consider magnetic excitations. Spin waves (magnons) in ferromagnetic iron are known from inelastic neutron scattering. Both experiment and theory find that, between approximately 100 and 200 meV, there are two magnon branches, one "acoustic" and one "optical," separated by a gap in which sharply defined spin waves do not exist. Assuming that the electrons couple predominantly to the lower, acoustic, branch provides a natural explanation of the observed effect. Independent evidence comes from spin-polarized electron-energyloss spectroscopy on the iron (110) surface. A loss structure at 170-200 meV is interpreted as the result of exchange scattering by spin waves from spin-down surface states into spin-up bulk states, in very good agreement with the ARPES data. The observations confirm fundamentally that mass enhancement seen by ARPES can result from coupling to magnetic excitations, an important prerequisite for models of high-temperature superconductivity.

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### NANO AND MATERIALS SCIENCE

#### Creation of an Antiferromagnetic Exchange Spring

Ferromagnetic metals can be made into permanent magnets through exposure to strong magnetic fields. Only a few metals are ferromagnetic; the most common are iron and its steel alloys (but not stainless steel). You can stick a magnet to the side of your steel refrigerator but not to an aluminum can. Antiferromagnetic materials, such as nickel oxide, are generally not affected by magnetic fields. The read heads in computer hard drives combine thin layers of ferromagnetic and antiferromagnetic materials to make use of their unique properties. An antiferromagnetic layer acts as a magnetic reference to pin, or hold steady, a first ferromagnetic layer. This layer in turn acts as a magnetic reference for a second ferromagnetic layer, which senses the stray field of magnetic domains (or bits) written on a hard disk. Scholl et al. have demonstrated that a novel structure known as an exchange spring forms at the interface between the two layers, a behavior that provides one more clue into the mystery of how the pinning phenomenon works.

In the ongoing quest for faster and more efficient magnetic data storage, devices such as read heads in computer hard drives are mostly produced by trial-and-error combinations of thin magnetic films with different properties. To speed up this search for better materials, researchers are striving for a better understanding of the microscopic structure and interactions between ferromagnet and antiferromagnet layers. Researchers from the ALS, Stanford University, and Italy have now solved a piece of this puzzle using an x-ray magnetometer at the ALS. They proved that antiferromagnets in contact with ferromagnets form an exchange spring system. An exchange spring combines the maneuverability of magnetically soft materials with the permanence of magnetically hard materials.

At the atomic level, ferromagnetic metals such as iron, cobalt, and nickel—consist of electron spins, each of which acts as a small magnet. Moreover, the electron spins are aligned in parallel, giving rise to a macroscopic field that strongly interacts with applied magnetic fields. In antiferromagnets, the spins alternately point in opposite directions, canceling each other to make the antiferromagnet insensitive to applied magnetic fields.

Exchange springs are structures consisting of magnetically hard materials and magnetically soft materials. Magnetically soft materials can be magnetized very easily, but their orientation remains sensitive to magnetic fields. Magnetically hard materials retain their magnetic orientation, even in strong magnetic fields. The ultimate hard-magnetic material is the antiferromagnet, because extremely high fields are required to change its magnetism. The benefit of an exchange spring is that the magnetism of the magnetically soft material is reinforced by the magnetically hard material.

When an antiferromagnet and a ferromagnet are combined in a layered structure—such structures are part of the read heads in computer hard drives—the hard antiferromagnet pins and holds the magnetization of the ferromagnet across the interface in the presence of an applied magnetic field, up to a certain field threshold. This pinning, known as exchange bias, results from atomic exchange forces across ferromagnet–antiferromagnet interfaces, which tend to align the magnetization of nearby atoms.

When a stronger magnetic field above the threshold is applied, abrupt movement of the ferromagnet is expected, leaving the hard antiferromagnet relatively unaffected. In reality, as the recent ALS experiments showed, the behavior is different. In these experiments, the magnetization of the soft layer dragged the magnetization of the antiferromagnet, winding it like a clock spring. The result is the creation of a domain wall between the rotated region at the surface of the sample and the unrotated region below (Figure 1). This behavior is common with ferromagnets but was unknown for antiferromagnets.

The experiments were conducted at ALS Beamline 4.0.2, home of an EPU, comple-



Antiferromagnetic exchange spring. A magnetic field (purple arrow) applied to a ferromagnetic (blue)-antiferromagnetic (green) bilayer rotates the magnetization and creates a domain wall.

mented by measurements at Beamline 7.3.1.1, which houses a photoemission electron microscope (PEEM-2). A recently built octupole magnet allowed rotation of a magnetic field up to one Tesla in any direction in space. The team studied thin cobalt (ferromagnet) layers on nickel oxide (antiferromagnet) single crystals because their magnetic properties are well known.

The researchers measured electron yield spectra of the topmost 5 nm of the antiferromagnet surface, expecting that this region would most strongly show a twisting of the magnetic structure and the formation of a domain wall. The response of the antiferromagnet was recorded using XMLD, a spectroscopic technique that quantitatively measures the angle between the magnetic moments of the antiferromagnet and the linear polarization direction of the x rays (Figure 2).



2 XMLD spectra of NiO demonstrate that a domain wall forms only if the ferromagnet Co is present (blue).

As expected, spectra measured on a pure nickel oxide showed no rotation, because the antiferromagnet alone was unaffected by magnetic fields. However, the cobalt–nickeloxide sample showed a clear rotation of more than 45 degrees when a magnetic field was applied (Figure 3). These results demonstrate that antiferromagnets in contact with ferromagnets form an exchange spring system, which is instrumental in explaining exchange bias and understanding the behavior of this complex magnetic system.

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#### PEEM Images Reveal Hidden Universal Behavior in Magnetic Stripe Domains

It's hard to imagine, but with today's highly sophisticated techniques for fabricating thin films, it is possible to create ultrathin crystals of iron more delicate than a butterfly's wing and that, under the right conditions, display patterns just as intricate. In a process called molecular beam epitaxy, for example, a beam of molecules is deposited, almost atom by atom, onto a substrate consisting of a single crystal, allowing exquisite control over layer thickness, composition, and structure. Although magnetic thin films have been around for many decades, techniques for their fabrication improved remarkably as their importance to the semiconductor and data-storage industries grew. In turn, improvements in fabrication techniques facilitate the discovery of new phenomena that have the potential to revolutionize industry and open up new fields of scientific research. Studies such as the one by Wu et al. are an integral part of this cycle of discovery, exploring the fundamental physics that underlie the technologies of the information age.

Ultrathin magnetic films a few atoms thick occupy a scientific "sweet spot" at the intersection of theory and application. Potentially lucrative as a medium for high-density data storage, such films are also of fundamental interest because of their low dimensionality, enabling scientists to study systems that model 2D magnetic behavior. Nanostructures of several ultrathin magnetic layers can be engineered to explore many interesting phenomena, including the formation of elongated (stripe) magnetization domains (Figure 4). With the ALS's photoemission electron microscope, PEEM-2, researchers from Berkeley and China looked at stripe domains in mag-



Rotation angle of the magnetization at the surface of the antiferromagnet as a

function of the applied field.



Magnetic stripe domains in 2.53-monolayer (ML) iron.

netic sandwiches of cobalt, copper, and iron/nickel. The results revealed a hidden universal dependence of the stripe domain width on variables such as film thickness and external magnetic field.

One issue in magnetic nanostructure research has concerned the presence of long-range order in a 2D magnetic material (for example, spins lined up so as to give rise to ferro- or antiferromagnetism). It has long been established that an isotropic 2D system of spins (a Heisenberg system) does not carry longrange order at nonzero temperature and therefore cannot exhibit magnetic properties—as long as the system is, in fact, isotropic. The magnetic order observed in today's ultrathin films is usually attributed to the existence of magnetic anisotropy—a preferred direction for the magnetic moment.

Magnetic anisotropy arises from two sources: the crystal lattice geometry (magnetocrystalline anisotropy) and the shape of a grain of the material (shape anisotropy). In an ultrathin film, the magnetocrystalline anisotropy dominates, and the magnetization is typically perpendicular to the plane of the film. As the film thickness increases, the competition between the two anisotropies results in a spin reorientation transition (SRT) point where the magnetization flips to lie in the plane of the film.

Because the two magnetic anisotropies cancel each other out at the SRT, a study of the magnetic phase at that point is expected to provide insight into the secret of 2D magnetic



Nanostructure "sandwich" of cobalt, copper, and iron/nickel on a copper (001) substrate. The SRT occurs in the iron/nickel layer. Interlayer coupling with the cobalt layer serves as a virtual magnetic field H tuned by the copper layer thickness.

long-range order. Early experiments showed that the macroscopic magnetization of a thin film breaks into stripes near the SRT, raising many challenging questions about the nature of this phase. Answering these questions requires observation of the magnetic stripes within an external magnetic field. However, such observations are inhibited by the difficulty of operating an electron microscope within a magnetic field. In this experiment, the issue was addressed by using magnetically coupled layers in which the interlayer coupling served as a virtual magnetic field.

A uniform thickness of ferromagnetic cobalt was separated from a wedge of ferromagnetic iron/nickel by a nonmagnetic wedge of copper (Figure 5). The SRT occurs in the iron/ nickel layer, with the magnetic anisotropy tuned by the iron film thickness. The interlayer coupling between the iron and cobalt layers serves as an in-plane virtual magnetic field whose strength is tuned by the copper spacer layer thickness. The experiment was performed using PEEM-2 with circularly polarized light from ALS Beamline 7.3.1.1. Magnetic domain images were obtained by taking the ratio of L<sub>3</sub> and L<sub>2</sub> edges, utilizing the effects of x-ray magnetic circular dichroism (Figure 6). Domain imaging of the iron/nickel layer revealed how the stripe domains change as a function of the magnetic anisotropy (iron film thickness) and the in-plane magnetic field (copper film thickness) (Figure 7).



6 Element-specific domain imaging reveals the stripe domains of the iron/nickel layer within the virtual magnetic field provided by the cobalt layer and the interlayer coupling. The iron/nickel stripe orientation was aligned with the cobalt magnetization.



**7** Stripe domains as a function of the magnetic anisotropy (K) and the magnetic field (H). An analysis of this image reveals a universal dependence of the stripe width on magnetic anisotropy and external magnetic field.

The iron/nickel stripe orientation was aligned with the cobalt in-plane magnetization, and the stripe domain width decreased exponentially with increasing the interlayer coupling between the cobalt and iron/nickel films. To understand the experimental observations, the researchers developed a theoretical model of the ultrathin iron/nickel film on a 2D square lattice, relating the stripe domain width to the interlayer coupling and the perpendicular anisotropy. The results agreed nicely with the experimental data, taking into account the exchange interaction, magnetic anisotropy, dipolar interaction, and magnetic Zeeman energy.

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#### A New Mechanism for Band-Gap Opening in a Triple-Band Peierls System

The phrase "electronic structure" is shorthand for a description of the way electrons behave in solids, liquids, molecules, and atoms. It underlies almost all of the everyday properties of matter from structural strength to electrical conductivity. For example, metals conduct electricity because some of their electrons have access to a continuous band of energies, whereas a break or gap in the band turns the metal into an insulator. As it happens, electronic structure is intimately tied to the atomic structure (where the atoms are), a relationship particularly evident in so-called low-dimensional solids, such as "atomic wires" only a few metal atoms wide, which thus provide a test bed for studying the details of the connection. When the wires are cooled, pairs of neighboring atoms along the length of the wire move a bit closer together, just enough to generate a band gap. Ahn et al. have found that atomic wires made of metallic indium deposited on a silicon surface undergo the expected metal-to-insulator transition, but in a heretofore unobserved way.

A "wire" of indium only one or a few atoms wide grown on a silicon surface constitutes an ideal test laboratory for studying 1D metals. A new example comes from a collaboration between researchers from Yonsei University in Korea, the ALS, and the University of Oregon, who have discovered that the phase transition from metal to insulator that occurs at low temperature in indium wires on the silicon (111) surface involves not only the expected shift in the electronic structure (bandgap opening) but also a band restructuring that gives rise to an energy gap in a second band.

Low-dimensional metals have attracted much attention because of their unique electronic properties, which often lead to exotic physics, including unconventional superconductivity, charge and spin density waves, and violations of the usual rules for interactions of electrons with either other electrons or lattice vibrations and other "excitations" (non-Fermi-liquid behavior). Research on 1D metals has been enriched by the synthesis of quite novel materials, of which carbon nanotubes and metallic atomic wires on surfaces are recent examples.

To make metallic atomic wires, researchers deposit metal atoms on insulating substrates, where the atoms form self-organized 1D atomic chain structures that are often macroscopic in length but truly nanoscopic in width, spanning just one or a few atoms. Successful recent syntheses are the formation of indium wires on a flat silicon (111) surface [the Si(111)4×1-In surface] and gold wires on a series of regularly stepped (vicinal) silicon surfaces [Au/Si(557), Au/Si(5512), and Au/Si(553)].

These atomic wires have well-defined 1D metallic electronic structures, commonly with one or more bands that are partially filled by electrons at energies up to the Fermi energy  $E_F$  and with nearly ideal band dispersions (continuous dependence of electron energy on momentum k). Moreover, metal-insulator transitions occur at transition temperatures ranging from about 100 to 300 K in which the

continuous bands are broken by an energy gap around  $E_F$ . Since they are accompanied by lattice-period-doubling lattice distortions, the transitions are assumed to be due to the Peierls instability that is inherent in a 1D metal, especially one with a half-filled band (Figure 8).

The Korean–American collaboration made its measurements of indium wires on silicon with the soft x-ray angle-resolved photoemission endstation (the Electronic Structure Factory) at Beamline 7.0.1, which provides unprecedented flexibility in collecting data in a large volume of the Brillouin zone (unit cell in momentum space) over a wide temperature range and in preparing samples in situ, two features that were crucial in the present study. The indium wires have three metallic bands, one of which is half filled while the others are less than half filled.

The team found that in the insulating state below 125 K, the expected band-gap opening of the half-filled band was accompanied



Atomic structure models of indium wires four rows wide running from left to right on silicon. Top: The metallic 4×1 phase. Bottom: The perioddoubled 4×2 insulating phase. The arrows indicate the major displacements of the indium atoms at low temperature.

by a restructuring in which the band with the smallest filling disappeared, owing to an interband interaction in which the electrons of the disappearing band transferred into the third band, which became half filled (Figure 9). Thus, the ground-state band structure consisted of two bands with energy gaps at the same momentum  $k_F$ , a condition giving an energy advantage to the period-doubling lattice distortion associated with a charge-density wave and a Fermi surface "nesting" vector  $q_{CDW} = 2k_F$  (Figure 10). Only the originally half-filled band exhibited nearly ideal 1D behavior, while some 2D (quasi-1D) behavior characterized the others (Figure 11).

The researchers believe that this first-ever observation of the band restructuring due to a strong interband interaction introduces a new gap-opening mechanism in a multiband metal. The physical origin of the direct interband charge transfer needs to be clarified but may be related to the complex interactions of the lattice with defects and with the complex multiple 1D bands with varying band fillings.



The measured energy bands of indium atomic wires in the metallic state (left) and in the insulating state at 45 K (right). The shallow  $m_2$  gap is 40–80 meV, and the deep  $m_3$  gap is 160 meV. Bands are indicated by bright regions of higher photoemission intensity. Binding energy is the energy relative to the Fermi energy ( $E_F - E$ ).



Schematic drawings of the triple bands in the metallic state with the nesting vector  $q_{CDW}$  (left) and the insulating state (right). In the metallic state,  $m_3$  (black) is the half-filled band. In the insulating state, electrons in  $m_1$  (green) transfer to  $m_2$  (blue), which becomes half filled. The two energy gaps are indicated by the bands turning down before they reach the Fermi energy  $E_F$ .



At four atoms wide, the wires are not perfectly 1D, so electrons can have a momentum component perpendicular to the wire  $(k_{\perp})$  as well as parallel  $(k_{\parallel})$ , and the energy band dispersion  $E(k_{\parallel})$  can be different for each  $k_{\perp}$  (quasi-1D). Photoemission intensity maps over the 2D momentum space defined by  $k_{\perp}$  and  $k_{\parallel}$  taken at a constant energy show band contours. The wiggling contours at the Fermi energy (binding energy = 0) for the metallic phase (left) and at 0.1 eV below the Fermi energy for insulating phase (right) demonstrate the deviation of  $m_1$  (green) and  $m_2$  (blue) from the nearly ideal 1D nature exhibited by  $m_3$  (black).

INVESTIGATORS J.R. Ahn, J.H. Byun, and H.W. Yeom (Yonsei University, Korea); H. Koh (Yonsei University, Korea, and ALS); E. Rotenberg (ALS); and S.D. Kevan (University of Oregon). **FUNDING** Ministry of Science and Technology of Korea through the Creative Research Initiative Program and U.S. Department of Energy, Office of Basic Energy Sciences. PUBLICATIONS J.R. Ahn, J.H. Byun, H. Koh, E. Rotenberg, S.D. Kevan, and H.W. Yeom, "Mechanism of gap opening in a triple-band Peierls system: In atomic wires on Si," *Phys. Rev. Lett.* **93**, 106401 (2004).

#### Twinning and Shear Stress in YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7-x</sub> High-T<sub>c</sub> Superconductor Thin Films

While solid-state physicists, both on the experimental and theoretical sides, are struggling to come up with a model that explains how "high-temperature" superconductors can carry electrical current without resistance at much higher temperatures than previous metallic superconductors, materials scientists are busy trying to make these superconductors in practical forms that can be used in applications, such as electrical power lines and magnets for MRI machines. The theory, when it comes, may not be of much direct help, because "real-world" superconductors (conventional or high-temperature) are complex, heterogeneous materials with compositional variations and structural features that are deliberately added to increase performance or deliberately removed to avoid degraded performance. Boundaries between domains or regions of the superconductor with different crystallographic orientations are a case in point. Depending on the type of boundary, they can be good or bad. Caldwell et al. have demonstrated for the first time that the strain near a type of boundary called a twin domain boundary can play a beneficial role.

High-T<sub>c</sub> superconductors, such as YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7.x</sub> (YBCO), develop crystallographic twins during processing, and magnetic hysteresis experiments on both twinned and untwinned samples show that the boundaries between twins could be effective vortex pinning centers. "Flux pinning" is highly desirable in superconductors because the motion of vortices produces a pseudo-resistance that degrades the material superconducting performance. To investigate the cause of pinning, an ALS-Stanford team has used the whitebeam x-ray microdiffraction facility on ALS Beamline 7.3.3 to study the microstructure of a YBCO thin film. Their work suggests that the intrinsic strain field associated with twin boundaries plays a significant role.

Microstructural characteristics (grain size, grain shape, grain crystallographic orientation, type of grain boundaries, distribution of local strains and stresses, precipitates, variation in chemical composition, defects, etc.) often have marked effects on a material's mechanical, electrical, magnetic, or optical properties. In YBCO, for example, it is known that, in contrast to the possibly beneficial influence of low-angle twin boundaries, largeangle grain boundaries are responsible for a dramatic decrease in critical current densities, which makes it important to develop techniques for making highly textured samples with fewer such boundaries. Quantitative measurements of parameters such as strain and stress across grain boundaries and microtexture are therefore of primary importance in designing performance-enhanced materials.

The ALS–Stanford team studied the microstructure of a 260-nm-thick YBCO thin film that was epitaxially grown with its c-axis normal to a  $SrTiO_3$  substrate. A significant advantage of the white-beam x-ray microdif-fraction technique, compared to other techniques such as reciprocal-space mapping, is its ability to completely characterize the reciprocal-space lattice with a single exposure on the order of 10 seconds. Moreover, the short exposure time and the submicron size of the beam allows for effective and rapid mapping of the microstructure of the sample by "scanning" it under the beam with a step size on the order of the size of the beam.

For YBCO, the researchers found that a single Laue pattern obtained with a CCD x-ray

detector in reflective geometry indicated that the film consists of a mixture of four uniquely oriented twin lattices due to the accommodation of the tetragonal-to-orthorhombic phase transition during post-growth cooling (Figures 12 and 13). Twins appear to be mirror images of each other across a twin boundary. Twinning in YBCO takes place across the basal diagonals of the orthorhombic unit cell and occurs in domains consisting of pairs of orientations that share the same basal diagonal twin plane.

The analysis of the Laue diffraction patterns taken at each step not only provides the relative proportions of the twin sets but also the local strain by measuring the deviation of the reflection positions on the CCD with respect to its calculated "unstrained" positions. Stress is calculated from the measured strain using the elastic constants of the material. The result is a high-spatial-resolution map of the twin domain distribution and of the strain and stress.

The measurements show that the partitioning of the film into twin domains is clearly correlated with the distribution of in-plane shear strain. The interiors of twin domains are rel-





Reciprocal-space lattice decorated by the four {110} twins, each in a different color. The average tetragonal reciprocal lattice is shown by the dashed frame.

Reciprocal-space projection of the (hk13) layer reflections of the diffraction pattern. Each box spans 0.02  $Å^{-1}$  on a side. Also shown is an angular profile through the ( $\bar{2}$ 013) reflection along the path indicated by the dashed white line. The data were reconstructed from a single 10-s-exposure white-beam diffraction pattern obtained with a large-area CCD x-ray detector.

atively strain free, because they consist of twins with orientations sharing coherent lattice boundaries. On the other hand, the data show that shear stresses can exceed 100 MPa at the interfaces between two different twin domains.

This work provides the first direct experimental measurement of the intrinsic strain field associated with twin domain boundaries. The inplane shear strain is a measure of the distortion of the YBCO basal plane containing the copper-oxygen sublattice where superconductivity is believed to occur. The deviation of the lattice from its equilibrium configuration at domain boundaries indicates that these regions are the most prone to revert to a nonsuperconducting state and preferentially trap magnetic flux. The interaction of such strain fields with flux lines is likely to be significant for flux pinning. INVESTIGATORS W.C. Caldwell, N. Tamura, R.S. Celestre, A.A. MacDowell, and H.A. Padmore (ALS); T.H. Geballe and G. Köster (Stanford University); and B.W. Batterman and J.R. Patel (ALS and Stanford Synchrotron Research Laboratory).

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#### Picosecond Magnetization Dynamics by Time-Resolved X-PEEM

Any desktop or laptop computer user knows how fast the storage capacity of hard disks is growing. The storage density now doubles every 12 months, significantly faster than semiconductor memory, which, according to the famous Moore's law, doubles every 18 months. During the last decade, the data rate, which limits the speed of a disk drive, also increased 20-fold. To maintain this pace, we require new tools to study magnetic materials in smaller areas and over shorter times. A type of x-ray microscope known as a PEEM can image the nanometer-sized magnetic bits on hard disks, thereby allowing examination of both the basic properties of magnetic media and the data-reading and -writing processes. Choe et al. have applied a new strobe-like PEEM technique to take snapshots of rapidly moving magnetic vortices, peculiar magnetic structures that appear in micrometer-size magnetic patterns. PEEM images that resolve the motion of the vortex core in response to a magnetic-field pulse provide clues to the mechanism driving the motion on very short time scales.

The data rate in modern disk drives will soon surpass 1 GHz. Subnanosecond magneticfield pulses like those of a write head initiate magnetization precession, a gyroscopic motion of the magnetization around an applied field (like a wobbling top). An ALS-Stanford-Berlin group has used a new time-resolved x-ray photoemission imaging technique to resolve the motion of magnetic vortices, peculiar magnetic structures that appear in micron-size magnetic patterns, in response to an excitation field pulse. Analysis of the observed gyrating trajectory of the core on such short time scales suggests that the precession is induced by a handedness, or chirality, in the magnetization pattern, thereby demonstrating that handedness plays an important role in the dynamics of microscopic magnets.

For data-storage purposes, magnetic vortices can be trapped in lithographically defined rectangular or circular magnetic patterns. They are of considerable technological interest because a low stray magnetic field leads to a magnetic stability and minimizes the crosstalk between adjacent vortices-two prerequisites for high storage densities. At low frequencies, magnetic friction (damping) governs the response as the magnetic moments rotate into the direction of an applied field. But at gigahertz frequencies and above, precession is the dominant process. For the microscopic study of such ultrafast magnetization dynamics, the collaborators developed a novel technique based on the 70-ps-long xray pulses of the ALS, which can be used like light flashes from a strobe to freeze the dynamics and to acquire a snapshot of the motion of the magnetization.







Top: Domain structure of magnetic vortices showing the directions of the magnetization (white arrows), the vortex handedness (hands), and the out-of-plane core magnetization (thumb direction and green arrows). Bottom: Simulated trajectories of left- and right-handed vortices. Red arrows are the vortex acceleration directions.


Top: Time-resolved PEEM images of left-handed  $1 \times 1 \ \mu m^2$  (I), left- and right-handed  $1.5 \times 1 \ \mu m^2$  (II and III), and left-handed  $2 \times 1 \ \mu m^2$  (IV) vortex patterns at various delay times after the driving field pulse. Bottom: The trajectories of the gyrating vortex cores at 100-ps intervals over 8 ns after the field pulse. Red stars correspond to the times indicated in the PEEM images.

In this experiment at ALS Beamline 7.3.1.1, a light flash from a laser activates a gallium arsenide photo switch, which is integrated into the sample, and launches a 300-ps-long electrical current pulse into a waveguide optimized for the transmission of short pulses. The current pulse generates a powerful magnetic field pulse that initiates the dynamics. After a controllable time delay, an x-ray pulse illuminates the sample, resulting in a photoelectron image that is then magnified a thousandfold by the optics of a photoemission electron microscope (Figure 14). A CCD camera accumulates the signal from millions of x-ray pulses until an image of sufficient quality characterizing the current state of the magnetization of the sample has been obtained.

About 40 magnetic structures of different sizes and shapes were patterned by focused ion-beam lithography into a 20-nm-thick, magnetically soft cobalt-iron alloy film on a copper waveguide. Four triangular magnetic domains meeting in the center of a structure give rise to a vortex where the domain walls intersect, so that the magnetization curls around the vortex center or core (Figure 15). XMCD at transition-metal L edges probes the direction and size of the element-specific magnetic moments within the domains. For the cobalt-iron samples, the researchers computed the images at 100-ps intervals over several nanoseconds as the ratio of two PEEM images acquired at the cobalt L<sub>3</sub> and L<sub>2</sub> absorption edges.

In this way, they observed two phases of vortex dynamics: an initial linear acceleration in response to the field pulse, followed by a gyrotropic (spiraling) motion of the vortex core around the pattern center (Figure 16). A "hidden" out-of-plane magnetization in the nanometer-scale vortex core induces a 3D handedness in the planar magnetic structure. The result is a precessional motion of the core parallel to the subnanosecond inplane field pulse. The displacement of the core causes an imbalance of the in-plane magnetization within the structure, creating a magnetostatic field perpendicular to the displacement that drives the vortex on a spiraling trajectory. The observed gyrotropic motion corresponds to a subgigahertz mode seen in micromagnetic simulations and recent magneto-optical experiments.

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# ENVIRONMENTAL AND EARTH SCIENCE

### Energetics of Hydrogen Bond Network Rearrangements in Liquid Water

For many of us, the main question about liquid water is whether to drink it straight from the tap or filter it first. However, water remains a focus of scientific research because some of its basic features, such as the weak (hydrogen) bonding between water molecules, that give it unique physical and chemical properties have yet to be nailed down. Consider the structure of the liquid, which is often visualized as a kind of floppy ice consisting of a 3D network of water molecules, each of which is hydrogen bonded to four neighbors. Previously, a group combining theory and experimental measurements proposed that liquid water actually has only about 50 percent as many chemical bonds as solid ice, resulting in a mixture of rings and chains rather than a network. However, Smith et al. have now presented new x-ray data for water from a novel liquid microjet apparatus that allowed them to determine the energy needed to break a bond and that supports the traditional model. The debate continues.

The unique chemical and physical properties of liquid water are thought to result from its highly directional hydrogen bonding (H-bonding) network structure and its associated dynamics. However, despite intense experimental and theoretical scrutiny, a complete description of this structure has been elusive. Recently, with the help of their novel liquid microjet apparatus, a UC Berkeley group derived a new energy criterion for H-bonds based on experimental data. With this new criterion based on analysis of the temperature dependence of the x-ray absorption spectra of normal and supercooled liquid water, they concluded that the traditional structural model of water is valid.

The standard description of water structure consists of a random tetrahedral network in which every molecule is H-bonded to its four nearest neighbors, an arrangement similar to that in hexagonal ice. In recent years, a number of XAS and related experiments have begun to characterize the H-bond structure in detail by assigning the observed spectral features to specific H-bonding configurations. However, in order for such an analysis to yield a quantitative description of the H-bond structure, it is necessary to establish an experimental definition of what actually constitutes an H-bond, or in other words, what degree of distortion of the H-bond network leads to a measurable change in the XAS.

Previously, only a geometric criterion had been established, which was derived by density functional theory calculations of a model cluster [P. Wernet et al., *Science* **304**, 995 (2004)]. Applying their theoretical H-bonding criterion to their x-ray Raman measurements, the authors had to invoke a picture of a liquid composed of monocyclic rings and linear chains—radically different from a tetrahedral network—to obtain agreement with theoretical calculations.

This latest experiment begins with injection of a small liquid microjet (10–30  $\mu$ m in diameter) into a high-vacuum chamber (Figure 1). The small size of the volatile sample makes it possible to maintain a relatively good vacuum (10<sup>-5</sup> Torr), which enables windowless coupling to both Beamlines 8.0.1 and 11.0.2. Furthermore, such low pressures allow for efficient transport of electrons generated by the x-ray absorption process away from the jet surface to a detector placed about 1 mm away from the interaction region.



A liquid microjet about 30  $\mu$ m in diameter. The nozzle is formed from a fused silica capillary with an inside diameter of 100  $\mu$ m, which is elongated by means of a commercial CO<sub>2</sub> laser pipette puller in order to obtain the final nozzle diameter.



2 Comparison of the total electron yield x-ray absorption spectra taken at two temperatures. The solid black curve was recorded at 288 K and the gray curve at 254 K.

The Berkeley group measured x-ray absorption by the total electron yield method. To obtain the temperature dependence, they recorded successive total electron yield spectra as a function of distance from the liquid jet nozzle. The microjet undergoes rapid evaporative cooling upon injection into the high-vacuum chamber, and therefore the liquid jet temperature continually decreases with distance away from the nozzle. The cooling rate had been thoroughly characterized in previous experiments by the group.

Upon cooling, a sizeable decrease in the preedge intensity, an XAS spectral feature previously assigned to broken or distorted hydrogen bonding configurations in water, was observed. A simultaneous increase in the post-edge intensity, a spectral feature assigned to highly symmetric ice-like configurations, was also observed (Figure 2). A plot of the logarithm of the ratio of peak areas ( $I_{post-edge}/I_{pre-edge}$ ) vs inverse temperature should be linear with a slope proportional to the energy difference between the two configurations (distorted and ice-like). From its temperature dependence measurements, the group found the difference in energy to be  $1.5 \pm 0.5$  kcal/mol (Figure 3). This is the experimentally derived energetic hydrogen bond criterion.

By this experimental criterion, the x-ray Raman measurements reported by Wernet et al. are consistent with the "standard model" for water after all. The Berkeley group would like to study the nature of the transition from the symmetric ice-like structure to the distorted structure described above via molecular dynamics simulations.



<sup>3</sup> Plots of the log of the ratio of the areas of the post-edge and pre-edge features versus inverse temperature from three separate experiments. The error bars represent twice the standard deviation in the Gaussian fits to the peaks. The solid lines represent the linear fit with a slope of  $\Delta E/R$ , where  $\Delta E$  is the difference in energy between the two different H-bonding distributions and R is the gas constant. The energy difference is determined to be 1.5  $\pm$  0.5 kcal/mol. Although each experiment is self-consistent, changes in the collection geometry, beamline calibration, and baseline cause variations in the measured slope and intercept of the fitted line. Therefore, the  $\Delta E$  reported here is the average of the three independent measurements shown, with the associated standard deviation.

INVESTIGATORS J.D. Smith, C.D. Cappa, B.M. Messer, R.C. Cohen, and R.J. Saykally (UC Berkeley and Berkeley Lab) and K.R. Wilson (Berkeley Lab).

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### Composition and Reactions of Atmospheric Aerosol Particles

Most people equate aerosols with hairspray and household cleaning products, but a large portion of the microscopic particles floating in the air actually originate from the incomplete burning of coal and oil and dust storms. According to mathematical models of the Earth's climate, if the particles remain airborne long enough, they can contribute to both atmospheric heating and cooling. In effect, the longer they linger, the more time they have to wreak havoc on Earth's climate. By means of high-resolution x-ray microscopy of particles collected at several locations around the world, Maria et al. have determined that carbon-containing aerosol particles oxidize more slowly than earlier estimates indicated. Since oxidized aerosols fall relatively rapidly back to the earth in rain, the slower oxidation buys them more time to do their atmospheric damage. These longer-lived particles will increase the carbon-containing aerosol burden on climate models by up to 70 percent.

Microscopic aerosol particles in the atmosphere contain carbonaceous components from mineral dust and combustion emissions released from around the world. How long these tiny particles remain in the atmosphere can have a huge impact on the global climate. Measurements based on high-resolution scanning transmission x-ray images obtained at the ALS have revealed chemical reactions on and in atmospheric aerosol particles that caused particle growth while changing organic composition by 13 to 24% per day, an oxidation rate significantly slower than is currently used in atmospheric models. Since oxidation has a strong effect on particle lifetime in the atmosphere, these results will help climate scientists refine the computer models used to predict climate change.

A large portion of the microscopic particles floating in the air originate from incomplete combustion of coal and oil and from dust storms. Once in the atmosphere, they can have either cooling or warming effects. Lighter-colored organic carbon particles cool regions of the planet by scattering sunlight back into space. Other aerosol particles composed of black carbon, or soot, warm the atmosphere by absorbing sunlight and heating the surrounding air. Impacts like these are why scientists want to know how long carbon-containing aerosols remain in the atmosphere.

One way to gauge an aerosol's ability to stay aloft is to determine its oxidation rate. Because oxidized aerosols absorb moisture and subsequently form clouds and fall as rain, the faster an aerosol particle oxidizes, the less time it spends in the atmosphere,



4 Source type and mechanism information for the four aerosol samples gathered from the Caribbean, the Sea of Japan, and New Jersey.

and the less impact it has on the climate. Hoping to learn more about aerosol particle oxidation rates and confident that measurements of aerosol particle composition could reveal signatures of atmospheric chemical reactions, such as oxidation, a multi-institutional collaboration based at UC San Diego examined a variety of carbon-containing aerosol particles that had undergone vastly different journeys.

Aerosol particles for STXM analysis were collected on silicon nitride substrates by impaction on the National Center for Atmospheric Research's C-130Q aircraft over the Caribbean Sea in July 2000 and over the Sea of Japan in April 2001. The sources of the particles collected were determined to be African mineral dust and Asian combustion, respectively (Figure 4). Additional aerosol samples representing eastern U.S. combustion were collected on lacey-carbon transmission electron microscopy grids in New Jersey in August 2003 on both clear and foggy days. In all, more than 120 particles were analyzed as part of eight samples from the Caribbean Sea, eastern Asia, and New Jersey.

The group carried out STXM measurements near the carbon absorption K edge at ALS



Images, speciated maps of detectable regions, and representative spectra of measured organic and inorganic species for marine boundary layer particles near St. Croix in the Caribbean. High-resolution soft x-ray images (a,e,i) show (a) an absorbance image at 300 eV for particles collected at 310 m and (e,i) images at 289.9 eV for particles at 30 m. Threshold contours (b,f,j) at the detection limits are drawn for the same three samples:  $R(C=C)R_0$  (purple) (285.0 ± 0.2 eV), R(C=0)R (cyan) (286.7 ± 0.2 eV), R(C=0)H (green) (288.7 ± 0.3 eV),  $\sigma^*$  transition for CNH (orange) (289.5 ± 0.1 eV),  $CO_3^{2-}$  (yellow) (290.4 ± 0.2 eV), K+ (red) (294.6, 297.2 ± 0.2 eV), and Ca<sup>2+</sup> (magenta) (347.9, 351.4 ± 0.4 eV). Enlarged maps (c,g,k) and spectra (d,h,l) for representative particles labeled (i–vi) illustrate detailed composition characteristics for each sample.

Beamlines 7.0.1 and 5.3.2 in a helium-filled sample chamber maintained at 1 atmosphere. X-ray transmission images, typically spanning an area of 64 µm<sup>2</sup>, were scanned sequentially at increasing photon energies in the range 279–305 eV to create a stack of images from which a spectrum could be extracted at each point (Figure 5). The jump in the carbon K-edge absorbance (namely the difference above and below the absorption edge), which is linearly related to the number of absorbing atoms, was used as a semi-quantitative measure of total carbon, with absorbance below the carbon edge

quantifying total mass. In this way, maps of carbon and total mass were constructed (Figure 6).

These measurements revealed surface- and volume-limited chemical reactions on and in atmospheric aerosol particles. The observed much slower oxidation rates mean that organic aerosols will reflect more radiation because of increased atmospheric lifetimes, producing a 70% increase of the organic aerosol burden. These changes in organic aerosol burden will change the radiation balance of the atmosphere, increasing cooling

by as much as 47%, while also causing offsetting warming changes of up to 61%.

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**FUNDING** National Science Foundation, James S. McDonnell Foundation, and U.S. Department of Energy, Office of Basic Energy Sciences.



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L.M. Russell, S.F. Maria, and S. Myneni, "Mapping organic coatings on atmospheric particles," *Geophys. Res. Lett.* **29**, 10.1029/2002GL014874 (2002).

**6** Two-dimensional spectrally resolved maps of organic composition for particles representative of four aerosol samples. The colors in the left column represent various ratios of total carbon to total mass; the colors in the right column represent various ratios of carbonyl carbon to total carbon.

### Primitive Origins of Organic Matter in Interplanetary Dust

They are not among NASA's most glamorous missions. They don't normally make headlines unless something goes spectacularly awry, as with the recent crash of the Genesis capsule in the Nevada desert. Genesis' mission was to collect particles thrown off by the sun in what's called the solar wind. A related mission, dubbed Stardust, was launched in 1999 to collect dust particles from the comet Wild 2. Benavente, the dust particle studied here by Floss et al., was collected closer to home, in the Earth's stratosphere, by high-flying aircraft. NASA has been collecting dust particles from the stratosphere since the 1970s, but their small size makes chemical and petrographic analysis challenging. With new and improved analytical techniques, scientists can extract from the grains of dust a "geological" record, not of the Earth, but of the solar system. By studying the components of the dust particles, specifically their isotopic content, we can gain knowledge, not only about the age of a sample, but about the physical conditions under which it formed in the dusty, distant past.

Carbonaceous (carbon-containing) dust particles are complex assemblages of primitive interplanetary material left over from the formation of the solar system (Figure 7). One such interplanetary dust particle (IDP), collected by NASA from Earth's stratosphere and nicknamed "Benavente," was analyzed by researchers from Washington University and LLNL by a variety of techniques, including synchrotron infrared spectroscopy at the ALS. The measurements revealed, for the first time in an IDP, an isotopically anomalous region that is both depleted in carbon-13 and enriched in nitrogen-15 and also located in a host phase that is organic in nature. These isotopic anomalies provide valuable clues to the history of the particle and, by extrapolation, the solar system.

Since long before life appeared on Earth, a constant flux of carbonaceous dust has rained down from the sky, at times accreting as much as a centimeter deep over the Earth's surface every million years. In the Milky Way galaxy, interstellar molecular

clouds are the principal formation sites of organic matter—that is, molecules based on carbon and hydrogen, where the carbon is arranged in chains (aliphatic hydrocarbons) or rings (aromatic hydrocarbons). Isotopic anomalies provide a fingerprint for tracing how abiotic interstellar organic matter was incorporated into the solar system. Organic molecules formed in cold, dense interstellar clouds will have isotopic ratios that differ from those formed in the relative warmth of the solar system, because the pathways for mass fractionation (which determines isotopic composition) depend on physical or chemical conditions.

A "heavy" isotope's greater mass results in slightly different chemical bonding characteristics. These differences become significant at low temperatures, when the difference in the binding energy between isotopes exceeds thermal energy. Past measurements of IDPs have found high levels of deuterium (heavy hydrogen) and nitrogen-15, consistent with origins in low-temperature interstellar clouds. Because these anomalies are associated with carbonaceous material, the lack of similar anomalies in carbon has been a major conundrum.

Using a new technique called NanoSIMS that allows isotopic imaging down to 100 nm, the researchers looked for carbon and nitrogen isotopes simultaneously. They noted that one region of the IDP Benavente, about  $0.5 \times 2$  $\mu$ m<sup>2</sup> in size, was strongly enriched in nitrogen-15 and depleted in carbon-13 relative to terrestrial isotopic compositions, the first observation of correlated nitrogen and carbon isotopic anomalies in an IDP (Figure 8). Transmission electron microscopy of this material at LLNL showed that the region is rich in glass with embedded metal and sulfides and amorphous carbonaceous material.

Infrared spectra of the carbonaceous material taken at ALS Beamline 1.4 showed a prominent absorption feature at a wavelength of 3.4 µm, corresponding to the stretching mode of the carbon–hydrogen (C–H) bond



Electron microscope image of an interplanetary dust particle collected in the stratosphere.





8 NanoSIMS images of the dust particle, showing a region of nitrogen-15 enrichment (left) associated with carbon-13 depletion (right).

(Figure 9). The positions of the bands within the feature are consistent with those of aliphatic hydrocarbons, confirming the organic nature of the carbonaceous material. Aromatic hydrocarbons are likely to be present too, but are probably dominated by the strong resonance of the C-H feature.

In the absence of carbon isotopic anomalies, it was previously not possible to determine whether the carbonaceous material was itself presolar or simply a relatively



Infrared spectrum of a section of the dust particle, showing the C-H stretch feature at 3.4 µm indicative of the presence of aliphatic hydrocarbons.

recent solar-system host substrate for the anomalous deuterium and nitrogen-15 species commonly found in IDPs. Now, the observation of correlated carbon and nitrogen anomalies establishes that IDPs indeed contain heteroatomic organic compounds of presolar interstellar origin: the material took organic form before the solar system existed and was then incorporated into the IDP. Theoretical models indicate that low-temperature formation of organic molecules in cold molecular clouds can produce C and N fractionations through gas-phase ion-molecule reactions. However, additional studies are required to determine whether processes exist that can produce both effects in the same material.

**INVESTIGATORS** C. Floss and F.J. Stadermann (Washington University) and J. Bradley, Z.R. Dai, S. Bajt, and G. Graham (Lawrence Livermore National Laboratory).

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## STRUCTURAL BIOLOGY

### 1.35-Å Structure Shows How the Membrane Protein AmtB Transports Ammonia

Like any factory, a biological cell takes in raw materials and energy and expels waste products. What goes in and out passes through the cell membrane that surrounds the cell's interior via channels and transporters that serve as carefully guarded entry and exit ports. Determining the mechanisms by which the membrane proteins accomplish these roles is a major challenge among life scientists. By means of x-ray crystallography, Khademi et al. have determined the first atomic structure of a channel that passes ammonia gas molecules through the bacterial cell membrane of *E. coli*. The structure allowed them to deduce how ammonia makes the transit without requiring an energy source to drive the process and without altering the electrical potential (voltage) that exists across the membrane. Since this membrane protein is related to similar ones in higher organisms, including the Rh factors in humans, the mechanism they deduced has broad implications for "gas channels" in general.

Membrane proteins provide molecular-sized entry and exit portals for the various substances that pass into and out of cells. While life scientists have solved the structures of protein channels for ions, uncharged solutes, and even water, up to now they have only been able to guess at the precise mechanisms by which gases (such as NH<sub>3</sub>, CO<sub>2</sub>, O<sub>2</sub>, NO, N<sub>2</sub>O, etc.) cross biological membranes. But, with the first high-resolution structure of a bacterial ammonia transporter (AmtB), determined by a team in the Stroud group from UC San Francisco, it is now known that this family of transporters conducts ammonia by stripping off the proton from the ammonium (NH $_4^+$ ) cation and conducting the uncharged NH $_3$  "gas."

Progress in determining structures of membrane proteins of all kinds has been slowed by the difficulty of obtaining sufficiently robust crystals that diffract to high resolution. A common strategy is to grow crystals of proteins from multiple organisms in which the protein is known to have evolved from a common ancestor (orthologs) and select the one that gives the best diffraction data. The UC San Francisco researchers cloned multiple orthologs of the integral membrane protein AmtB belonging to the Amt/MEP/Rh superfamily. To define any preferred sites for ammonia or methyl ammonia  $(CH_3NH_2)$  and to clarify the mechanism for transport or conductance of these molecules, crystals were grown in the absence of any ammonium derivative and in the presence of ammonium sulfate or methyl ammonium sulfate.

Diffraction data from crystals of AmtB from the bacterium *Escherichia coli* were collected at ALS Beamline 8.3.1 with a CCD area detector. Phases were calculated from MAD data from a selenomethionine (SeMet)-substituted protein. After data processing (solvent flattening and phase extension to 2.0 Å), the



Ribbon representation of the AmtB trimer is viewed from the extracellular side. Each monomer contains a channel that conducts ammonia. Three  $NH_3$  molecules (blue) are in each channel, while  $NH_4^+$  ions (orange) remain near the channel entrance.



A stereo view of the monomeric ammonia channel viewed down the quasi-twofold axis. Corresponding related helices are shown in the same color. The extracellular side is uppermost. The brown rectangle represents the inferred position of the hydrophobic portion of the bilayer. Three  $NH_3$  molecules seen only when crystallized in the presence of ammonium sulfate are shown as blue spheres. The orange sphere represents an  $NH_4^+$  ion at the vestibule.

model was refined to 1.35 Å, the highestresolution structure of any membrane protein to date.

Overall, the structure shows that AmtB is a trimer, with each monomer containing a channel conducting ammonia (Figure 1). The monomer protein chain includes two structurally similar motifs of opposite polarity. Each motif spans the cell membrane between the periplasm (region between the cell wall and the membrane) and the cytoplasm (cell interior) five times (Figure 2).

Comparison of the structures with and without ammonia and with methyl ammonia enabled the team to identify a wider vestibule site at the periplasmic side of the membrane that recruits  $NH_4^+$  and a narrower 20-Å-long hydrophobic channel midway through the membrane that lowers the dissociation constant of NH4+, thereby forming NH3, which is then stabilized by interactions with two conserved histidine side chains inside the channel. In a second vestibule at the cytoplasmic end of the channel, the NH<sub>3</sub> returns to equilibrium as  $NH_4^+$  (Figure 3). An ammonia conduction assay was devised using stopped-flow kinetics and, together with the structural result, proved that it is only neutral NH<sub>3</sub> that is conducted by the channel. This is the first time that the structure and mechanism of a "gas channel" has been determined.

Conductance of uncharged NH<sub>3</sub>, versus the NH<sub>4</sub><sup>+</sup> ion, solves several biological problems. Transport of only uncharged NH<sub>3</sub> assures selectivity against all ions. NH<sub>4</sub><sup>+</sup> or any other ion would be unstable in the center of the hydrophobic bilayer, while NH<sub>3</sub> is not. Passage of uncharged NH<sub>3</sub> would not result in a net change of protons across the membrane nor would it change the membrane potential, thus neither energy nor any negative counter ion to balance the charge is needed to accumulate ammonia.

The structure of AmtB and the mechanism of gas transport are common to other members of the superfamily in eukaryotic cells. For example, related Rh proteins in humans



Summary of mechanism of conductance. Two vestibules reside at the top and bottom of the channel. Amino acid residues (blue, red, and gray ball-and-stick models) that line the pore of the outer vestibule stabilize  $NH_{4^+}$  (green and yellow). After a proton (orange) departs, the channel narrows midway through the membrane for a 20-Å distance and is hydrophobic. Here, two pore-lining histidine residues (light and dark blue) stabilize three  $NH_3$  molecules through hydrogen bonding. Farther on, with the addition of a proton (orange), the molecules return to equilibrium as  $NH_{4^+}$  in the inner vestibule.

are thought to be critical players in systemic pH regulation in the kidney, in amino acid biosynthesis, and in the central nervous system.

INVESTIGATORS S. Khademi, J. O'Connell III, J. Remis, Y. Robles-Colmenares, L.J.W. Miercke, and R.M. Stroud (UC San Francisco). FUNDING National Institutes of Health.

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L.J. Miercke, and R.M. Stroud, "Mechanism of ammonia transport by Amt/MEP/Rh: Structure of AmtB at 1.35 Å," *Science* **305**, 1587 (2004).

### Transcription Initiation and Elongation by RNA Polymerase II

Every cell of the human body contains the same DNA. The variation in cell types—such as blood, nerve, and liver cells comes from the selection of genes chosen to be copied from DNA into messenger RNA by an enzyme called RNA polymerase. RNA polymerase, which is regulated by transcription factors, is made up of several protein subunits with different roles. RNA polymerase II (pol II) is the protein complex responsible for all messenger RNA production, the first step in gene expression. The structure of the pol II enzyme provides the basis for understanding all gene activity in the cells of higher organisms, such as yeast, plants, and humans. TFIIB and TBP are transcription factors that interact with pol II to start the transcription assembly line. The study of the structure and function of pol II and its transcription factors is the key to translating an organism's genetic code and understanding the flow of information from gene to protein, as revealed in two reports by Bushnell et al. and Westover et al.

RNA pol II is the protein complex responsible for all messenger RNA production. TFIIB and TBP are transcription factors that interact with pol II to start the transcription assembly line. Protein crystallography structures from the ALS and SSRL have helped researchers from Stanford University to analyze the inner workings of RNA and its role in turning DNA's genetic blueprint into working proteins. In two studies, the researchers determined the structure and function of pol II–TFIIB complexes and further characterized the elongation phase of transcription by pol II, thus offering the first real understanding of the defining events of DNA transcription.

Genetic information is carried by two kinds of nucleic acid molecules, DNA and RNA. The master blueprint from DNA must be copied, or "transcribed," into messenger RNA before a cell can grow or differentiate. To understand this transcription process, which is critical to all living things, scientists must study the inner structure of the RNA polymerase enzyme. Guided by helper molecules known as transcription factors, RNA polymerase binds to the start of a gene, unwinds the DNA double helix, and manufactures an RNA message.

The eukaryotic cells of higher organisms contain three forms of RNA polymerase, made up of 10 to 15 polypeptides. These enzymes require the help of general transcription factor molecules to recognize a promoter (the region of DNA in front of a gene that binds RNA polymerase to promote gene expression) and initiate transcription. Structural similarities among RNA polymerases and general transcription factors hold the key to understanding the universal features of the transcription mechanism.

RNA pol II, a 12-subunit protein complex, is responsible for all messenger RNA production. Previous experiments demonstrated that a mutant 10-subunit pol II could not recognize a promoter to initiate transcription two additional subunits, Rpb4 and Rpb7, were required. These subunits are normally found in substoichiometric amounts, a problem overcome by the researchers, who successfully crystallized a 12-subunit pol II. To initiate transcription from a promoter, pol II also requires the help of five general transcription factor molecules. Two of these factors, TFIIB and TBP, are responsible for promoter recognition and interaction with pol II.

Crystals of pol II–TFIIB complexes were studied at ALS Beamlines 5.0.2 and 8.2.2, and diffraction data complete to 4.5-Å resolution were collected at SSRL Beamline 9-2. These observations revealed three features that are crucial to transcription initiation: an N-terminal zinc ribbon of TFIIB that "docks" with the polymerase near the path of RNA exit from a transcribing enzyme; a "finger" of TFIIB inserted into the active center of the polymerase, possibly to slow down the transcription process so that the strands of DNA and new RNA can separate properly; and a C-terminal that orients DNA for unwinding and



RNA polymerase II pre-initiation complex model.

transcription (Figure 4). In addition, the researchers observed that TFIIB may interact with the DNA template strand to determine the location where transcription starts. TFIIB may also define the roles of other transcription factors during initiation.

The team also studied the elongation phase of transcription (the growth of a polypeptide chain) by pol II. Previous studies of the elongating polymerase had problematic structures that failed to separate newly synthesized RNA from the template DNA strand. The researchers drew on their considerable expertise in the preparation of protein crystals to add pol II to a preassembled DNA–RNA scaffold. These crystal complexes diffracted on ALS Beamline 5.0.2 to 3.6 Å.

Structures from these complexes revealed proper separation of the RNA strand from the DNA template. The separation was achieved by a network of interactions between three previously unobserved protein loops in pol II



5 Close-up of strand separation. RNA (red) and DNA (blue) strands are separated by a network of interactions with three protein loops. The loops limit the extent of RNA separation (orange), stabilize the separated single strand, and form part of the RNA exit pore (green and pink). and the RNA–DNA phosphate backbone (Figure 5). The strand–loop network also moved the pol II so that the binding site for an incoming nucleotide triphosphate was empty. Future work can exploit the empty binding site for studies on the mechanisms of nucleotide selection and addition.

**INVESTIGATORS** K.D. Westover, D.A. Bushnell, R.E. Davis, and R.D. Kornberg (Stanford University).

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PUBLICATIONS D.A. Bushnell, K.D. Westover, R.E. Davis, and R.D. Kornberg, "Structural basis of transcription: An RNA polymerase II-TFIIB cocrystal at 4.5 angstroms," *Science* **303**, 983 (2004).

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### Structure of a Sliding DNA Clamp–Loader Complex

Imagine a car racing along a track at 300 miles per hour. Now imagine the car spinning and spiraling as it careens, each blurred movement perfectly coordinated. Such are the acrobatics performed by protein structures during DNA replication. Kuriyan et al. have captured a split-second glimpse of a speedy protein complex that plays an essential role in DNA's ability to make copies of itself. Their work reveals for the first time how a ring-shaped protein called a sliding clamp may target a special DNA structure generated during replication, in which a polymerase enzyme adds free nucleotides to a single DNA strand. As part of this process, the polymerase uses the sliding clamp like a seatbelt to tether itself to the new DNA double helix.

Sliding clamps are ring-shaped proteins that encircle DNA and enable polymerasesenzymes that replicate DNA-to relax and regain their hold on DNA strands without losing their place, despite the considerable torque that results from the production of double-helical DNA. In addition to their role in DNA replication, sliding clamps are also involved in several other processes that require a mobile contact on DNA. Hoping to shed light on this important but still poorly understood mechanism, a trio of researchers from Berkeley and New York have obtained the crystal structure of a sliding clamp in complex with a clamp loader assembly that is "powered" by the hydrolysis of ATP. The researchers found a spiral structure in the

clamp loader with a striking correspondence to the grooves of the DNA double helix. The crystal structure suggests a simple explanation for how this interaction with the double helix triggers ATP hydrolysis and the release of the sliding clamp.

The clamp-loader protein assembly churns through 1000 base pairs per second, moving 30 times its length every second. At a human scale, that's the equivalent of racing at almost one-half the speed of sound. But the protein complex doesn't just race. It also rotates 100 times per second as it follows DNA's spirals. And further complicating matters, the polymerase moves in only one direction, while the two DNA strands to be replicated are arranged in opposite directions. This means that while one DNA strand can be smoothly replicated by the polymerase, the other strand can only be duplicated in many shorter stretches, with a second polymerase hopping from one piece to another, and its sliding clamp continuously clamping and unclamping from DNA like an automated claw on an assembly line. The complexity of its speed and movement is mind-boggling, but nature is very smart and its solutions are tremendously simple.

To determine how the sliding clamp targets DNA that is ready to replicate itself, encircles it, then lets go when the replication is complete—all in the blink of an eye—the research group turned to ALS Beamline 8.2.2. There, they used x-ray diffraction to reveal the structure of a sliding clamp from a yeast species as it is bound to a clamp loader, a five-subunit protein motor that both opens and closes the clamp and targets it toward freshly unwound DNA strands that are ready for replication (Figure 6). The researchers were able to capture this protein assembly precisely when the clamp loader is poised to release the sliding clamp around its target DNA.

The result is a 3D protein structure (Figure 7) that reveals how the clamp loader simultaneously binds to the clamp and ATP, a highenergy molecule that fuels the motor. From this structure, scientists can begin to under-



6 Schematic of the clamp loading cycle. PCNA is the clamp, RFC is the clamp loader. Hydrolysis of ATP releases the loader from the clamp.

stand how the protein assembly recognizes DNA strands that are ready for replication a fundamental process that is conserved in every branch of life. The clamp loader recognizes the junction where DNA changes from



The clamp loader (blue) bound to the clamp (gold), with double-stranded DNA modeled through the clamp and against the underside of the clamp loader. The clamp loader recognizes the junction where DNA changes from double stranded to single stranded, and it couples this recognition with a structure that forces the clamp loader to release the clamp from the DNA. double stranded to single stranded, and it couples this recognition with a structure that forces the clamp loader to release the clamp from around the DNA.

This work marks yet another milestone for this research group, which was the first to solve the structure of the clamp protein more than a decade ago. Next, to gain a more global understanding of how clamp loading works, the scientists hope to determine how the entire protein assembly is configured on DNA. The group's ultimate goal is to determine the structure of the entire replication assembly at this level of atomic detail. While it may take a while to accomplish that task, the resolution of this first structure of a DNA clamp–loader complex in action using x-ray crystallography is an exciting step in the right direction.

**INVESTIGATORS** G.D. Bowman and J. Kuriyan (UC Berkeley and Berkeley Lab) and M. O'Donnell (The Rockefeller University).

FUNDING National Institutes of Health.

**PUBLICATIONS** G.D. Bowman, M. O'Donnell, and J. Kuriyan, "Structural analysis of a eukaryotic sliding DNA clamp–clamp loader complex," *Nature* **429**, 724 (2004).

### The Structure and Activation of Vinculin in Focal Adhesions

Cell adhesion proteins on the surface of all cells bind them to their neighbors and to molecules outside the cell, a process necessary for the development of all multicellular forms of life, including humans. Since cell membranes have little structural strength, adhesion receptor proteins, which penetrate through the membrane, anchor to an internal (intracellular) structure known as the cytoskeleton, which provides the cell with a solid framework. This interaction results in the formation of adhesion complexes, which attach cells to each other and to the surfaces on which they are growing. However, relatively little is known about how these adhesion complexes are formed or regulated. Izard et al. have focused on how one class of these adhesion receptors, termed integrin transmembrane receptors, are linked to the cytoskeleton. The key protein establishing these links is vinculin, which was known to be essential for binding integrin receptors to the cytoskeleton. The structures they obtained for vinculin allowed them to construct a model that explains how it transitions from a nonbinding or resting state to the activated state that occurs when adhesion complexes are formed.

When cells come in contact with components of the extracellular matrix (supporting material in a tissue that is not part of a cell), adhesion complexes form that direct changes in the cells' internal structural scaffolding (the cytoskeleton), which then allows the cells to migrate and to undergo shape changes. The proteins talin and vinculin are essential for proper formation of specific complexes, called focal adhesions, at the cell membrane, but the structures of these proteins and how they interact to direct changes in the actin cytoskeleton were unknown. To address this problem, a group led by researchers from St. Jude Children's Research Hospital (Memphis, Tennessee) has obtained the crystal structures of human vinculin in its resting and activated states and used the structure to clarify the mechanism of vinculin activation.

Focal adhesions are directed by integrin transmembrane receptors that connect the actin cytoskeleton to ligands in the extracellular matrix. The cytoskeletal protein talin helps link the integrin to the cytoskeleton. Talin, in turn, is linked to actin through its association with vinculin. Vinculin is a large (about 116 kDa) protein that was known to be maintained in its resting state through intramolecular interactions of its tail (Vt) domain (a fivehelical bundle structure) with an undefined N-terminal domain present in its head (the Vh1 domain), but the structures of this complex and of full-length vinculin were unknown. Furthermore, although some studies suggested that acidic phospholipids activate vinculin by disrupting the Vh1-Vt interaction, the researchers thought it likely that other, more direct, links to its partners, such as talin, would trigger vinculin activation.

The conformational plasticity of vinculin made the group's crystallographic studies particularly challenging at every stage. Difficult crystal morphology, unit-cell variability, radiation sensitivity, and limited data resolution combined to make structure determination and refinement highly demanding. X-ray diffraction data sets collected at ALS Beamline 5.0.2, with the help of its automated inverse-beam protocol, enabled the solution of the first vinculin substructure (the Vh1–Vt complex), which proved essential in solving all subsequent structures, for which data was gathered at the Advanced Photon Source.

The initial crystal structure solved was vinculin's N-terminal Vh1 domain when in complex with its Vt domain. This structure established that these two domains form extensive hydrophobic contacts and that the Vh1 domain was a seven-helical bundle structure that contains two subdomains joined by a long centrally shared  $\alpha$  helix. The Vh1–Vt crystal structure then allowed the group to solve the crystal structure of the entire human vinculin molecule. This structure showed that, in its resting state, vinculin is a series of helical



B Structure of inactive vinculin. The space-filling representation reveals the overall architecture of its five domains. The collection of loosely packed helical bundle domains is largely held together through the hydrophobic interactions of the seven-helical bundle of the Vh1 domain (yellow) with the five-helical bundle of Vt (cyan). The seven-helical bundle domains Vh2 (orange) and Vh3 (magenta) are very similar in their structure to Vh1, whereas the four-helical Vt2 domain (dark blue) is very similar to Vt. A disordered proline-rich region that serves as a hinge between the Vt2 and Vt domains is shown as a dark gray beaded string.



<sup>9</sup> Vinculin activation in focal adhesions. Following the formation of focal adhesions, the vinculin binding site of talin (red), itself an amphipathic  $\alpha$  helix, inserts into the Vh1 domain and displaces Vt to a more distant location. Displacement occurs by provoking dramatic movements and changes in the conformation of the N-terminal helical bundle of Vh1 by a process called helical bundle conversion. The net result is that the Vt domain swings free from the remainder of the molecule, allowing it to bind to other partners, such as F-actin.

bundles connected by short linkers that divide the protein into five discrete domains. Three of these domains (Vh1, Vh2, and Vh3) are juxtaposed and structurally related sevenhelical bundles. The protein also contains a four-helical bundle whose structure is most closely related to that of Vt (the Vt2 domain), and which is joined to Vt by a flexible proline-rich linker that serves as a hinge for the molecule (Figure 8). This structure also revealed that the helical bundle domains of vinculin are loosely packed and are clasped together by the Vh1–Vt interaction.

Most importantly, the Memphis groups' crystal structures of vinculin's Vh1 domain in complex with two of talin's vinculin binding sites, along with their biochemical and biological studies, revealed that talin functions as the trigger that activates vinculin by binding to the Vh1 domain and displacing Vt from a distance. It accomplishes this by provoking remarkable changes previously unknown in protein structures by means of a process the group calls helical bundle conversion (Figure 9). The group's studies have thus not only resolved how vinculin is activated but, coupled with their most recent work, have revealed that reorganization of the actin cytoskeleton by focal-adhesion signaling involves a chain reaction of structural alterations that ultimately allow vinculin to change the structure of actin networks.

**INVESTIGATORS** T. Izard and P.R.J. Bois (St. Jude Children's Research Hospital, Memphis, Tennessee); G. Evans, G. Bricogne, and C. Vonrhein (Global Phasing Limited, Cambridge, England); and R.A. Borgon and C.L. Rush (University of Tennessee, Memphis).

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#### Exposing the Secrets of the p75 Nerve Growth Factor Receptor

There are approximately 100 billion neurons in your brain. Each neuron is connected to about ten thousand other neurons. There are about one quadrillion synapses, the points of contact between the axon of one cell and the dendrite of another. The electrical firings and chemical messages passed between neurons are what produce your thoughts, feelings, memories, and other sensations. Babies are born with all the neurons they will ever have, but a new phase of brain development begins after birth—the wiring phase. Synaptic links form, and nerves begin firing. The environment then takes over the brain development process. This stage is the equivalent of creating telephone trunk lines between the right neighborhoods in the right cities. The brain must then sort out which wires belong to which house, and this is how learning takes place. Memories are stored in the wiring between the houses. Researchers He and Garcia have discovered a critical step in the mechanism for reproducing nerve growth factor (NGF), one of the most important molecules in the nervous system.

In a breakthrough that can now be directly applied to drug design for treating neurodegenerative conditions such as Alzheimer's disease or spinal cord injuries, researchers from Stanford University have discovered a critical step in the mechanism for reproducing NGF. One of the most important molecules in the nervous system, NGF and its other neurotrophin family members control the development of the nervous system in the embryo and the maintenance of nervous tissue and neural transmission in the adult. The researchers used the ALS to obtain the 3D x-ray crystallography structure of a complex of NGF bound to a p75 cell surface receptor, thereby demonstrating the mechanism for receptor activation that has eluded drug companies for many years.

Neurons are the basic functional unit of the nervous system. They are specialized cells responsible for all sensation and direction of movement in the body. Stimulated by NGF, each of these nerve cells extends an axon or dendrite projection that connects it to other neurons, muscle, or skin, and these projections provide the wiring for information sent between the brain and the spinal cord. Many of these connections between neurons and other tissues are also necessary for the continued survival of these cells. Neurons that are lost through aging, disease, or injury are unable to be replaced because most neurons are not able to divide to produce new neurons.

Neurotrophins are a family of proteins essential to the nervous system. Each neurotrophin can signal through two different types of cell surface receptor-the Trk receptor, tyrosine kinase, and the p75 neurotrophin receptor, which may have an important role in the control of axonal regeneration. During development of the brain, the binding of neurotrophins to their receptors is necessary to match the correct number of neurons with their targets. NGF also regulates axonal and dendritic growth, the formation of synaptic structure and connections, and neurotransmitter release. Neurotrophins are capable of promoting neuronal cell survival, or cell death, depending on the environment. Alterations in neurotrophin levels may underlie several medical conditions, including pain, depression, obesity, and disorders in nerve regeneration, learning, and memory.

The Stanford researchers provided a detailed glimpse of how NGF binds to the p75 receptor by creating a 3D atomic model that shows how a molecule with two symmetrical components, such as NGF, can simultaneously activate two different receptors on its surface (Figure 10). For the last



Structure of the NGF-p75 complex. p75 binds along one side of the NGF homodimer.

15 years, neurobiologists have wondered how NGF specifically selects one of each type of receptor, p75 and Trk, instead of two of the same type.

Receptors and ligands are the locks and keys of molecular biology, allowing the trans-

mission of specific information across cell membranes. The researchers showed that the NGF key combines with the p75 lock in a 2:1 ratio. When this binding occurs, a second p75 interaction is prevented—essentially, the NGF key changes shape after it enters the lock. This allows the other NGF receptor, Trk, to bind on the other side of the NGF molecule, forming a three-way signaling complex.

The researchers determined the structure by imaging crystals of the molecular complex of NGF with its low-affinity neurotrophin receptor, p75, using x rays produced at ALS Beamline 8.2.1, and refined the structure to a resolution of 2.4 Å. This dimension is about 100,000 times smaller than a cell—a resolution that is critical for an accurate picture of how the thousands of atoms in the neurotrophin–receptor structure are assembled.

With the definition of this crystal structure, drug companies can now work on stimulating or blocking the actions of NGF, potentially repairing the damage done by degenerative diseases of the brain. **INVESTIGATORS** X. He and K.C. Garcia (Stanford University).

**FUNDING** Paralyzed Veterans of America, Spinal Cord Research Foundation; American Heart Association; Christopher Reeve Paralysis Foundation; Keck Foundation; and National Institutes of Health.

**PUBLICATIONS** X. He and K.C. Garcia, "Structure of nerve growth factor complexed with the shared neurotrophin receptor p75," *Science* **304**, 870 (2004).

#### Snapshots of Ribozyme Reaction States Reveal Structural Switch

Did an earlier form of life exist in which RNA did it all—providing the material for replication and catalyzing the chemical reactions that engendered the replication process? For example, retroviruses (such as hepatitis delta) carry their genetic blueprint in the form of RNA, not DNA. Recent discoveries about the role of RNA lend further credence to the theory that it could have been the precursor molecule. Francis Crick, co-discoverer of the DNA double helix, speculated in 1968 that RNA could function as an enzyme. In 1982, Thomas Cech moved speculation into fact when his laboratory discovered that an intron (a bit of messenger RNA removed before protein synthesis) spliced itself without requiring assistance from any protein enzyme. Up to this point, all enzymes were thought to be proteins. This self-splicing RNA, and other RNAs capable of catalyzing chemical transformations, became known as ribozymes. Ke et al. have obtained atomic structures of a ribozyme from the RNA of a hepatitis delta virus that shows how it engages in catalysis, a finding with medical implications.

RNA, like protein, can sometimes function as an enzyme (ribozyme) to speed biochemical reaction rates. But how does RNA, a simple polymer with just four different chemical building blocks, enhance reaction rates by at least a million fold? Recently, a group from UC Berkeley and the Howard Hughes Medical Institute obtained high-resolution xray crystallographic structures of a ribozyme trapped in different states of its catalytic cycle, showing how a change in the RNA conformation governs the reaction mechanism.

Most ribozymes catalyze the cutting and pasting of RNA molecules at specific sites, snipping out (cleaving) extraneous sequences not needed in the final functional form of an RNA. In the hepatitis delta virus (HDV), a human pathogen with a small circular RNA genome, a ribozyme contained within the viral sequence cuts the RNA at a single site during replication to enable packaging of new virions, the extracellular virus particles that allow the virus to infect a host and replicate. Understanding how the ribozyme works is of interest both for defining the fundamental principles of RNA-catalyzed reactions and for discovering a possible Achilles' heel in this deadly pathogen.

The hepatitis delta virus is so small that it cannot replicate on its own, needing hepatitis B for the process and therefore only infecting patients who already have that form of the disease. Unfortunately, superinfection with the delta virus causes a severe, fulminant form of hepatitis that is often lethal. In its replication cycle, HDV resembles small infectious RNAs called viroids, covalently closed circular RNA molecules that are found in plants. In both the delta virus and plant viroids, self-cleaving ribozymes encoded within the viral genome slice the RNA copies into unit-length pieces for viral packaging. The delta virus ribozyme is unique, however, in that once the RNA is cleaved, the ribozyme is somehow inactivated, "switching off" and preventing further RNA

cleavage or re-ligation of the separated RNA strands.

To comprehend how such inactivation might occur and to determine the chemical mechanism by which the delta virus ribozyme does its work, the researchers used x-ray crystallography at the ALS to examine ten molecular structures of ribozymes trapped in the precleaved state. The catalytic site in the precursor ribozyme contains a hydrated divalent magnesium ion, which is adjacent to the phosphorus-oxygen bond to be broken (Figure 11). A cytidine base that is part of the ribozyme sequence is positioned in the active site on the other side of the labile phosphorus-oxygen bond. Together with supporting biochemical data, these structures suggest that the cytidine from the ribozyme activates the RNA for self-cleavage, while a magnesium-bound water molecule stabilizes the RNA as the bond is broken.

Comparison of these trapped precursor



**11** The compact catalytic core of the HDV ribozyme comprises five helical segments connected as an intricate nested double pseudoknot. The gold ball represents the catalytically critical magnesium divalent metal ion at the active site. The green partial segment represents the RNA substrate strand that is "snipped" during the ribozyme-catalyzed reaction.

structures to each other and to the structure of the "product"—a (previously determined) self-cleaved form of the delta ribozyme—shows that the RNA undergoes a significant conformational change in the region where the cleavage reaction occurs (Figure 12). This structural change destroys the binding site for the catalytic magnesium ion and also moves the critical cytidine base beyond striking distance of the reactive groups in the RNA, thereby explaining the inactivation of the ribozyme.

This unique quality of the HDV ribozyme to slice specific RNA molecules and then inactivate itself provides a mechanistic explanation for its activity during the HDV viral life cycle, information that could be useful in developing antiviral therapies that target the ribozyme.



Structures of the HDV ribozyme in precleavage (left), transition (center), and postcleavage (right) states. The magnesium ion is shown as a yellow ball; the phosphorus–oxygen bond to be broken is denoted by an asterisk (\*); the cytidine base (a part of the ribozyme sequence) is on the opposite side of the phosphorus–oxygen bond and is labeled C75.

INVESTIGATORS A. Ke, F. Ding, and J.H. Cate (UC Berkeley); K. Zhou (Howard Hughes Medical Institute); and J.A. Doudna (UC Berkeley, Berkeley Lab, and Howard Hughes Medical Institute).

**FUNDING** National Institutes of Health and Howard Hughes Medical Institute.

**PUBLICATIONS** A. Ke, K. Zhou, F. Ding, J.H. Cate, and J.A. Doudna, "A conformational switch controls hepatitis delta virus ribozyme catalysis," *Nature* **429**, 201 (2004).

### Substrate Recognition Strategy for Botulinum Neurotoxin

The best thing one can say about botulism is that it is relatively rare. At worst, botulism can ultimately result in death due to respiratory failure resulting from paralysis of the breathing muscles by the neurotoxin produced by the bacterium *Clostridium botulinum*, which can be ingested with contaminated food, enter the body through wounds, or (in the case of infants) germinate in the intestine from spores. Given early after onset of symptoms, an antitoxin exists than can prevent further damage, but a more effective treatment for this and other neurotoxin-caused illnesses, such as tetanus, await a more detailed understanding of how the toxin works at the molecular level. Breidenbach and Brunger have taken a step toward this goal with the first structure of a key component of botulinum neurotoxin while bound to its target molecule, known as SNAP-25. The new structure allowed the team to generate a detailed model of how the binding between the botulinum neurotoxin component and SNAP-25 comes about. The model may lead to the development of inhibiting agents that prevent the binding.

Clostridal neurotoxins (CNTs) are the causative agents of the neuroparalytic diseases botulism and tetanus. By inhibiting release of the neurotransmitter acetylcholine, for example, the neurotoxin produced by the bacterium *Clostridium botulinum* interferes with nerve impulses and causes a paralysis of respiratory and skeletal muscles that can cause death. Researchers from Stanford University have now determined the first structure of a CNT in complex with its target. The structure, at a resolution of 2.1 Å, together with enzyme kinetic data, reveals an array of active sites that give the CNT its deadly specificity.

CNTs contain enzymes that do their damage by impairing neuronal exocytosis (the process by which neurotransmitter is released into a synapse). In normal function, it is believed that assembly of SNAREs (soluble N-ethylmaleimide-sensitive factor attachment protein receptors) into a low-energy ternary complex catalyzes membrane fusion, which precipitates the neurotransmitter release.

CNTs interfere with this process by degrading SNAREs, a process called proteolysis. Toxins like botulinum neurotoxins are two-chain polypeptides with a heavy chain joined by a disulphide bond to a light chain. CNT light chains are part of a unique group of zincdependent endopeptidases (enzymes) that catalyze hydrolysis of peptide bonds within other proteins. When such chains catalyze SNARE hydrolysis at specific sites, membrane fusion is attenuated and neurotransmitter release inhibited.







Exosite-based model of BoNT/A substrate recognition. Left: SNAP-25 attaches to a presynaptic membrane via palmitylation sites (black) on its linker domain (purple). Center: Helix formation at the  $\alpha$  exosite probably initiates binding of BoNT/A (blue) to the SNAP-25 C-terminal domain (green), and the anchor points along the domain (green notches) increase substrate specificity. Right: The resulting enhanced binding at the  $\beta$  exosite induces conformational changes at the active site (AS) that allow cleavage of the SNAP-25.

The means by which a CNT properly identifies and cleaves its target SNARE has been a subject of much speculation. It is thought to use one or more regions of enzyme–substrate interaction (exosites) remote from the active site where hydrolysis occurs. To address this question, the Stanford team used x-ray diffraction data from ALS Beamlines 8.2.1 and 8.2.2 and SSRL Beamline 9.2 to determine the first structure of the light chains of a CNT endopeptidase (the protease botulinum neurotoxin serotype A or BoNT/A) in complex with its target SNARE (human SNAP-25).

In their structure (Figure 13), an  $\alpha$  exosite is formed by BoNT/A light-chain helices  $\alpha 1-\alpha 4$  that bind to the helical N-terminal of the substrate SNAP-25. Contacting side chains between the SNAP-25 substrate and the BoNT/A light chain at the  $\alpha$  exosite are located along the helices. A  $\beta$  exosite resides on the opposite face of BoNT/A. The C-terminal of SNAP-25 forms an antiparallel  $\beta$ sheet along with a portion of a "250 loop," which is separated from the zinc-containing active site where substrate cleavage occurs by a "370 loop." Additional exosites (anchor points) also include side-chain contacts between the substrate and the light chain.

Based on their structure and available kinetic data for several mutant SNAP-25 substrates, the researchers concluded that most of this unusually large enzyme–substrate interface serves to provide a substrate-specific boost to catalytic efficiency by reducing  $K_M$  (the Michaelis constant), so that the substrate is properly oriented with respect to the light chain. They also observed significant structural changes near the toxin's catalytic pocket upon substrate binding, probably serving to render the protease competent for catalysis.

A general model of the strategy used by BoNT/A to recognize and cleave SNAP-25 is presented in Figure 14. SNAP-25 attaches to a presynaptic membrane via palmitylation (fatty acid binding) sites on its linker domain. The N-terminal (sn1) and C-terminal (sn2) domains are unstructured or flexible in uncomplexed SNAP-25. Binding of BoNT/A is probably initiated by helix formation at the  $\alpha$  exosite, and

the anchor points along the extended portion of SNAP-25 serve as additional determinants of substrate specificity. These sites reduce  $K_{\rm M}$  and enhance binding at the  $\beta$  exosite, thereby inducing conformational changes at the zinc active site that render the endopeptidase competent to cleave its substrate.

Ultimately, the novel structures of the substrate-recognition exosites could be used for designing inhibitors specific to BoNT/A.

INVESTIGATORS M.A. Breidenbach (Stanford University) and A.T. Brunger (Howard Hughes Medical Institute, Stanford University, and Stanford Synchrotron Radiation Laboratory).

**FUNDING** National Institutes of Health and Howard Hughes Medical Institute.

**PUBLICATIONS** M.A. Breidenbach and A.T. Brunger, "Substrate recognition strategy for botulinum neurotoxin serotype A," *Nature* **432**, 925 (2004).

# LIFE SCIENCE

### X-Ray Tomography Views Whole Yeast Cells at 60-nm Resolution

Our relationship with *Saccharomyces cerevisiae*, the budding (or brewer's) yeast, began thousands of years ago with bread and alcohol. In modern times, researchers find *S. cerevisiae* to be a valuable model system for biochemical, molecular, genetic and, recently, proteomic analyses. This organism was the first eukaryote sequenced. Eukaryotes, unlike bacteria, have nuclei. Some are single celled, like budding yeast, but with the nucleus also came the evolution of multicelled organisms, such as plants and animals. It was found that at least 31% of proteins encoded by yeast genes have mammalian equivalents, or homologs. Therefore, yeast are important model organisms for understanding cellular processes in higher eukaryotes. In fact, our connection to the budding yeast is even more ancient than originally believed. Nearly 50% of human genes implicated in heritable diseases have yeast homologs, making this distant relative a good predictor of human gene function. *S. cerevisiae* has a short, 90-minute, life cycle, so Larabell and Le Gros have been able to use an imaging technology called x-ray tomography to visualize the entire process of cell development.

X-ray tomography is the first high-throughput imaging technology that generates images of whole, hydrated cells at better than 60-nm resolution. With it, researchers from Berkeley Lab have obtained 3D views of the internal structure of whole, hydrated Saccharomyces cerevisiae cells, bridging the mesoscale resolution "gap"-the middle area between light (200 nm) and electron microscopy (3 Å). Using this technology, researchers can now rapidly examine phenotypic consequences of genetic mutations and knockouts and observe changes not detectable with light microscopy. It is also possible to obtain quantifiable, 3D information about the localization of molecules throughout an entire cell.

With light microscopy, a glass lens focuses visible light onto the sample. With x-ray microscopy, an x-ray zone plate is used to focus photons. The photons illuminating the sample at a 2.4-nm wavelength (photon energy of 517 eV) are in a range known as the "water window." This means that the structures in the cells absorb approximately an order of magnitude more strongly than the surrounding water. The resulting natural contrast generates unprecedented views of the internal cellular architecture in a natural, albeit frozen, state. After tomographic reconstruction, computer algorithms can process data to reveal features of interest.

Data were obtained with XM-1, the Center for X-Ray Optics (CXRO) transmission x-ray microscope. (A dedicated biological x-ray microscope, dubbed "XM-2," will be in operation at the ALS by 2006.) Light microscopy was used to position and examine rows of living yeast in their capillary container before the living *S. cerevisiae* cells were rapidly frozen and placed in the x-ray microscope. The cells remained fully hydrated throughout image collection.

With the ALS transmission x-ray microscope, data collection was fast (under three minutes) and relatively easy (like light microscopy), producing high-resolution, absorption-based images (like electron microscopy) that provide contrast between cellular structures and allow for discernment of individual structures. After data collection, tomographic techniques were used to reconstruct the original information into quantifiable 3D views of the entire cell. Through the use of computer algorithms, the researchers then processed the reconstructed data to create made-to-order images of whole cells and their internal structures (Figure 1).

Because of the alignment of the yeast in their capillary container, tomographic data sets could be collected from multiple cells by simply advancing the capillary into the field of view. Cells were rotated through 180 degrees and images collected every 4 degrees. A fully automated cryorotation stage has recently



1 High-magnification view of a budding yeast. Left: Projection image showing numerous superimposed organelles. Right: Computer-generated sections through the yeast reveal numerous organelles after tomo-graphic reconstruction; the most dense (bright white circles) are filled with lipid.

been developed that will enable collection of more images with 0.5- to 1.0-degree intervals, yielding higher-resolution data.

To get volume information, the researchers started with the surface of the yeast. They then took it away to reveal internal vesicles and organelles. To get density information, they color coded the structures by measuring x-ray absorption (Figure 2). In this way, the researchers were able to quantify information and differentiate cellular regions. Density information can also be superimposed on top of volume information to determine what densities are associated with what structures.

In sum, x-ray tomography generated unique 3D reconstructions of whole yeast (Figure 3) without the need for chemical fixatives or contrast-enhancement reagents. Because the high-resolution data set was based on tomographically reconstructed local x-ray absorption, the information in these reconstructions was quantifiable, and because the cells were rapidly frozen from the living state and remain fully hydrated, the information retained biological fidelity.

**INVESTIGATORS** C.A. Larabell (Berkeley Lab and UC San Francisco) and M.A. Le Gros (Berkeley Lab).

**FUNDING** National Institute of General Medicine and U.S. Department of Energy, Office of Health and Environmental Research.

PUBLICATIONS C.A. Larabell and M.A. Le Gros, "X-ray tomography generates 3-D reconstructions of the yeast, *Saccharomyces cerevisiae*, at 60-nm resolution," *Molecular Biology of the Cell* **15**, 957 (2004).



2 Reconstructed data using different volume-analysis algorithms. Left: Opaque surface. Center: Transparent surface showing internal vesicles. Right: Volume-rendered thick-slice section: dense lipid droplets are white, least-dense vacuoles appear gray, structures of varying densities appear green, orange, and red.





Video sequence of reconstructed data-the structural organization of the entire yeast.

# ATOMIC AND MOLECULAR SCIENCE

### Tracking Particle Motion in Deuterium Molecules

Molecular fragmentation can be initiated by collision with a charged particle, by exposure to a strong laser pulse, or by the absorption of a single photon. When a molecule absorbs enough energy, bonds are broken and ions can form, splitting the molecule into component parts (electrons and nuclei) that can react with neighboring molecules. A natural example of this process occurs in Earth's upper atmosphere, where solar ultraviolet radiation prompts molecular ionization and fragmentation to create a dense layer of free electrons in the ionosphere. In the case of deuterium (a "heavy" isotope of hydrogen) molecules, a "Coulomb explosion" occurs in the rare event when two electrons—the glue holding the molecule together—are released (double ionization) and the two remaining nuclei explode apart in opposite directions because they both have positive charges and repel each other. Weber et al. have used a unique "momentum microscope" to study Coulomb explosions in molecular deuterium, resulting in the most detailed description of the process yet.

Nothing in the universe stands still. The study of particle motion in molecules allows physicists to probe the fundamental properties of molecules and how they work, which is crucial to understanding the molecular mechanisms behind chemistry, biology, and pharmaceutical development. Researchers from Berkeley Lab, Kansas State University, and institutions in Germany, Australia, and Spain used a pulsed beam of photons from the ALS to ionize the electrons in a deuterium molecule, causing it to fragment in a Coulomb explosion. The team then used position and timing data to construct a 3D "photograph" of the simultaneous motion of all the electrons and nuclei at the moment of fragmentation. In the process, they discovered that even simple molecular hydrogen is full of surprises.

A molecule's properties are determined by the initial-state wave function of its electrons and nuclei. To determine these properties, experimentalists study what happens when the molecule fragments into its constituent parts. The outcome of such a reaction is determined by its initial state, the fragmentation process itself, and the interaction of all four particles in the final state. It is very difficult for theorists to do a calculation that correctly takes all these contributions into account. On the other hand, experimentalists have to measure the momentum of each charged particle, which sounds quite simple but is actually rather complex.

To study the motion of multiple particles, the researchers needed a delicate way to fragment a molecule while preserving some of



Artist's rendition of the momentum spectrometer. The deuterium molecules, prepared in a supersonic jet going from the bottom to the top, intersect the pulsed photon beam in the middle of the copper rings, which define a homogenous electric field. The large coils are a Helmholtz pair that establish a uniform magnetic field parallel to the spectrometer axis. The charged nuclei (ions) are guided to a position-sensitive detector to the left while the electrons spiral to a similar detector on the right in the magnetic field. Unlike the light electrons, the motion of the heavy ions is not significantly influenced by the magnetic field.

its internal motion. Rather than "smashing open" a molecule with charged particles, they decided to insert a single photon, which has no mass or charge and does not disturb the momentum of the particles inside the molecule. The photon can quietly transfer its energy, like a cold virus sneaking into a cell, to "kick-start" the fragmentation process. The international team used a pulsed beam of linearly polarized photons from ALS Beamline 4.0.2 to illuminate a jet of deuterium molecules in their COLTRIMS apparatus. The researchers used deuterium instead of ordinary hydrogen because its greater mass provided a thicker target for the photon beam. (A hydrogen nucleus only contains one proton, while a deuterium nucleus contains a proton and a neutron.) Absorption of a photon usually ejects only one of the molecule's electrons, but can sometimes eject both of them, in the process driving the two remaining equally charged nuclei apart in the Coulomb explosion.

After the explosion, electric and magnetic fields in the COLTRIMS apparatus (Figure 1) accelerated the electrons and nuclei away from each other, where they drifted onto microchannel plate detectors. Ultrafast timing techniques ensured that the pairs of detected electrons actually came from the same molecule. For each charged particle, the position of impact on the detector and the flight time from the explosion were measured. With the data from this "microscope for motion" (momentum spectrometer), the team was then able to calculate the initial, simultaneous momentum of all four particles and build a 3D image of the fragmentation (Figure 2).

The results of this experiment show electron behavior that is strongly influenced by the separation of the nuclei at the instant the photon is absorbed. The escape directions of the electrons do not solely depend on the polarization of the synchrotron's photon beam. The reason for this electron behavior is



<sup>2</sup> 3D view of photon-induced fragmentation of a deuterium molecule, showing the angular distribution of one ejected electron in the plane containing the molecular and light polarization axes. Another escaping electron of the same energy is emitted upwards out of the plane. The direction of the molecular axis is given by the exploding nuclei (green).

likely hidden in the entangled motion of the electron pair in their initial molecular binding state. Quantum mechanical theory predicts an electron emission pattern shaped like a dipole, but the researchers observed highly structured angles of escape. In addition, the team's observations of particles simultaneously moving together in a few-particle system do not match theoretical predictions.

This experiment provides insight into the quantum dynamics of many-particle systems, ultimately leading to a better understanding of countless physical and chemical processes, but providing a challenge to theorists. For the moment, the experimentalists are ahead of the theorists. However, nothing in the universe stands still, including molecular theory.

INVESTIGATORS Th. Weber (Universität Frankfurt, Berkeley Lab, and Kansas State University); A.O. Czasch, O. Jagutzki, A.K. Müller, V. Mergel, H. Schmidt-Böcking, and R. Dörner (Universität Frankfurt); A. Kheifets (Australian National University); E. Rotenberg, G. Meigs, M.H. Prior, and S. Daveau (Berkeley Lab); A. Landers (Auburn University); C.L. Cocke and T. Osipov (Kansas State University); and R. Díez Muiño (Donostia International Physics Center and Unidad de Fisica de Materiales, Spain).

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### Spin-Resolved Photoelectron Spectroscopy Probes the Molecular Environment

How does the presence of neighboring atoms affect the local environment of an atom in a molecule? Within the close quarters of a molecule, even electrons in the tightly bound inner shell of an atom feel the effects of the complicated molecular field generated by the atoms next door. Carbonyl sulfide and hydrogen sulfide are both simple triatomic molecules that contain a single sulfur atom in different configurations. Both are well-studied molecules found in planetary atmospheres and are of great interest in biological, astronomical, and fundamental research. To better understand phenomena such as the chemistry of the sulfur cycle in the Earth's atmosphere or spectroscopic data from interstellar space, scientists obtain detailed information about the molecules' electronic structures by measuring the energies and ejection angles of electrons emitted when the molecules are exposed to soft (long-wavelength) x rays. With this work, Turri et al. have now demonstrated the ability to further probe the molecular environment with exquisite sensitivity by also detecting the spin of ejected inner-shell photoelectrons.

Inner-shell electrons, localized on a single atom, are sensitive site-specific probes of the molecular environment, unlike valence electrons, which can be delocalized over the whole molecule. At ALS Beamline 4.0.2, an international collaboration (U.S., Germany, Finland, and Russia) has, for the first time, used spin-resolved photoelectron spectroscopy to study molecular effects on the inner-shell electrons of two simple sulfurcontaining molecules, carbonyl sulfide and hydrogen sulfide. The researchers show that this technique is very sensitive to the molecular environment in the selected cases by comparing with previous atomic results. Binding energies of inner-shell electrons for an atom vary depending on the electron density around that atom modified by the electron-donating and -withdrawing properties of the surrounding atoms. Furthermore, the molecule's geometry can remove the degeneracy of inner-shell electrons, separating them depending on the orientation of their orbitals within the molecule. Such phenomena do not occur in atoms, and hence the investigation of inner-shell photoionization in molecules is considerably more complex.

Carbonyl sulfide (OCS) and hydrogen sulfide (H<sub>2</sub>S) are simple sulfur-containing molecules of fundamental, biological, and astrophysical interest. These molecules have different geometries: OCS is linear with a terminal sulfur atom, whereas H<sub>2</sub>S is bent with a central sulfur atom. The 2p inner-shell level of the isolated sulfur atom has six electrons arranged into three orbitals separated by spin-orbit splitting: one sulfur 2p1/2 level with two electrons and two degenerate sulfur 2p<sub>3/2</sub> levels with four electrons. In the anisotropic field of the OCS and H<sub>2</sub>S molecules, however, the degeneracy of the sulfur  $2p_{\scriptscriptstyle 3/2}$  level is removed, splitting it into two levels with slightly different binding energies and resulting in two closely spaced peaks in the photoelectron spectrum (Figure 3). These molecular effects obviously cannot be explained using a purely atomic model, but rather require the use of more complex molecular models.

Measurements were performed using circularly polarized light from the EPU at Beamline 4.0.2. Spin-resolved photoelectron spectra were measured using a TOF electron spectrometer, combined with a Mott polarimeter of the Rice type. In the Mott detector, electrons emerging from the TOF spectrometer are accelerated up to 25 keV and scattered off of a thorium foil. Depending on their spin, the electrons will preferentially scatter into one of two detectors, thus determining their spins.

The spin polarizations of the two field-split components of the sulfur  $2p_{3/2}$  levels were graphed as a function of photoelectron kinetic energy for OCS and H<sub>2</sub>S (Figure 4). A negative spin polarization here indicates that the electrons are preferentially emitted with spin parallel, rather than antiparallel, to the direc-



Photoionization spectrum of sulfur 2p shell of  $H_2S$  as measured at 54.7° with 200-eV photon energy. The 2p inner shell of isolated sulfur has six electrons arranged into three orbitals: one sulfur  $2p_{1/2}$  level (A) with two electrons and two sulfur  $2p_{3/2}$  levels with four electrons with slightly different binding energies and resulting in two closely spaced peaks in the photoelectron spectrum (B and C).



Spin polarizations of the two components of the sulfur  $2p_{3/2}$  levels (green = peak B and blue = peak C from Figure 3) as a function of photoelectron kinetic energy. For the H<sub>2</sub>S molecule, the unresolved  $2p_{3/2}$  doublet (B + C, red) is also shown. Solid lines are calculations for a comparable fully atomic model (argon 2p).

tion of photon propagation. To explore the effects of the molecular environment, the researchers compared their experimental results with values calculated for a fully atomic model. In both molecules, the sulfur atom has a filled outer shell and thus has the same electronic configuration as argon.

Calculations of the spin polarization for argon 2p photoionization have been published pre-

viously and are depicted in the graph as solid lines. The atomic model is in good agreement with the spin polarization of both field-split sulfur  $2p_{3/2}$  lines in OCS, while those for H<sub>2</sub>S deviate both from each other and from the calculations over a wide energy range. However, when compared with data at lower spectral resolution that does not resolve the splitting of the sulfur  $2p_{3/2}$  lines, the argon calculations do reproduce the observed spin polarization in H<sub>2</sub>S.

It is clear that the different molecular environments of the sulfur atoms in OCS and  $H_2S$  affect the spin polarization of the photoelectrons from the 2p shell. The molecular effects disappear when the results are integrated over the field-split sulfur  $2p_{3/2}$  levels, restoring somehow the spherical symmetry found in the atomic case. Similar, albeit less intense, behavior has been observed for the angle-resolved photoionization cross sections for these molecules.

INVESTIGATORS G. Turri, G. Snell, and S.E. Canton (Western Michigan University and Berkeley Lab); B. Langer (Max Born Institute, Germany); M. Martins (Universität Hamburg, Germany); E. Kukk (University of Oulu, Finland); N. Cherepkov (State University of Aerospace Instrumentation, Russia); J.D. Bozek and A.L. Kilcoyne (Berkeley Lab); and R.C. Bilodeau and N. Berrah (Western Michigan University).

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PUBLICATIONS G. Turri, G. Snell, B. Langer,
M. Martins, E. Kukk, S.E. Canton,
R.C. Bilodeau, N. Cherepkov, J.D. Bozek,
A.L. Kilcoyne, and N. Berrah, "Probing the molecular environment using spin-resolved photoelectron spectroscopy," *Phys. Rev. Lett.*92, 013001 (2004).

### Electron Trapping by Molecular Vibration

Philosopher of science Karl Popper once described science as "the art of systematic oversimplification." Indeed, many valuable insights can be gained by reducing a system to its bare essentials. For example, the basic description of atomic and molecular structure, in which electrons with specific energies inhabit "orbitals" around immobile nuclei, has resulted in remarkably useful explanations of spectroscopic data, complete with specific rules that predict which electronic states are accessible and which are not. Popper believed that good scientific theories must include such predictions because they make the theories falsifiable. Then again, violations of predicted rules offer an excellent opportunity to explore more complex phenomena underlying the simplified theoretical picture. In the work described here, Rathbone et al. observe a nominally "forbidden" electronic transition that is activated by molecular vibrational modes that break the molecule's symmetry. Their observation and analysis of this unprecedented behavior provide valuable insight into the subtle interplay between electronic transitions.

In photoelectron spectroscopy experiments performed at the ALS, a group of researchers from Louisiana State University, Texas A&M University, and the ALS has found that electronic states normally thought to be inaccessible (i.e., forbidden via transitions from the ground state) are excited in conjunction with certain types of molecular vibrations. Specifically, they found that photoelectrons became temporarily trapped in guasi-bound states known as shape resonances that were thought to be unreachable because of their symmetry. These forbidden transitions were found to occur only when accompanied by the excitation of asymmetric molecular vibrations. These recent experiments demonstrate that the well-accepted rules about the symmetry of accessible shape resonances are broken as a result of this novel vibrationally activated mechanism. This process represents a novel type of symmetry-breaking phenomenon that

has not been observed previously but appears to be widespread.

Using the HiRAMES endstation at ALS Beamline 10.0.1, the researchers performed vibrationally resolved photoelectron spectroscopy studies of gas-phase carbon disulfide  $(CS_2)$ , a simple molecule consisting of a central carbon atom with two sulfur atoms on each side, 180 degrees apart. This molecule has one bending vibrational mode and two stretching modes: one symmetric and one antisymmetric (Figure 5). The group investigated how the vibrational structure in the photoelectron spectrum changes as the incident photon energy is varied. They found that when the incident photon energy is tuned to the shape resonance (about 40 eV), the peaks corresponding to the bending and asymmetric stretch modes are dramatically enhanced (Figure 6).

This is a new resonance phenomenon: the observed shape resonance is the result of coupling between vibrational modes and electronic transitions that are "forbidden" by selection rules. However, such rules are based on simplifying approximations, and nominally forbidden behavior can occur as the result of unanticipated processes. Thus, exceptions to the rules provide opportunities to gain deeper insight into how electronic motion and nuclear motion are intertwined. In the case of  $CS_{2i}$ the forbidden behavior is observed only when the photoelectrons are tuned to specific resonant energies and become trapped, or quasibound, when the molecule is distorted from its equilibrium geometry. This point is made dramatically clear in plots of the relative probabilities (branching ratios) of the various vibrational modes versus incident photon energy (Figure 7). The resonance peak appears vividly for the two asymmetric vibrations but is



5 Vibrational modes of CS<sub>2</sub>: Bending mode (top), symmetric stretching mode (center), and anti-symmetric stretching mode (bottom).

absent in the plot for the symmetric vibrational mode.

In addition to the symmetry-breaking observation, the researchers note another aspect that is equally interesting. Specifically, the shape and width of the curves for the bending mode and the antisymmetric stretching mode are very similar; only their amplitudes are different. This indicates that the resonance trapping does not depend on the specific type of distortion in the molecular geometry, only on the fact that the motion breaks the molecule's symmetry. Such behavior is also unprecedented for these quasi-bound shape-resonant states, but the researchers have found that this type of behavior is exhibited in other molecules and is likely to be widespread. In addition to these experimental results, they have performed accurate electron-molecule scattering calculations, and these theoretical results were largely responsible for the qualitative explanations provided here.

The results demonstrate that there are reso-



6 Photoelectron spectra with incident photons on-resonance at 40 eV (left) and off-resonance at 30 eV (right). The peaks for the bending and antisymmetric stretching vibrational modes are greatly enhanced on-resonance. The peak representing the case with no vibration (red) is provided for reference.

nances with little sensitivity to distortions in bond length. Because it is common to correlate shape resonance position with changes in bond length, this has implications for studies that use vacuum ultraviolet or x-ray probes for analyzing complex or exotic structures. More generally, the results provide a natural means of examining coupling between nuclear and electronic degrees of freedom and for developing tools based on the connections between them. Such coupling between electronic motion and nuclear motion becomes increasingly important as scientists learn more about the geometry and dynamics of novel chemical structures such as those found in nanodevices and transient chemical species, and the results have implications for studies that use photoelectron spectroscopy as a diagnostic tool.

INVESTIGATORS G.J. Rathbone and E. Poliakoff (Louisiana State University), J. Bozek (ALS), and R. Lucchese (Texas A&M University).

FUNDING U.S. Department of Energy, Office of Basic Energy Sciences; Robert A. Welch Foundation; and Texas A&M University Supercomputing Facility.

**PUBLICATIONS** G.J. Rathbone, E.D. Poliakoff, J.D. Bozek, and R.R. Lucchese, "Observation of the symmetry-forbidden  $5\sigma_u \rightarrow k\sigma_u CS_2$ transition: A vibrationally driven photoionization resonance," *Phys. Rev. Lett.* **92**, 143002 (2004).



7 Branching ratios as a function of energy for different vibrations. Note that the resonance peak appears vividly for the two vibrations that break the molecular symmetry but not for the symmetric stretch, which does not.

### Studies of Flame Chemistry with Photoionization Mass Spectrometry

The old saying that "the solution to pollution is dilution" no longer applies to the Earth's atmosphere. The other approach is to minimize pollutant production at the source. But researchers are finding that detailed mathematical models of the complex chemistry that describes pollutant (e.g., soot and nitrogen oxides, or  $NO_x$ ) formation in the combustion of hydrocarbon fuels, the thermal decomposition of hazardous waste, or the ignition of solid rocket propellants are critical for the design of improved engines, power plants, incinerators, and munitions. Such models may incorporate thousands of chemical reactions involving hundreds of transient species (reaction intermediates) that form on the way toward completion of the process. The key to making the models quantitative is measuring the chemical parameters that populate the models, so-called thermophysical data. To this end, Taatjes et al. have combined mass spectrometry of ions excited by VUV light in a special laminar-flame apparatus with chemical theory to extract the energy needed to remove an electron (ionization energy) from nitrous acid, an important player in atmospheric chemistry.

VUV photoionization mass spectrometry with a synchrotron light source is a powerful new approach for studies of flame chemistry and the properties of combustion intermediates. Designed to study the formation and destruction of nitrous acid (HONO), an important chemical species in tropospheric chemistry and a key reaction intermediate in the combustion of solid propellants, recent laminar-flame experiments by researchers from Sandia National Laboratories and Cornell University have yielded a direct measurement of the HONO ionization energy, a benchmark piece of thermochemical data.

HONO emitted in automobile exhaust is an important air pollutant, as demonstrated in 1995 studies performed in the Caldecott Tunnel in Oakland, California [T.W. Kirchstetter et al., Environ. Sci. Technol. 30, 2843 (1996)]. The photolysis of HONO is a direct source of atmospheric hydroxyl (OH) radicals that promote ozone formation. Despite the importance of HONO in combustion and atmospheric chemistry and the fundamental interest in its properties, the ionization energy of HONO has not previously been directly measured. The Sandia and Cornell researchers combined photoionization mass spectrometry with a low-pressure, 1D laminar flame to make this measurement under well-characterized experimental conditions.

For their studies of a low-pressure (20-Torr) hydrogen–oxygen–argon flame doped with NO<sub>2</sub>, the researchers used a "flat flame" burner (Figure 8) on a branch of the Chemical Dynamics Beamline 9.0.2 equipped with a 3-m



A schematic representation (altered photograph) of the flat flame burner and molecular beam sampling assembly. The luminous zone of the flame used in these experiments has an unusual "peach" color attributable to chemiluminescent emission from electronically excited NO<sub>2</sub>. Hydrocarbon flames typically have a blue-violet or blue-green color associated with chemiluminescence from electronically excited CH and C<sub>2</sub>.

off-plane Eagle monochromator. The ability to precisely tune the photon energy over a wide range from 7.25 to 17 eV with good energy resolution [ $\Delta$ E (FWHM)  $\approx$  0.02 to 0.04 eV] afforded by the Eagle monochromator often enables selective detection of a single isomer. Experimental determinations of the isomeric composition of flame species are important in describing chemical reaction mechanisms that lead to soot formation with hydrocarbon fuels.

Premixed reagent gases enter the flame chamber through the porous flat face of a burner located at the left of the figure. The burner can be translated horizontally relative to a fixed quartz sampling cone and nickel skimmer. Flame gases are sampled through



Section of a mass spectrum of a low-pressure (20-Torr) hydrogen-oxygenargon flame doped with NO<sub>2</sub>. The spectrum, taken 0.5 mm from the burner at a photon energy of 11.33 eV, shows NO<sub>2</sub> (m/e = 46) and HONO (m/e = 47).

Experimental PIE curves for trans-HONO. Data were taken at energy resolutions  $\Delta E$  (FWHM) = 40 meV (blue) and 60 meV (red).

a 200-micron pinhole in the quartz cone and expanded to a pressure of  $10^{-4}$  Torr before passing through the skimmer to form a molecular beam. The molecular beam enters a differentially pumped ( $10^{-6}$  Torr) ionization chamber, where it is crossed by the tunable VUV beam from the ALS. Photoions are extracted using a pulsed-field technique and mass-analyzed with a 1.3-m linear TOF mass spectrometer.

A mass spectrum obtained in this way at a photon energy of 11.33 eV and sampled very close (0.5 mm) to the burner face exhibits peaks at mass-to-charge ratios of 46 and 47, which correspond to  $NO_2^+$  and  $HONO^+$ , respectively (Figure 9). The integrated ion signal for m/e = 47, recorded for photon energies from 10.83 to 11.63 eV, generates the photoionization efficiency (PIE) spectrum for HONO shown in Figure 10.

A Franck–Condon simulation based on calculated geometries and force constants of the positively ionized and neutral trans-HONO isomer, including the effects of Duschinsky rotation (a symmetry operation connecting vibrational modes), is used as a fitting function to estimate the adiabatic ionization energy from the experimental data of Figure 10. The contribution of the cis-HONO<sup>+</sup> isomer is neglected because its ionization energy is calculated to be 0.3 eV higher. The measured ionization threshold of 10.97  $\pm$  0.03 eV is in excellent agreement with recent ab initio calculations.

The present measurement provides a direct benchmark for the thermochemistry of HONO and  $NO_2$ . Values of the heat of formation of the HONO<sup>+</sup> cation and the proton affinity of  $NO_2$  derived from this value are in good agreement with existing indirect thermochemical estimates.

INVESTIGATORS C.A. Taatjes and D.L. Osborn (Sandia National Laboratories) and T.A. Cool and K. Nakajima (Cornell University).

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### Determination of Absolute Photoionization Cross Sections of Reactive Species

Molecules are complex entities characterized by a rich spectrum of electronic orbitals, atomic vibrations, and molecular rotations. Which orbitals, vibrations, and rotations are active in the molecules participating in a chemical reaction determines what the outcome will be (e.g., the quantities of the various possible reaction products). A key step in analyzing reaction processes in such detail is the use of VUV light to ionize the products for identification in a mass spectrometer or some other detection device. It turns out that VUV photoionization is itself a reaction whose cross section (probability) needs to be known to extract information from the experiment. So far so good, but what happens when the product molecules are so reactive that they don't stick around long enough to be analyzed? Robinson et al. recently developed a general procedure to attack this problem for photoionization reactions involving highly reactive species known as free radicals and are now applying it to the measurement of photoionization cross sections.

In experiments ranging from photodissociation and molecular-beam scattering experiments to flame diagnostics, VUV radiation is typically used to photoionize reaction products that can then be measured by a number of detection schemes. Extraction of information such as product branching ratios from such experiments requires knowledge of photoionization cross sections for each chemical species probed. While cross sections for a wide array of closed-shell molecules are known, the high reactivity of radical molecules makes the determination of their photoionization cross sections quite difficult. A UC Berkeley and Berkeley Lab team, which recently developed a general method for the determination of such cross sections, has used this technique to measure the absolute cross sections for the formation of  $C_3H_5^+$  by photoionization of two isomers (allyl and 2-propenyl radicals) of  $C_2H_5$ .

Based on the use of tunable synchrotron radiation, the general method for the determination of photoionization cross sections developed by the Berkeley group combines the technique of photofragment translational spectroscopy and tunable VUV photoionization of momentum-matched photofragments. If one of the photofragments has a known photoionization cross section, one can then determine the cross section of the other fragment, even if the system exhibits complex photodissociation dynamics.

The group performed their photoionization experiments on allyl ( $CH_2CHCH_2$ ) and 2-propenyl ( $CH_2CCH_3$ ) radicals with the use of

a rotating-source/fixed-detector crossedmolecular-beams instrument located on the Chemical Dynamics Beamline 9.0.2 at the ALS. A pulsed valve (frequency 100 Hz, nozzle diameter 0.5 mm, pressure 200–300 Torr, temperature  $\approx$  80 °C) generated a molecular beam of either allyl chloride or 2-chloropropene, both about 2%, in helium. This molecular beam was then photodissociated by a 193-nm argon fluoride (ArF) excimer laser beam propagating orthogonally to both the molecular beam and detector axes.

Photofragments resulting from the laserexcited photodissociation enter the detector and travel 15.1 cm before they are ionized by tunable VUV synchrotron radiation, mass-selected by a quadrupole mass filter, and counted as a function of time with a multichannel scaler. The product is a set of angle-resolved TOF spectra for ions with a specific mass-to-charge ratio. Owing to the tunability of synchrotron radiation, ionization energies could be set to minimize ionization associated with VUV-excited dissociation of the photofragments (dissociative ionization).

In the experiments, two types of photodissociation measurements were performed. First, to determine a translational energy distribution in the center-of-mass frame for each process, a set of TOF spectra were taken for each m/e pertinent to the channel of interest over a range of ionization energies. Integration of this series of measurements



Absolute PIE curves for m/e = 41 ( $C_3H_5^+$ ) photoproducts for allyl chloride (left) and 2-chloropropene (right). Data were taken with the detector set at an angle of 30° from the molecular beam. The solid squares represent the data points with 2 $\sigma$  error bars.

(following normalization by VUV photon flux, laser shots, laser power, etc.) yielded a PIE curve, showing relative photoionization cross sections as a function of photon energy. By comparing the data from the radical of interest to the chlorine photofragment (the fragment with a known photoionization cross section), absolute photoionization cross sections were determined and used to place the PIE curves on an absolute scale.

Shown in Figure 11 are the absolute PIE curves obtained for allyl and 2-propenyl radi-

cals. Data were taken with the detector set at an angle of 30° from the molecular beam. As can be seen, the PIE curves are similar but not identical, suggesting that the detected  $C_3H_5$  products are different species and that scrambling between  $C_3H_5$  isomers after C–CI bond cleavage but before ionization does not occur. Nonetheless, the measured photoionization cross sections offer future chemical dynamics researchers the ability to more cogently utilize the experimental possibilities offered by synchrotron radiation. **INVESTIGATORS** J.C. Robinson (UC Berkeley, Berkeley Lab, and Intel Corporation) and N.E. Sveum and D.M. Neumark (UC Berkeley and Berkeley Lab).

**FUNDING** U.S. Department of Energy, Office of Basic Energy Sciences.

**PUBLICATIONS** J.C. Robinson, N.E. Sveum, and D.M. Neumark, "Determination of absolute photoionization cross sections for isomers of C<sub>3</sub>H<sub>5</sub>: Allyl and 2-propenyl radicals," *Chem. Phys. Lett.* **383**, 601 (2004).

#### A Hollow-Ion Resonance of Unprecedented Strength

Our understanding of how electrons move within an atom is, in general, based on the assumption that individual electrons are sensitive only to the average positions of the other electrons in the atom. While it is true that electron correlation (the effect that one electron has on another) is usually insignificant compared to the attraction between the nucleus and electrons, it becomes especially important in negative ions that have more than their normal contingent of electrons (three instead of two for He<sup>-</sup>). These electron–electron interactions can be the key to determining the physical properties of an atom and are thus of basic importance in many fields, such as astronomy, plasma chemistry, and x-ray laser development. Bilodeau et al. have investigated what happens when photons are used to excite electrons deep inside a negative helium ion's inner (1s) shell. The resulting hollow ion, with all three of its electrons in excited states, is a particularly valuable test system, as it offers a challenging yet tangible target for future theory development.

A so-called hollow ion is formed when core electrons are removed or excited to higher energy levels, leaving an empty inner shell. Such states can be produced in He<sup>-</sup>, a fundamental three-electron system and prototypical negative ion. The nuclear Coulomb attraction is efficiently screened in negative ions, greatly enhancing the effects that the electrons have on each other and providing an ideal opportunity to verify and further motivate theoretical models of electron correlation. Our understanding of these basic interactions can elucidate processes of importance in many fields, from the interpretation of cosmic spectra to x-ray lasing efforts using innershell ionization and hollow-ion formation. At the ALS, researchers from Western Michigan University, the University of Nevada, Reno, and the ALS have detected in negative helium ions a resonant simultaneous double-Auger decay of unprecedented strength, evidence of a triply excited hollow-ion state that has eluded observation for 25 years.

In contrast to valence-electron excitations, decay pathways of core excited states are highly correlated phenomena, typically involving multi-electron processes such as Auger decay. States located above the double-ionization limit (such as triply excited hollow-ion states) can decay via two-electron emission in a single step if one electron is demoted with the simultaneous emission of two others (double-Auger decay). The significant challenges presented by these complex and exotic multi-electron processes to high-level theoretical models make detailed studies in computationally accessible three-electron prototype systems of prime interest.

The first experimental investigation of Heindicated that some of the observed structure was inconsistent with predictions and stimulated renewed theoretical interest. Included in these new ab initio calculations were detailed investigations of hollow-ion resonances. The positions, widths, and cross sections of these resonances present sensitive parameters for evaluating the calculations; however, such measurements remained unavailable. In addition, while the lowest triply excited quartet state in He<sup>-</sup> (the  $2s2p^{2}$ <sup>4</sup>P state) was predicted 25 years ago, until now it has eluded observation. In fact, this state has not been observed in photoexcitation of any threeelectron system.

At Beamline 10.0.1, researchers were able to measure, for the first time, the photo-excitation widths, line shapes, and absolute cross sections of He<sup>-</sup> triply excited (hollow-ion) states. A rubidium-vapor charge-exchange ion source was used to produce a 9.96-keV He<sup>-</sup> beam in the 1s2s2p <sup>4</sup>P<sup>o</sup> ground state. A 60-nA beam of He<sup>-</sup> was merged with a counterpropagating photon beam, leading to excitation of the He<sup>-</sup> from its ground state to the 2s2p<sup>2</sup> <sup>4</sup>P, 2p3s3p <sup>4</sup>D, and 2p3s3p <sup>4</sup>P states. Subsequent Auger decay in the merged region led to two-electron loss (Figure 12). The



**12** Top: Absorption of a photon by an He<sup>-</sup> ion in the 1s2s2p <sup>4</sup>P<sup>o</sup> ground state boosts a 1s electron into an empty 2p orbital, forming the triply excited hollow-ion 2s2p<sup>2</sup> <sup>4</sup>P state. Bottom: In double-Auger decay, one electron decays to the 1s orbital, while the other two electrons are simultaneously ejected, forming He<sup>+</sup>.

resulting He<sup>+</sup> ions (the signal) were deflected by a demerging magnetic field and counted to obtain the cross sections (i.e., probabilities) of the various resonances versus incident photon energy (Figures 13 and 14).

Because the 2s2p<sup>2</sup><sup>4</sup>P state lies below the 2s<sup>2</sup> threshold, there is no intermediate state to accommodate sequential (two-step) Auger decay. The observed signal must therefore be due to a double-Auger process, involving all three electrons of the ion simultaneously. This represents the first observation of double-Auger decay from a photoexcited negative ion, and its strength is three to four orders of magnitude larger than similar observations in other systems. Calculations of double-Auger decay in He- are not yet available and would be of great value in improving our understanding of this unexpectedly strong reso-



Measurement of double-Auger decay from the 2s2p<sup>2</sup> <sup>4</sup>P state with the best-fit profile. The filled circle is the absolute cross-section measurement.





nance. Otherwise, theory is in good general qualitative agreement with the new data, except for differences in the position and shape of certain features. A fourth feature in the spectrum, resolved for the first time, is observed to be Lorentzian in shape, contrary to predictions (Figure 14). The researchers concluded that, while our understanding of this three-electron system has advanced considerably in the past few years, further improvements in theory are still needed. **INVESTIGATORS** R.C. Bilodeau and G. Turri (Western Michigan University and ALS), J.D. Bozek and G.D. Ackerman (ALS), A. Aguilar (ALS and University of Nevada, Reno), and N. Berrah (Western Michigan University).

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### Facility Report





### ALS Strategic Plan

With the approaching full realization of Director Daniel Chemla's original strategic plan, the ALS stands at a pivotal point in its history. The available straight sections are built out or spoken for, and only a few of the superbend lines remain uncommitted. An early vision of the future was offered in 2003 as part of the DOE's Office of Science Twenty-Year Facilities Roadmap. We proposed an orderly upgrade, at modest cost, having three components: an upgrade of the source, an upgrade of the older insertion devices, and new application-specific beamlines. A more detailed strategic plan was fleshed out in 2004 through a series of retreats with our user community (Figure 1) and with input from our SAC. The plan dovetails neatly with the scientific priorities of DOE BES. It is also responsive to the needs of our users, not only in the provision of scientific tools, but also in the provision of a safe and congenial research environment. The emphasis is on keeping the ALS at the cutting edge for the next decade and beyond by honing our existing stock and by creating sharper tools that exploit the very significant advances in accelerator and insertion-device technology that have occurred since the ALS began operation.



### Building a Foundation for the Future

The ALS, a world-class facility optimized for advanced spectroscopies, is in a position to address many fundamental questions as it enters its next phase: Where are the electrons? Where are the atoms? Where are the spins? Some of the challenging areas that can be addressed include the following:

- Size-dependent and dimensional-confinement phenomena at the nanoscale.
- Correlation and complexity in physical, biological, and environmental systems.
- Temporal evolution, assembly, dynamics, and ultrafast phenomena.

Our focus throughout the strategic planning process has been on the qualitatively new science that would be enabled by upgrading the source—initiatives that will continue to make it possible to address grand scientific and technological challenges with incisive world-class tools.

### Upgrades and Additions

Our highest priority is to begin top-off operation, in which electrons in the storage ring are replenished approximately every minute, resulting in increased brightness and beam stability. This will require a booster upgrade, significant changes to the radiation-protection system, and a variety of other hardware and control improvements. The use of small-gap in-vacuum undulators will further enhance brightness, especially in the important energy range above 500 eV. Concurrent development of superconducting undulators will extend the reach of ALS undulators in the multi-keV range. The combination of top-off mode and these new insertion devices will allow an increase in brightness from 8 to over 100 times, depending on the specific undulators and photon energy range (Figure 2).

Our second priority in the machine area is to further study the possibility of a picosecond

bend-magnet source. Based on a concept put forward by A. Zholents (Center for Beam Physics, Berkeley Lab), it was found that by inserting rf deflecting cavities into two adjacent straight sections, vertical beam height can be traded for pulse length on the bendmagnet beamline located halfway between them (Figure 3). This will then be an exceedingly powerful source of, roughly, 1-ps pulses, creating opportunities for high-repetition-rate, ultrafast timing experiments.

Currently there are 37 simultaneously operating beamlines operating at the ALS. While some of the older beamlines will be retired as



Members of the Users' Executive Committee meet with ALS management and staff at a spring 2004 retreat to discuss the strategic plan.



ALS brightness curves. The combination of top-off mode and new insertion devices—in-vacuum (left) and superconducting (right)—will allow an increase in brightness from 8 to over 100 times.

more powerful ones come online, the rest need to be upgraded to take full advantage of the increased brightness made possible by top-off operation. Many endstations depend on high-resolution focusing devices—zone plates and mirrors—for world-class performance. The continued development of these optics, as well as an orderly program to replace them on highly productive older beamlines, is essential to the future success of the facility.

Available detectors are also not well-matched to the capabilities of the ALS and other highbrightness synchrotrons. A broad-based program, based in part on high-energy-physics detector developments, is needed to create high-rate pixel detectors. In addition, highspeed streak cameras are needed to fully utilize the femtosecond sources coming online. The ALS, in cooperation with Berkeley Lab's Engineering Division, has begun work in these areas. Because of its importance to our user program, we plan to expand detector development and bring it to a successful conclusion via technology transfer to a commercial supplier.

### **New Beamlines**

We plan to exploit the accelerator developments described above to extend our capabilities for high spatial and temporal resolution and utilize the remarkable coherence properties of the ALS. Top-off operation will make possible the replacement of our 11year-old 5-m-long undulators with pairs of chicaned 2-m-long modern insertion devices with superior performance, feeding a new generation of beamlines that will address the outstanding problems of the coming decade. Three "waves" of such proposed beamlines are outlined below.

In addition, five beamlines are already funded or under construction—three based on undulator sources (PEEM-3, the ultrafast x-ray facility, and MERLIN—all funded by DOE BES), one based on a regular bend magnet (the soft x-ray microscope XM-2), and one on a superbend (a migration of the microdiffraction program from Beamline 7.3.3).

PEEM-3 is a third-generation photoemission electron microscope with a spatial resolution



3 Schematic of the effect on electron bunches (top, green) of rf deflecting cavities (also known as "crab cavities") in the ALS lattice (bottom, blue).



In PEEM-3, electrons are focused by an electrostatic objective lens before being deflected 90° into an electrostatic electron mirror designed to cancel aberrations introduced by the lens.

of a few nanometers (Figure 4). The system will be primarily used for studying phenomena that require extremely high resolution instruments, such as pinning mechanisms in magnetic domains. The ultrafast x-ray facility being built in Sector 6 will allow the study of atomic motion at the molecular-vibration time scale. This beamline will use an undulator version (Figure 5) of the laser-driven electron-beam-slicing source currently in use on bend-magnet Beamline 5.3.1. MERLIN is an undulator beamline designed to provide ultrahigh energy resolution for ARPES and IXS. It will operate in the VUV energy range below 150 eV, where low-energy excitations are crucial to understanding the behavior of strongly correlated systems. XM-2 is a bendmagnet beamline for high-resolution soft x-



5 The ultrafast x-ray facility will be the first at the ALS to use a small-gap, in-vacuum undulator source for increased brightness.


CAD model of the XM-2 beamline to be built in Sector 2.

ray microscopy and tomography of biological cells (Figure 6). It is being constructed as part of a National Center for X-Ray Tomography funded jointly by the NIH and DOE BER. Funds have also been secured from NSF to migrate our highly successful microdiffraction program from bend-magnet Beamline 7.3.3 to a new home on superbend Beamline 12.3.2.

### WAVE ONE

As our highest priority, we propose to establish in half of straight section 12 a beamline to provide coherent light in the 0.5–2 keV range with full polarization control. The motivation for this initiative has several parts: (a) nanoscale tomography—3D imaging of the internal structure of complex, fine-grained materials at high spatial resolution of materials from labyrinthine, mesoporous catalysts to electronic devices; (b) whole-cell imaging at molecular resolution-a tomographic singleparticle imaging technique that can identify and locate large proteins or macromolecular assemblies of known crystallographic structure within a cell; and (c) the time evolution of mesoscopic systems. One branch of this beamline will serve the soft x-ray coherent scattering community, where much of the interest is in magnetic phenomena. This approach is designed to study time correlation as well as magnetic-field and temperaturedependent correlation and hysteresis phenomena. The other branch will be devoted to diffraction microscopy. This new form of lensless imaging is designed to provide 3D structures to 10-nm resolution for frozen hydrated biological specimens and even higher resolution where radiation damage is not a limitation.

In the other half of straignt section 12, we propose a "nanoARPES" facility for the study of surfaces and structures that cannot be prepared in large formats and for nanostructures created in the Molecular Foundry. ARPES has emerged as a leading technique for understanding the electronic structure of high-temperature superconductors and other complex oxides. Often, the most interesting materials are intrinsically, or extrinsically, inhomogeneous (i.e., in nanoscale phase segregations). Small probe sizes enable the isolation of more homogeneous materials than can be achieved by interrogating the entire sample. In some other cases (as with transuranics), larger specimens would pose

unacceptable hazards. We propose to create a 100-nm probe for a nanoARPES specializing in valence-shell photoemission at 92 eV. The other branch of this beamline will be devoted to continuing development and testing of EUV optics.

The third proposal in Wave One is a new superbend beamline for time-resolved SAXS. This facility will make it possible to follow, in real-time and with elemental discrimination, the synthesis and self-assembly of novel nanostructures. The topic of self-organization spans a broad range of topics, from correlated electron systems to protein folding, to surfactant-coated nanoparticle ripening to form monodispersed size distributions, and beyond (to the organization of the cosmos). The new materials studied apply to many national missions such as space exploration, the construction of particle accelerators, medical advances, and the U.S. energy problem, which has become a homeland security and environmental issue. Development of this beamline will facilitate the development of joint programs with the Molecular Foundry, Berkeley Lab's Nanoscale Science Research Center (NSRC), and Beamlines 11.3.1 (small-molecule crystallography) and 10.3.2 (micro-XAS).

### WAVE TWO

Each of the above facilities will open new, unique capabilities at the ALS in service of the user community. They are well-matched to the capabilities of the upgraded storage ring and serve the core constituency of the ALS. In addition, the large majority of the older ALS beamlines are in need of a significant upgrade. Most importantly, we need to keep our flagship beamlines, which have been operating for a decade in an ever-more oversubscribed mode, at the cutting edge. The highest priority is to chicane the Sector 10 straight section and give each branch-the photoemission branch and the atomic/molecular physics branch—a separate EPU for full polarization control and a separate beamline so they can run simultaneously. This beamline has been exceedingly productive in terms of high-profile publications and citations. Each of the new, separate beamlines will be application-specific, optimized for the scientific program of the two user communities, without the need for

the compromises of the shared beamline in current use.

How fast can you demagnetize a magnet? What are the mechanisms? Studies of fast, time-dependent magnetic effects will shed light on both basic and technologically important problems involving domain switching, vortex dynamics, and exchange interactions. We plan to place an EPU in the empty half of straight section 6 to be time-shared between a new, dedicated program in ultrafast magnetism and the soft x-ray branch of the slicing source. This new facility will focus a confluence of experimental and computational interest into problems that overlap synergistically with the mission of the Molecular Foundry and the community that is coalescing around ultrafast phenomena in general.

While MERLIN is designed for the ultimate energy resolution below 150 eV, there is a great need to extend the capability for ultrahigh-resolution IXS investigations to energies at least as high as 1 keV, so as to be able to scan the momentum (q) vector out to the Brillouin zone boundary (Figure 7). The ability to map the q-dependent dispersion relations of exotic elementary excitations in complex media is key to understanding many outstanding problems in condensed-matter physics. The elemental, spin, and orbital sensitivity of resonant soft x-ray scattering offers a unique combination of capabilities that will lead to many high-impact experiments. We plan to build on the experience at MERLIN in designing a q-resolved inelastic scattering beamline (QERLIN), which should fit into Sector 2



**2** QERLIN will allow us to map the momentum vector q beyond our current capability, out to the Brillouin zone boundary.

with a modest rearrangement of accelerator components. This beamline will have to be extra long, and this is the only location at the ALS where the necessary length is available. The incorporation of very high resolution photoemission in the 1-keV range would also be considered.

### WAVE THREE

The flagship beamlines in Sectors 7 and 8 are prolific generators of world-class research and high-profile publications. Yet each would benefit from the replacement of the old 5-m undulators with brighter EPUs and new optics. Chicaning these straight sections to add beamlines is also under consideration.

If the use of rf deflecting (crab) cavities makes a picosecond bend-magnet source viable, attention will turn to finding an appropriate location. One possibility would be to place the cavities in Sectors 7 and 8, thereby delivering picosecond pulses from the 7.3 bend-magnet ports. The picosecond nanomagnetism studies already underway on the PEEM-2 microscope on Beamline 7.3.1 would benefit greatly from the shorter pulses. Following the planned migration of the microdiffraction program to a superbend, the 7.3.3 port would become available for an ultrafast program.

## Safety, Staffing, and Infrastructure

The safe operation of the facility and user program is the top priority of both ALS management and the ALS community. As the user community grows and the experimental floor becomes more crowded, maintaining and further improving our excellent safety record becomes an ever-increasing challenge. We will continue and enhance the safety training of staff and users alike and will redeploy staff to increase the coverage of beamline coordinators to provide more safety support to users.

The scientific staffing level of most of the beamlines is barely half of what is considered optimal. It is generally observed that staffing levels go hand-in-hand with scientific productivity; hence the facility is significantly underutilized. The intellectual excitement of the ALS as a forefront science facility has been a powerful tool in the recruitment and retention of outstanding staff, but additional sustained efforts are required to increase diversity both in gender and in underrepresented groups. To build a more diverse scientific staff, the ALS has to contribute to the "pipeline" of qualified applicants. The ALS Doctoral Fellowship Program has been very successful in attracting graduate students and providing them with high-level technical training. We intend to expand this program with special emphasis on underrepresented groups. We also envision starting a distinguished postdoctoral fellowship program with the same emphasis, to increase and diversify our pool of candidates for beamline scientist positions.

Both safety and productivity are jeopardized when there is inadequate lab and office space. Adequate housing and meal service is also essential to any user facility that operates around the clock. The ALS and Berkeley Lab have proposed both a User Support Building (Figure 8) to relieve overcrowding on the



Artist's conception of the User Support Building.



Possible site for a Berkeley Lab Guest House in relation to the ALS and the Molecular Foundry.

experiment floor and a Berkeley Lab Guest House to be located within walking distance of the ALS and the Berkeley Lab cafeteria (Figure 9). Both projects are very high priorities for the ALS, and requests for funding (from DOE for the User Support Building and from UC for the Guest House) are pending.

In the longer term, we are eager to construct CIRCE, the leading candidate for a highly stable terahertz source based on coherent synchrotron radiation. This source is designed to make use of the ALS injection system, would sit on top of the booster ring, and would serve eight beamlines (Figure 10). The facility will provide ultrashort pulses and be well suited to a wide variety of pump–probe experiments.

While the ranking of the projects above reflects the current sense of priorities, we recognize that priorities can change. The planning process is ongoing, with further workshops and reviews planned to validate the scientific need, organize the teams, and create detailed designs for each major component of the plan.



10 A national workshop on terahertz science and its future concluded that, as the community grows and matures, the scientific case for a terahertz user facility such as CIRCE will become stronger.



## Operations and Availability

The mission of the ALS is to "support users in doing outstanding science in a safe environment." Critical to that support is the delivery of high-quality beam. Delivering beam according to the published schedule, along with an efficient, effective safety program, allows ALS researchers to make maximum use of the limited beam time. In 2004, the ALS maintained its exemplary operations record while continuing to make significant improvements in beam quality and reliability. In addition, the Operations groups worked with the Experimental Systems Group and other groups at Berkeley Lab to bring online two new beamlines, including a beamline for examining materials under conditions of

extremely high pressure and temperature and a beamline optimized for x-ray tomography. Both of these beamlines use superbends, the superconducting bend magnets installed in the ALS several years ago, as the source of hard x rays.

The research community at the ALS has become accustomed to high operational efficiency and reliability, and it was not disappointed during this period. As shown in Figure 1, the ALS delivered beam to users over 95% of the time scheduled for user operations in FY 04, doing slightly better than the previous year.

As in years past, we look very carefully at our different systems to determine where to focus our resources to improve reliability. Figure 2 shows our "lost user-beam analysis" over the past several years. These figures allow us to pinpoint the most frequent causes of lost user-beam time. Improvements in beam time lost due to water and power supplies in 2004 resulted from attention paid to these areas since 2003. As a result of the 2004 analysis, we are continuing to install higher-order mode (HOM) dampers that should reduce time lost due to the longitudinal feedback systems in future years.

### Changes in User and Instrument Hours

The monthly operations schedule continued to include the minimum number of maintenance and installation periods consistent



ALS operational availability (percentage of scheduled user-beam time actually delivered).

■10 ■20 □30 □40

#### ■ FY00 ■ FY01 ■ FY02 ■ FY03 ■ FY04



Lost user-beam analysis. The bars represent the percentage of user-beam time lost over the last four fiscal years, separating out the various machine systems responsible. THC/LBF = third-harmonic cavities/longitudinal feedback; SR RF = storage-ring rf power.).

with safe, efficient operation, which has been our practice for the last several years. Allowing approximately three days per month for needed maintenance and installation of new instrumentation has provided the maximum number of hours for user operations. In addition, this year we had one five-week installation shutdown primarily to install a new wiggler in Sector 5. This wiggler will serve the protein crystallography beamlines in that sector as well as the needs of the femtosecond slicing source to be installed in Sector 6. In addition, we replaced the superbend cryogenic coolers, which require rebuilding annually. The delivered operating hours remained at about the same level in FY 04 as in previous years.

With the constant number of operating hours and the installation of new beamlines, we were able to increase the number of instrument hours (user hours multiplied by the number of beamlines that can simultaneously accept beam). We finished the fiscal year with 37 beamlines operating simultaneously, up from 35 at the end of the previous fiscal year. Figure 3 shows the growth in instru-





ment hours since the first full year of ALS operations. This year's growth resulted in

the delivery of about 190,000 instrument hours, an increase of 13% over FY 03.

### Facility Growth

In this year's shutdown, we installed the new wiggler (described above), the first optic for the PEEM-3 beamline, and a new liquid nitrogen tank to supply users. Two superbend beamlines, one for research on materials at high pressure and temperature (CALIPSO) and another to provide x-ray tomography on various geological and biological materials, were commissioned early in the fiscal year. These new beamlines have enhanced our ability to serve local users, opening up major new capabilities for geoplanetary, geological, and biological research using the hard x-ray capabilities of the ALS spectrum.

### Beam Quality Highlights

#### Christoph Steier

Over the last five years, EPUs have been used very successfully at the ALS to generate high-brightness photon beams with arbitrary polarization. However, all three EPUs installed so far cause significant changes in the vertical beam size, especially when the row phase is changed to adjust the polarization of the emitted photons. Detailed beam-based measurements showed that this is caused by a row-phase-dependent skew quadrupole term in the EPUs (Figure 4). Based on those results, very detailed magnetic and mechanical measurements were carried out on the third EPU before it was installed in the ring. These measurements finally revealed the exact reason for the effect. Magnetic forces between the permanent-magnet blocks create shift-dependent micrometer-size motion of the holder modules on which the blocks are mounted. This results in fairly significant skew quadrupole field errors and, ultimately, beam size variations.

To reduce the impact of the EPU-related variations on experiments at the ALS, an active feedforward system, using four wires installed in grooves of the EPU vacuum chamber along the full length of the EPU, was tested. Figure 5 shows the results of the initial tests. At small baseline coupling (amplifying the effect of the EPU), the system is capable of nearly perfectly compensating for the skew



Results of beam measurements of the shift-dependent skew quadrupole strength of the first two EPUs installed in the ALS.



5 Shift-dependent variation of the beam size measured at Beamline 3.1 (vertical beta function of 24 m) with and without the skew quadrupole feedforward (FF).

gradient effect on the beam size using a predictive feedforward table. With the larger nominal ALS emittance (for Touschek lifetime reasons), the relative variation is even smaller. A complete feedforward algorithm has been implemented and is being used for one of the devices in routine user operation since the beginning of June 2004.

To ensure optimum performance, the complete storage ring is routinely realigned (about every other year). After each realignment, the ring's closed orbit is optimized to coincide with the magnetic centers of the realigned quadrupoles. In this year's realignment, the moves were smaller than in previous years and the realigned storage ring is performing well. The alignment was carried out in close consultation with all users, and three days of dedicated beam time were added at the end of the startup period to optimize and realign beamlines if necessary.

Several stable high-resolution beam-position monitors (BPMs) were added around the center bend magnets in the five sectors (1, 2, 3, 6, 11) that were not equipped with these before. Now all sectors have BPMs surrounding the center bend magnets, ensuring muchimproved long-term orbit stability in all arcs.

An improved lattice now provides 33% lower vertical beta functions in the straight sections and 15% lower beta functions in the center bend magnets (and slightly larger beta functions in the outer bend magnets). This results in a smaller beam size (but larger divergence) in the straights, which in combination with the diffraction limit corresponds to an increase in brightness of up to 15%. More importantly, the lattice provides a better dynamic momentum aperture (i.e., slightly longer Touschek lifetimes), will facilitate the use of smaller-gap vacuum chambers in the straights, and is less sensitive to disturbances due to insertion-device motion.

Over the last few years, there has been a significant effort to damp higher-order modes in the main and third-harmonic rf cavities of the ALS. The purpose of these dampers is to reduce the driving terms for multibunch instabilities and therefore reduce the requirements for the multibunch feed-

back systems. The efforts have resulted in much greater reliability of the multibunch feedback systems. Problems with harmonic cavities and multibunch feedback systems were the largest source of lost beam time about five years ago; last calendar year they accounted for next to no losses. During the 2004 shutdown, additional HOM dampers were installed in the third-harmonic cavities, completing the system of dampers.

# Fast Orbit Feedback in Routine User Operation

Christoph Steier, Eric Williams, Ed Domning, Tom Scarvie

A fast global orbit feedback system has been implemented at the ALS and is currently being employed during user operation. The system has two main purposes. The first is to meet the demands of some users for even greater (submicron) short-term orbit stability. The second is to enable the use of more sophisticated insertion-device compensation schemes (e.g. tune, beta-beating, coupling) for fast-moving insertion devices such as EPUs without the deterioration of orbit stability. The fast orbit feedback has been used since June 2004 and has been extremely reliable and stable. It works in close cooperation with the already existing slow orbit feedback and all potential interference problems between the two systems have been solved successfully.

The main reason it was necessary to keep two somewhat independent orbit feedback systems is that there are not enough corrector magnets with high bandwidth (80 Hz). Only 22 high-bandwidth corrector magnets exist in each plane. To achieve the required long-term orbit stability, significantly more low-bandwidth corrector magnets (2 Hz) are used in the slow feedback system. Since there are no demonstrated solutions incorporating corrector magnets with very different bandwidths into the same feedback system, a layout with two separate feedback systems was chosen.

This layout has the potential to cause unintended interference effects between the two systems, leading to oscillations or periodic steps or spikes in the orbit. In the past, frequency deadbands were implemented, so that the frequency response of the two systems do not significantly overlap, with some success in reducing interference effects. However, this approach has one main disadvantage: to work, the deadband has to be fairly wide, leaving a reasonably large range of frequencies where neither of the systems is effective. Often this deadband happens to be exactly in the range where transient orbit distortions due to insertion-device motion occur.

An improvement over the pure deadband approach was implemented earlier at the APS and adapted for the ALS. In that approach, the fast and slow orbit feedbacks communicate. At the ALS, the slow orbit feedback updates the setpoint values of the fast orbit system with its update rate (i.e., 1 Hz). The new setpoints are based on the current orbit, plus the action the slow feedback anticipates doing in its current step. The results of this approach to avoiding interference between the fast and slow orbit feedbacks are very good (Figure 6). No interference has been observed at all. The combination of the two systems behaves exactly like the sum of the positive effects of each of the systems.

The long-term orbit stability at the ALS is very good; however, it does not yet reach the submicron level of the short-term stability. The long-term drift over the course of a week is approximately 3 microns rms in both horizontal and the vertical planes. Figure 7 shows the evolution of the horizontal and vertical rms orbit error over the course of 1.5 days. The reason the rms error does not start at zero is that only a limited number of corrector magnets (smaller than the number of BPMs) was used in the orbit feedback. However, this systematic error is very stable over time. It changes on the time scale of about a year, as the misalignment of the storage ring increases. It is not of importance, since the beamline alignment drifts on a similar time scale by larger amounts relative to the storage ring.

With the combined use of fast and slow orbit feedback systems, the ALS now

achieves submicron stability in the vertical plane for frequencies higher than 0.01 Hz. Anticipating future user needs, we will continue to improve the orbit feedback systems in a steady, evolutionary process. There are still significant upgrades planned for the fast orbit feedback, including networking upgrades, improvements in processor speed, better digital/analog converters, and better optimized digital filters. For the slow orbit feedback system, there are plans to incorporate additional stable BPMs and to monitor the physical motion of BPMs online.





Step response of different combinations of fast and slow orbit feedbacks.



Long-term change of the rms orbit distortion with slow orbit feedback.

# **ACCELERATOR PHYSICS**

David Robin, Accelerator Physics Group Leader

### Introduction

The Accelerator Physics Group (Figure 1) plays several important roles in the ALS mission of supporting users in doing outstanding science in a safe environment. The first is to make certain that the ALS provides high-quality beam in a reliable manner to users. The second is to strive to understand and continually improve the performance of the facility, keeping it at the forefront of synchrotron radiation sources. The third is to ensure that machine upgrades are implemented smoothly with minimal adverse impact to users. The fourth is to study potential facility upgrades that will enhance the capabilities and capacities of the ALS.

This year significant gains were realized in understanding and improving the quality of the beams delivered to users. One area of improvement was in beam stability. During the 2004 shutdown, higher-order-mode dampers were installed in the third-harmonic rf cavities. These dampers reduced the strength of the HOMs in these cavities that were responsible for driving transverse instabilities. Before the dampers were installed, it was necessary to properly adjust the cavity temperature and cavity tuners for stable operation. On a number of occasions during the previous year, cavity parameters drifted, resulting in unstable beam. Since the HOM dampers were installed, there has been no loss in transverse stability. During the 2005 shutdown, HOM dampers will be installed, in the main rf cavities to reduce the longitudinal modes in those cavities. This should significantly reduce the load on the longitudinal feedback system and might make the cavities passively stable.

This was the first year of routine operation with the fast orbit feedback system. The system is able to operate with an update rate of about 1.1 kHz. Before the fast feedback was installed, there existed a slow orbit feedback system with an update rate of about 1 Hz. The slow orbit feedback was only capable of suppressing noise below 0.05 Hz. With only the slow orbit feedback, the integrated steadystate closed-orbit motion in the insertion-



Accelerator Physics Group. Christoph Steier, Greg Portmann, David Robin, Agusta Loftsdottir, Hiroshi Nishimura, Fernando Sannibale, Walter Wittmer, Tom Scarvie, Linda Snow, Weishi Wan and Warren Byrne.

device (ID) straight sections in the frequency range between 0.05 and 500 Hz was below 2 microns in the vertical plane and about 4 microns in the horizontal plane. With the fast orbit feedback, the rms orbit motion in the same frequency range has been reduced to less than 1 mircon vertically and less than 2 microns horizontally. The suppression of residual transient orbit distortions caused by ID motion is significantly larger than the reduction in steady-state orbit noise. The fast orbit system has been operating extremely reliably, causing a total accelerator downtime of only a couple of hours during its first year of operation. The availability of the fast feedback was significantly larger than 99%.

Another improvement was an increase in the photon beam brightness seen by users. This year we began operation with smaller vertical beta functions in the ID straights. This was accomplished by increasing the vertical tune from 8.2 to 9.2, thus reducing the beta function from 3.65 m to 2.25 m in the straights. This resulted in up to a 40% increase in brightness for some ID users (depending on the length of the IDs). In addition, to maximize the performance of individual beamlines and therefore the photon brightness delivered at the end of the beamlines, three days were dedicated to beamline alignment at the end of our annual shutdown. During this time diagnostic orbit bumps were put in to determine the relative storage-ring to beamline alignment.

Two additional areas where significant progress was made were the upgrades of the high-level controls software and the study of the generation of terahertz radiation following the femtosecond slicing interaction. Both of these areas are discussed in more detail in separate sections below.

Since the last report, two new IDs have been installed in the storage ring. The first was the W11 wiggler replacing an older W16 wiggler. The W11 wiggler is now simultaneously used as a wiggler for protein crystallography and as a modulator for the femtosecond slicing experiment. The W16 wiggler was removed because its parameters did not allow optimized, simultaneous operation of the two experiments. An improved carbon filter assembly was designed and installed on the wiggler beamline, significantly reducing outgassing and necessary scrubbing time after vacuum work, as well as eliminating the need for annual carbon filter replacements. The second ID installed was an EPU with a 5-cm period, which will be used for photoemission electron microscopy.

During the 2005 shutdown, a third ID, an invacuum undulator (the first such device at the ALS), will be installed in the storage ring to act as the radiator for the femtoslicing experiment. Its minimum vacuum gap will be about 5.2 mm, significantly smaller than the present 8.9 mm. There was concern that the small gap may affect the performance of the storage ring-primarily its lifetime and injection efficiency. The effect of the smaller gap on the performance of the ALS has been extensively modeled. In addition, measurements have been performed using vertical scrapers to simulate the effect of the gaps. We found that with the vertical dispersion wave, the effect of the smaller gaps was not significant down to vertical apertures of about 5 mm. This was not the case when the beam size was controlled by linear coupling, where the lifetime was already affected by the vertical gap size around the previous apertures of about 9 mm.

The highest priority in the near term is the upgrade of the ALS to continuous top-off injection operation. With top-off injection operation, the ALS will benefit from increased time-averaged current (in our case, a 100% increase) and much-improved beam stability due to a constant heat load on the vacuum chamber and especially on beamline optics. The status of the top-off upgrade is discussed in a separate section below. There is also a plan to construct and install a quasiperiodic long-period EPU for inelastic scattering experiments. This undulator will have more challenges than previous EPUs: it will have stronger fields and possibly stronger perturbations to the beam dynamics. This year our tracking codes have been modified to include EPUs, and their impact is being studied.

The ALS went through an extensive planning exercise this year to develop a strategic plan to keep it on the cutting edge of synchrotron light sources over the next two decades (see "ALS Strategic Plan: Building a Foundation for the Future" elsewhere in this report). One interesting possible upgrade would be to insert rf deflecting cavities into two adjacent straight sections to create a bend-magnet picosecond source. Next year we will study the feasibility of such a source as well as develop the scientific case.

### An Accelerator Control Middle Layer Using Matlab

#### Gregory J. Portmann

Precise control of the ALS electron beam requires the tight coordination of many systems. There are thousands of control points and monitors in the control system distributed on many computers. High-level control is orchestrated by a commercial software package called Matlab, which uses a matrixmanipulation language and has been shown to be well suited for accelerator control.

Matlab was first used at the ALS in the early 1990s, shortly after commissioning. It was primarily used as a scripting language for machine physics shifts, but because it proved very reliable, it is now used in storage-ring operations and machine setup as well. Matlab has appeal for accelerator physics because of its combination of a matrix-oriented programming language, an active workspace for system variables, powerful graphics capability, built-in math libraries, and platform independence. Because Matlab is reliable enough to run operational code, one can develop and deliver algorithms using the same language.

At SSRL, parallel Matlab developments in the late 90s led to the Accelerator Toolbox (AT) for

machine simulations and Linear Optics from Closed Orbits (LOCO) for accelerator calibration. In a collaborative effort between the ALS and SSRL, many of the control functions developed at the ALS were ported to SSRL, restructured, and made more acceleratorindependent. As a result, the methodology and structure of the control routines and functions can now be easily ported to other machines. The resulting "Middle Layer" software simplifies application program development, buffers the user from the details of the Experimental Physics and Industrial Control System (EPICS), and hides cumbersome control system channel names.

As shown in Figure 2, the Middle Layer software provides a library of functions that access either the machine hardware or a simulator. Most control systems reference hardware devices by channel names and typically use units that represent the hardware (e.g., amperes for a power supply). Accelerator physicists, however, often think in terms of functional families (dipoles, quadrupoles, etc.) and attributes of the family that are in physics units (radians, k-value, gain, etc.), not necessarily physical units. The naming scheme used by Middle Layer tries to mimic accelerator tracking codes but also has the necessary hardware and control system details to map the nomenclature used by physicists to the hardware units of the actual accelerator. Thus Middle Layer can be a simulation analysis tool or an online control tool.

The primary purpose of Middle Layer is to simplify script construction for machine studies



and high-level application programming for machine control. Scripts rely heavily on Middle Layer to perform correlated perturb and measure studies. Application programs can be dominated by user-interface software but, again, benefit from Middle Layer for machine control and data handling. Middle Layer also provides high-level functions for many common accelerator physics tasks and a framework for saving operational data.

There are three main Matlab toolboxes written for accelerator physics-Middle Layer, AT, and LOCO. All three are well integrated and have proven to be quite useful for machine studies and control at several operating machines. The relatively user-friendly software and almost machine-independent programming language have fostered a number of collaborations. Most scientists find the syntax quite intuitive, making it possible for visitors to participate in machine development studies with minimal training. To date, the software has been installed on six machines (the ALS, the Canadian Light Source, SPEAR3, the Pohang Light Source, and the NSLS's vacuum ultraviolet and x-ray rings) and has received large interest from other laboratories. Synchrotron facilities under construction in Australia, the UK (Diamond), France (Soleil), and Spain (ALBA) all have plans to use Middle Layer. The software does take some up-front effort and expertise to install. With help from an experienced person, Middle Layer can be made functional for most applications within a few days and fully operational in a few weeks. Developing a fully calibrated online model (magnet hysteresis, calibration factors, beam-position monitor errors, etc.) is the most time-consuming part.

Use of the same high-level software by multiple laboratories has many advantages. Not every laboratory has to spend the resources to write the same algorithms. For new laboratories, it is a very inexpensive and fast way to acquire high-level control and simulation software that has also been thoroughly tested on other machines. Also, software development is not only expensive from a labor point of view, it is very expensive to test and commission new software from a beam-time perspective. Having the same software package debugged at many laboratories improves reliability. Thousands of dedicated accelerator hours have been spent testing, improving, debugging, and exercising the Middle Layer, AT, and LOCO software packages. As with the EPICS collaboration, software expansion, suggestions, and new ideas come from a larger pool of people. The number of physicists and engineers trained on Middle Layer is growing rapidly, and visiting scientists so trained can begin work immediately with very little hand-holding.

Since it is easy to switch between different accelerators in a simulated mode, it is easy to test algorithms on different accelerators. This is often an informative procedure when developing new algorithms. Writing software in a machine-independent way is somewhat more time-consuming, but the final product tends to be better written and more robust. Orbit correction, beam-based alignment of quadrupoles, and LOCO are examples in which effort was spent to make algorithms machine-independent.

### Coherent Synchrotron Radiation Activities

Fernando Sannibale

Accelerator physicists who design bunch compressors or damping rings for free-electron laser or linear-collider applications typically consider coherent synchrotron radiadion (CSR) a detrimental phenomenon that could jeopardize the performance of their devices. On the other hand, because the radiated power depends quadratically on the number of particles per bunch, CSR has the potential to be used in revolutionary new sources in which the photon flux is much higher than in "conventional" synchrotron light sources, where the radiated power depends only linearly on the number of particles.

CSR in storage rings was being discussed over 50 years ago, but only recently have a considerable number of observations been reported. Intense bursts of CSR with a stochastic character were measured in the terahertz frequency range at several synchrotron storage rings. The CSR study group at the ALS (J.M. Byrd, Z. Hao, A. Loftsdottir, M.C. Martin, D.S. Robin, F. Sannibale, R.W. Schoenlein, M. Venturini, A.A. Zholents, and M. Zolotorev) provided the first experimental evidence that this bursting emission of CSR is associated with a single-bunch instability, usually referred to as microbunching instability, driven by the fields of the synchrotron radiation emitted by the electron bunch itself [J.M. Byrd et al., *Phys. Rev. Lett.* **89**, 224801 (2002)].

At BESSY II in Berlin, CSR of a remarkably different character was observed when the storage ring was tuned to a special operational mode. Instead of the quasi-random bursting observed elsewhere, a powerful and stable flux of broadband CSR in the terahertz range was emitted, demonstrating the possibility of constructing a stable broadband source with extremely high power in the terahertz region. The ALS CSR group, in collaboration with BESSY and SLAC, developed a model that accounts for the BESSY II observations and indicates that the case is actually quite general and typical when relativistic electron storage rings are tuned for short bunches [F. Sannibale et al., Phys. Rev. Lett. 93, 094801 (2004)]. The theory showed that, in the regime where bunch lengths are a few picoseconds, the electromagnetic fields associated with the synchrotron radiation emitted by the electrons can generate a stable distortion of the equilibrium longitudinal distribution of the bunches from a Gaussian shape to a sawtooth-like shape. Such a distortion strongly extends the production of CSR toward higher photon energies, increasing the interest and the possibility of using storage rings as a powerful source of CSR. The model provides a scheme for predicting and optimizing the performance of ring-based CSR sources with a stable broadband photon flux in the terahertz region of up to about nine orders of magnitude larger than in existing "conventional" storage rings. Such a scheme is of interest not only for the design of new sources but also for the evaluation and optimization of CSR performance in existing storage rings.

Currently, BESSY II has dedicated CSR shifts for users, and several other laboratories are investigating the possibility of CSR operation in their existing or future machines. At the ALS, the design for a Coherent Infrared Center (CIRCE), a new ring optimized for CSR, is at an advanced stage, and the project has been included in the next five-year strategic plan. A comprehensive collection of papers concerning the work done on CSR in storage rings (with several contributions from people in our group) can be found in the ICFA Beam Dynamics Newsletter No. 35.

This year, CSR activity at the ALS concentrated on the characterization and understanding of a new way of producing CSR in the terahertz frequency range [J.M. Byrd et al., EPAC 2004, p. 2448]. At Beamline 5.3.1, the interaction of an electron bunch with a femtosecond laser pulse co-propagating through a wiggler produces a large modulation of the energy of the electrons within a short ~100-fs slice of the bunch. Such energy-modulated electrons are then spatially separated from the main bunch in a dispersive section of the storage ring. While the entire bunch generates synchrotron radiation, the spatially displaced femtosecond pulses of x-rays are selected by means of an aperture. In addition, the energy-modulated bunch propagating around the storage ring develops a longitudinal density perturbation due to the longitudinal dispersion of electron trajectories. The characteristic length of this perturbation is much shorter than the bunch length, causing the electrons to emit short pulses of terahertz CSR automatically synchronized with the modulating laser. We have measured such pulses at Beamlines 1.4 and 5.3.1, and the example in Figure 3 shows the scope track of the signal from a bolometer. The 1-kHz structure (modulating laser repetition rate) of the signal is clearly visible. Such a signal is now routinely used as a diagnostic for the tune-up of the proper time and spatial overlap between the laser and the electron beam during slicing experiments.

The CSR produced during slicing presents some very interesting opportunities. The synchronization between the modulating laser and the terahertz CSR pulse opens the possibility of pump–probe experiments. Additionally, by changing the shape of the modulating laser pulse, it is in principle possible to control the shape of the terahertz pulse as well, allowing for experiments using coherent learning con-



CSR signal when the slicing is on.

trol methods. Another intriguing phenomenon occurs when the current per bunch is above the threshold for the microbunching instability and the ALS is in a particular configuration of the lattice. In this situation, the slicing seems to seed the generation of the CSR burst associated with the instability. In other words, a significant part of the CSR bursts, usually random in time when the slicing is off, becomes synchronous with the modulating laser when the slicing is switched on. In this configuration, the CSR power associated with these synchronous bursts grows exponentially with the current per bunch (Figure 4). Future effort will be focused on better characterization and understanding of these slicing-induced CSR effects and on the investigation of their potential as a CSR source.

### Top-Off Mode

Upgrading the ALS injection system to enable full-energy injection and top-off operation (i.e., quasi-continuous injection) is the highestpriority machine upgrade currently underway. It will result in significant improvements in brightness and stability and keep the ALS competitive with newer light sources for the next decade. The scientific motivation for the upgrade as well as expected performance parameters have been described previously.

During the past year, significant progress was made. A project team was formed and a con-

ceptual design report (CDR) was developed. The project successfully passed internal and external reviews. During the conceptual design phase, all items that presented a significant technical risk were studied in detail and no showstoppers were found. One particular area of risk involved the pulsed extraction magnets in the booster ring and the pulsed injection magnets in the storage ring. However, after extensive simulations and measurements with newly built pulsers and newly assembled spare magnets as well as modifications of the injection geometry, it was determined that all existing pulsed magnets could be upgraded relatively easily for full-energy injection.

As part of those studies, we looked at the transient orbit distortions that the injection process produces on the stored beam. As reported last year, we found that only a small subset of users was adversely affected by these transients. To further reduce the number of affected users, the stray field of the septum magnets was studied in detail. Simulations showed that a simple modification of the thick septum magnet pulser should make it possible to reduce the delayed stray field by about one order of magnitude. Measurements both on a magnetic measurement bench and using the beam in the storage ring verified this improvement (Figure 5).

One very important aspect of the top-off upgrade is radiation safety. Since injection will occur with safety shutters to all beamlines open, new challenges arise. In addition, the higher beam current and smaller emittances producing higher brightness after the upgrade will also increase the electron loss rate from the storage ring, potentially increasing overall radiation levels. To address these challenges, the ALS will combine the best solutions from other facilities that already employ top-off injection (APS, ESRF, the Swiss Light Source, and SPring-8). These solutions include the installation of additional interlock systems, interlocked radiation monitors, locally shielded beam-defin-





CSR power vs current per bunch in the "seeded" bursting mode. The solid blue curve is an exponential fit with an imposed saturation value. PFT = Power Fourier Transform;  $\alpha_c$  = momentum compaction; G = gain.

Transient horizontal orbit distortion induced by delayed eddy currents in the thick septum magnets. Using a full-sine current waveform instead of a half-sine reduces the magnitude by a factor of 10.

ing apertures, and extensive simulation studies and measurements using the storage ring. Also, because the ALS storage ring has the lowest beam energy, there are additional challenges. Touschek lifetimes at the ALS are shorter, and the first beamline optics at the ALS are in general openly accessible with minimal shielding instead of being surrounded by large hutches and exclusion zones.

As part of the migration to top-off injection, the ALS must obtain regulatory approval to change its Final Safety Analysis Document. To prepare, we received approval to perform initial injection studies after significantly upgrading the shielding on one of the ALS beamlines (Figure 6). Radiation levels measured with the safety shutter open and large missteering of the injected beam were generally acceptable, verfying that radiation safety even without hutches around beamline optics is not a showstopper.

The top-off upgrade received authorization for significant funding from DOE this year. The funding total is \$3.5M for the upgrade and \$0.5M for the CDR phase. Given this funding and additional commitments from the ALS, the plan is to complete the injector upgrade for full energy injection in late spring 2006 and migrate to top-off injection the following summer. The funding is not sufficient to complete the full scope of the upgrade project as detailed in the CDR; in particular, the capability to operate with cleaned bunches in two-bunch operation will have to be postponed.



6 Additional lead shielding installed on ALS Beamline 4.0.2 to enable top-off injection tests to study radiation levels with the safety shutter open.

# **EXPERIMENTAL SYSTEMS**

Howard Padmore, Experimental Systems Group Leader

### Introduction

The role of the ESG (Figure 1) can be split into several categories: (1) to design and build beamlines and endstations based on the demands of the user program, (2) to conduct forefront research in science and instrumentation that will push the boundaries of the application of synchrotron radiation techniques, and (3) to give support to existing user programs, usually in areas of high technical complexity. Approximately 50% of the group's activity is in this latter area of direct user support. This short report gives several examples of work in the two former areas and summarizes the group's activity over the broader range of its work.

### Optical Metrology Laboratory

The main assignment of the Optical Metrology Laboratory (OML) at the ALS is the characterization, understanding, and adjustment of synchrotron radiation optics. This work, led by V. Yashchuk, is of growing importance as the ALS increases in brightness because of machine improvements and the use of new small-gap undulators. At the same time, our experiments are becoming more sophisticated, with emphasis on achieving small foci and reducing scattering. The OML carries out its mission using a number of metrology instruments, including a Micromap-570 interferometric microscope, a ZYGO GPI interferometer, a second-generation long-trace profiler, and a Polytec laser Doppler vibrometer. At the same time, the OML is working to investigate and improve the performance of these instruments and measurement techniques. As an example, one of the results of this work is reported here.

The Micromap-570 is a basic metrology tool for highly accurate testing of the surface finish of x-ray optics with sub-angstrom rms roughness. The standard list of output parameters of a Micromap measurement includes values of roughness averaged over



Experimental Systems Group. First row: Cathy Cooper, Phil Heimann, Tony Young, Tim Kellogg, Malcolm Howells, Ariana Gleason, Congwu Cui. Second row: Jim Patel, Wayne McKinney, Simon Clark, Philipp Dietrich, Tony Warwick, Aberto Comin, Matthew Church. Third row: Jamie Nasiatka, Steve Irick, Martin Kunz, Andrew Doran, Ernie Glover, Nobumichi Tamura. Back row: Andreas Scholl, Valeriy Yashchuk, Bryan Valek, Sander Caldwell, Greg Morrison, Rich Celestre, Howard Padmore, Andreas Bartelt.

an area and along a sample line. However, the task of designing high-performance, lowscatter x-ray optical systems requires the development of sophisticated x-ray scattering calculations based on rigorous information about the optics.

One of the most insightful approaches to these calculations is based on the 2D power

spectral density (PSD) distribution of the surface height, allowing for the evaluation of three-dimensional distributions of x rays scattered by the optics. A straightforward attempt to transform the area distribution of the residual surface heights available from the Micromap data file into a 2D PSD distribution fails because of the spectral distortion in the PSD caused by an unknown spatial





frequency response function of the instrument. The distortion appears as a significant difference between the tangential and sagittal PSD spectra deduced from the 2D PSD distribution of an isotropic surface.

A detailed investigation of the origin of the anisotropy was performed at the OML, and a special procedure and relevant software were developed. An accurate 2D PSD can now be determined. The Micromap PSD measurement has been compared with measurements obtained using AFM and XRS. The measurements were performed on gold-coated stainless-steel substrate mirrors. The surface finish of the mirrors (fabricated by InSync) was found to be essentially isotropic, allowing straightforward comparison of the 1D PSD spectra obtained by convolution of the 2D PSD distributions measured with the Micromap, the AFM, and the 1D PSD spectra extracted from the XRS experiment (Figure 2).

The main conclusion from the cross-check is

that all three techniques provide essentially consistent results. At spatial frequencies from ~0.1 to 50  $\mu$ m<sup>-1</sup>, the XRS measurements agree reasonably well with the AFM measurements. The frequency range available for the Micromap measurement is shifted to the lower frequencies, 0.001 to 2  $\mu$ m<sup>-1</sup>; nevertheless, in the overlapping range, good agreement between the PSD magnitudes can be seen. Moreover, the measurements are complementary, allowing for correction of the specific spatial-frequency-dependent systematic errors of the instruments.

The need for the evolution of mirror specifications to include the PSD characterization, and not just the rms roughness, requires development of a universal method to test and to calibrate the PSD measurement instruments available at different optical metrology laboratories at vendors and at user facilities around the world. Such a test method based on a specially designed pseudo-random grating is under development at the OML.

### High-Pressure X-Ray Diffraction on Beamline 12.2.2

A new facility for x-ray diffraction and x-ray absorption spectroscopy from samples held at high pressures and temperatures has been built on Beamline 12.2.2, by a team led by S. Clark. This facility constitutes a central component of a center for high-pressure science being established at the ALS in support of the West Coast extreme-conditions community. It is designed to operate using diamond-anvil high-pressure cells with either resistive or laser heating, allowing combined temperatures and pressures in excess of 3000 K and 1 Mbar. The beamline benefits from the hard x rays generated by an ALS superbend. Useful x-ray flux is available between 5 and 35 keV.

The radiation is transferred from the superbend to the experimental enclosure by brightness-preserving optics. These optics consist of a vertically deflecting plane parabolic collimating mirror that provides parallel radiation in the vertical for a double-crystal monochromator (two flat crystals or two flat multilayers) followed by a toroidal focusing mirror. The various distances of the beamline components from the source are 6.5, 16.5, 18.8, and 28.2 m for the plane parabola, monochromator, toroid, and sample, respectively. This optical arrangement with the toroid in the 2:1 horizontal demagnification geometry results in the elimination of low-order aberrations and achieves a focus spot of high fidelity.

To cover the expected range of experimental requirements, two endstations are installed on a  $3.6 \times 1.2$  m optical table, which in turn is placed within a spacious ( $5.4 \times 3.2$  m) hutch. After entering the hutch, the beam passes through a set of absorption foils, a fast shutter, a set of horizontal and vertical aperture slits, and a clean-up pinhole.

Endstation 1 has just been commissioned and is shown in Figure 3. It is optimized for the measurement of accurate unit-cell parameters to determine thermal equations of state of solid and liquid materials.



Photograph of endstation 1 of Beamline
12.2.2, complete with Brucker CCD detector.
The KB mirror vessel and laser-heating system can be seen on the left.

Resistively heated diamond-anvil cells are mounted on a goniometer. The goniometer consists of the following stages from bottom to top: (1) a horizontal-translation stage perpendicular to the x-ray beam (x-direction), (2) a rotation stage with vertical axis; (3) a vertical stage (y-direction), (4) a second horizontaltranslation stage perpendicular to the beam (x-direction), and (5) a horizontal-translation stage parallel to the beam (z-direction). This arrangement enables the vertical rotation axis to be centered on the beam using stage 1 and the placement of the sample onto the rotation axis and beam using stages 4 and 5. This scheme allows the use of the rotation axis as a reference position relative to the detector plane, and thus to accurately determine the sample-to-detector distance.

The size of the collimated beam was measured by scanning a single blade of the slit assembly across the optimized beam. Beamline acceptance was 1.0 (h) × 0.22 (v) mrad. The measured size is 115 × 78  $\mu$ m FWHM. This endstation uses a Brucker SMART 6000 CCD detector.

Two benchmarks for experiments on this endstation have been performed. First, the pressure determined using spectroscopic methods was compared to an internal diffraction standard. The agreement between the two independent methods is good, giving us confidence in the capability of the beamline to produce reliable compressibility data (Figure 4). Second, the integral uncertainty on refinable parameters of a Rietveld refinement (atomic coordinates) was determined. The



Comparison of pressures measured using x-ray diffraction from sodium Piermarini scales, demonstrating the overall system accuracy (better than 0.2 GPa) of Beamline 12.2.2.

relative precision of lattice parameters is  $\Delta a/a = 10^{-4}$  and the value for refined bond distances is  $\Delta r/r = 10^{-3}$ .

Endstation 2 is designed to operate with diamond-anvil cells and laser heating. When endstation 2 is in use, endstation 1 can be slid to one side to allow the x-ray beam to pass to the endstation 2 position. The x-ray beam diverges from the endstation 1 focus and will be refocused with a set of KB mirrors to a 5  $\times$  5  $\mu$ m focal spot. At the moment, this KB mirror system has been installed and is awaiting commissioning. A laser-heating system has already been installed and commissioned and has a focused laser spot size of 20 µm. The endstation has a set of goniometers similar to endstation 1 for sample alignment and uses a Mar345 imaging plate detector.

# PEEM-3 Beamline and Endstation

Beamline 11.0.1 is a new undulator beamline for PEEM studies at the ALS, built under the direction of T. Warwick. A 50-mm-period EPU is operational and delivering light into the new line, which is now being commissioned. This undulator is the third EPU to come into use at the ALS and the first to share a straight section by means of a chicane. Beamline 11.0.1 sits close to Beamline 11.0.2 (which serves a large Molecular Environmental Science program and STXM), separated by six degrees at the shared first mirror system behind the storage-ring shield wall.

The new beamline employs a VLS grating to generate an erect focal plane at the location of the exit slit. This puts the zero-order light approximately in focus so that it can be tracked as the grating rotates, providing a way to stabilize the energy scale of the monochromator to a level of precision much higher than the spectral line width of the instrument. Typically, this beamline will operate with a resolving power around 3000, and the goal is to stabilize the energy calibration to one part in 10<sup>6</sup> against the relative thermal motion of the entrance slit, exit slit, and grating. This is very important in a beamline that serves magnetic dichroism experiments. The goal is to allow the subtraction of spectra taken consecutively with negligible artifacts due to small changes in the energy scale from one scan to the next. Figure 5 shows the monochromator layout and a schematic of the stabilization scheme. The monochromator features a triple VLS grating with a set of grooves optimized for 280, 700, and 1500 eV. With full linear and elliptical polarization control and continuous

coverage optimized in these three energy regions, this will be an attractive facility for polarization-contrast PEEM studies of organic and magnetic materials.

The design of the endstation, led by A. MacDowell, has continued this year, with the instrument entering its final production phase. The instrument is designed as an aberration-corrected PEEM with a spatial resolution of approximately 5 nm. The sample is illuminated with soft x rays, and the emitted photoelectrons are accelerated to high kinetic energy in a small anode-cathode gap. The aberrations produced in this acceleration and in subsequent focusing are balanced by the actions of an electron mirror with opposite low-order aberrations. To direct electrons to and from the electron mirror and to then separate the beam paths, a dipole separator magnet is used. This has to be aberration-free to high order, resulting in a highly complex design. Following the separator, the image is magnified to a final image plane at a phosphor-fiber-CCD camera by regular electrostatic lenses.

The system without the magnetic separator and electron mirror will initially be commissioned in November 2005 to function similarly to the existing PEEM-2 instrument on Beamline 7.3.1.1 with a resolution of about 30 nm. Its advantages over PEEM-2 will be a flux density from the beamline a factor of 100 higher, polarization control, and a more sophisticated sample preparation environment, including the use of a novel five-axis, high-stability flexural sample stage that can be cooled down to 60 K. A drawing of the system is shown in Figure 6. While the initial phase is being commissioned, the magnetic separator, electron mirror, and sample preparation chamber will be completed, then added in 2006.

One reason for this two-stage approach is that there have been recent advances in separator design (from W. Wan of the Accelerator Physics Group) that appear to give significant advantages in performance, tenability, and simplicity over the conventional design. Essentially, the new design separates the functions of focusing and steering into separate elements of quadrupoles and dipoles,



5 Layout of the PEEM-3 Beamline 11.0.1.



**6** PEEM-3 endstation. X rays from undulator Beamline 11.0.1 are focused by the KB mirrors onto the sample inside the microscope. The transfer arms insert the sample into the microscope and the sample preparation chamber.

simplifying the design enormously. However, adoption of this new scheme late in the design phase would have slowed the project, and hence we have decided on the twophase approach. The last two optics of the beamline are a pair of KB mirrors that focus the x rays to a spot size of ~5  $\mu$ m on the sample. The microscope itself is housed in a large vacuum tank that has three layers of mu-metal magnetic

shielding necessary to reduce magnetic field strengths to less than  $2 \times 10^{-7}$  G. Such a low field is required as the path length is long (~1 m) for this microscope. Significant effort has been put into making the installation of the sample into the microscope user friendly. The same mechanism design has been used for moving samples into the preparation chamber. While samples are prepared in this chamber, the microscope can be used to study other samples, thus ensuring a high throughput rate.

### Streak-Camera Development

Streak-camera technology is being developed for use in a variety of ultrafast dynamics experiments by a team led by J. Feng in collaboration with the R. Falcone group (UC Berkeley) and a group led by J. Byrd at Berkeley Lab's Center for Beam Physics (CBP). The camera consists of a photocathode, a pair of meander-type deflection plates, a photoconductive switch, a magnetic focusing lens, and an image plane detector. The deflection plates are located before the magnetic focusing lens to minimize the transit time from the anode to the deflection plate and reduce the space charge effect. The photoconductive switch used to laser-trigger the camera (~60 mJ) is produced in-house and operates at 5 kHz. The base material of the switch is a semiinsulating GaAs wafer. It also has an annealed 200-Å Sn layer and 200-Å Ge layer to help form an ohmic contact, a 1200-Å gold contact layer, and a SiO<sub>2</sub> protection layer.

The performance of the switches is good, but we want to push into the MHz switching region, with higher voltages, to gain signal and improve temporal resolution. We are therefore investigating a range of new switch designs, including avalanche types. We are also working on the characterization of photocathodes. It is clear from initial work that traditional high-efficiency cathodes such as CsI suffer unacceptable radiation damage at our flux density levels. So far we have used gold cathodes, but we are looking at other materials such as negative-electron-affinity diamond, in combination with grazing incidence as a way to an optimum photocathode. We have used static and dynamic imaging to characterize the camera. Static imaging gives a resolution of ~25 microns when used with a direct-electron-illumination CCD camera. The dynamic imaging performance is tested using 267-nm light generated by a third-harmonic  $BaB_2O_4$  (BBO) crystal system from 800-nm, 30-fs Ti:sapphire light. Two ultraviolet pulses with a known delay are used for calibration purposes, and so far, a resolution of 900 fs has been achieved for 5000 shots (Figure 7).

The resolution is limited by the chromatic nature of the emission from the photocathode, by the extraction field, by the deflection system, and by the resolution of the final detector. To improve the meander deflection system, the time-dependent fields are modeled using Microwave Studio software and then entered into the IMPACT code (developed at Berkeley Lab by J. Ji of CBP). The latter propagates a description of the source through the electron optical system, including time-dependent fields and space charge. The code has been benchmarked against other approaches using Parmela and MAFIA. The results for one end-to-end model (using a 10-kV/mm extraction field and a gold photocathode) and one without energy spread are shown in Figure 8.

Deflector modeling helps us understand the system in detail and has already allowed us to design a lower-loss, higher-efficiency system. To go to higher temporal resolution, we can increase the extraction field, but the upper limit is around 30 kV/mm. To go well beyond this, we have to correct the chromaticity of the system. At present with our "straight shot" system, a higher-energy secondary electron from the photocathode takes a shorter time to reach the deflector and is hence deflected a larger distance off axis than a lower-energy electron. To correct this, we need to introduce a system that makes a high-energy electron take a longer time, and this can be done with dispersive systems. The trick is to do this in a system that is achromatic and double focusing. Wan from the Accelerator Physics Group has proposed a design for such a system that can theoretically achieve resolutions less than 50 fs. To use this performance, the deflection system has to be substantially improved, and we are looking at various options, including x-band rf deflection, locked to our laser oscillator.



Streak-camera data, averaged over 5000 shots, demonstrating 900-fs resolution.



Image plane of the streak camera showing two 50-fs pulses separated by 10 ps, with (red) and without (green) energy spread.

### Femtosecond Slicing Beamlines

Beamlines 6.0.1 and 6.0.2 are under construction for ultrafast x-ray science using femtosecond slicing techniques. The beamline work is led by P. Heimann in collaboration with R. Schoenlein of Berkeley Lab's Materials Sciences Division. The source is an in-vacuum undulator produced at Sumitomo (Figure 9). The 3-cm-period undulator is the first in-vacuum insertion device at the ALS and will have a minimum magnetic gap of 5.5 mm. It produces x rays over a wide photon energy range, from 150 eV to 10 keV, through the use of undulator radiation at low energies and wiggler radiation at high energies. Beamline 6.0.1, the soft x-ray beamline, will cover the photon energy range from 150-1800 eV while Beamline 6.0.2, the hard x-ray beamline, will provide photons from 2.2-10 keV.

The beamlines are designed specifically for the electron-beam-slicing technique, which can produce x-ray pulses of 200-fs duration. To interact with the electron beam and



9 In-vacuum undulator (3-cm period) for use at the femtosecond slicing beamlines in Sector 6.

excite samples, a high-average-power femtosecond laser system is being built. In electron-beam slicing, a femtosecond laser pulse modulates the energy of a slice of the electron bunch, which overlaps in time with the optical pulse. Dispersion in the storage ring lattice introduces a spatial separation of the modulated electrons.

The first section of the beamlines includes mirrors that image the x-ray source onto slits

that select the femtosecond x-ray pulses. High-speed choppers reduce the average power on samples in pink beam and on the downstream optics. The chopper design is based on a spinning disk, which is water cooled through a ferrofluidic vacuum seal. The scattering from the first mirrors is critical because it determines the background underneath the femtosecond x-ray pulses. Research and development contracts were placed with two mirror vendors to improve the sagittal roughness of cylindrical mirrors. In addition, we have developed computational methods to calculate the distribution of scattered x rays using metrology data from a mirror's optical surface.

The soft x-ray beamline includes a chamber for positioning transmission samples in the pink beam. A soft x-ray spectrograph allows the measurement of an entire x-ray absorption spectrum at one time. The optical elements are a spherical mirror (producing a vertically converging beam), a VLS plane grating, and a horizontally focusing plane elliptical mirror. The mechanical design of the spectrograph is a modification of the Beamline 11.0.2 monochromator design. At the end of the beamline is a gateable imaging detector. This detector can also operate as a streak camera. On the hard x-ray beamline, crystals produce a monochromatic beam for experiments inside a hutch. Here the optical elements are a vertically collimating cylindrical mirror, two Ge(111) crystals, a vertically focusing cylindrical mirror, and a horizontally focusing plane elliptical mirror. The Ge(111) crystals were chosen because of their high integrated reflectivity.

The femtosecond laser system operates at a high repetition rate, 20 kHz, in order to use a larger fraction of the available pulses of synchrotron radiation. To accommodate the high average power, cryogenic cooling is applied to the Ti:sapphire amplifier crystals. A pulse energy of ~1 mJ is provided in two amplifier arms: one for the interaction with the electron beam and another for exciting a dynamical process in the sample. The undulator, soft x-ray beamline, and laser system will be ready for commissioning in July 2005. The hard x-ray beamline will be completed about nine months later.

# SCIENTIFIC SUPPORT

Zahid Hussain, Scientific Support Group Leader John Bozek, Scientific Support Group Deputy Leader

### Introduction

The primary mission of the SSG (Figure 1) is to support the efforts of researchers at the ALS through scientific and technical collaboration and scientific outreach. Working with the users, the SSG plays an important role in developing novel instrumentation that enables cutting-edge science. Depending on the needs of the user, the degree of collaboration can range from technical assistance with the beamline and instrumentation to full partnership in developing new research programs.

## Scientific Outreach

The SSG strives to expand the scientific program of the ALS and broaden its user base through publications and presentations. The group organizes a variety of seminars, including the weekly ALS/Center for X-Ray Optics (CXRO) seminar series and a targeted weekly SSG lecture series. The weekly lectures cover a wide range of topics and are given by world-renowned scientists. The group also organizes the quarterly ALS Colloquium. This year a reference library and small meeting room with several computers for data analysis and communication were set up in the ALS mezzanine.

Working together with the UEC, the SSG also helps to organize workshops exploring new scientific opportunities and needs for new beamlines or experimental facilities. During the 2004 ALS Users' Meeting, six such workshops were heavily attended by enthusiastic scientists, triggering many fruitful discussions that should spark further advances at the ALS.

The ALS Doctoral Fellowship in Residence program, established in 2001, has been very popular among doctoral students and has been received with much appreciation. Doctoral fellowships enable students to acquire hands-on scientific training and develop professional maturity for independent research. More details are given at the ALS Web site (www-als.lbl.gov/als/fellowships/).



Scientific Support Group. Front row: Jinghua Guo, Adriana Reza, Bruce Rude, Karine Chesnel, Jonathan Spear, Per-Anders Glans, Timothy Learmonth. Middle row: Alex Kouprine, Simon Mun, Fred Schlachter, Bill Bates, Aran Guy, Zahid Hussain, Yi-De Chuang, David Kilcoyne, Alexei Fedorov. Back row: Feng Wang, John Pepper, Max Rossi, Jonathan Denlinger, Byron Freelon, Mike Martin, Eli Rotenberg, Stephan Kashtanov, John Bozek, Aaaron Bostwick.

A selection committee consisting of D. Lindle (Chair, UEC), A. Nilsson, Z. Hussain, S. Bader (Chair, SAC), and N. Smith recommended the following recipients for doctoral fellowships for academic year 2005 (Figure 2):

- Christopher Cappa (UC Berkeley, physical chemistry)
- Yulin Chen (Stanford University, spinresolved photoemission spectroscopy)
- Henry Fu (UC Berkeley, correlated electron physics)
- Johnathon Holroyd (Montana State University, physics/magnetic materials)
- Timothy Learmonth (Boston University, physics)



ALS Doctoral Fellows. Michelle Weinberger, Henry Fu, John Paul Strachan, and Johnathon Holroyd (not pictured: Chris Cappa, Yulin Chen, Timothy Learmonth, and Feng Wang).

- John Paul Strachan (Stanford University, condensed matter physics/magnetism)
- Feng Wang (University of Michigan, photoemission and spectroscopy of correlated systems)
- Michelle Weinberger (UC Los Angeles, physical/materials chemistry)

### **SUPPORT**

SSG members are responsible for the operation, upgrade, and maintenance of most of the facility beamlines and many of the permanent endstations at the ALS. The undulator-based beamlines-4.0.2, 7.0.1, 8.0.1, 10.0.1, a photoemission branchline on 12.0.1, and a coherent science branchline 12.0.2-typically have one or two SSG staff members responsible for their continued operation. The group is also playing an active role in optimizing the operation of the chemical dynamics complex (Beamline 9.0.2), which is operated by Berkeley Lab's Chemical Sciences Division under separate funding from DOE BES. A major SSG activity is the construction of a new, BES-funded, meV-resolution beamline (MERLIN) optimized for the study of inelastic x-ray scattering and ultrahigh-resolution photoemission. An important breakthrough this year was the development of a spectrograph with unprecedented energy resolution and efficiency (described in more detail below) for use with the MERLIN beamline. Members of the SSG put great emphasis on developing novel instrumentation that is

more efficient and user friendly. Also in 2004, the group designed and developed several new experimental systems, some of which are described below.

### **MEMBER RESEARCH**

Staff scientists within SSG are expected to maintain scientific and technical excellence in areas of synchrotron radiation research. Participation in active scientific programs is essential for such development, and all of the SSG scientists are active members of research programs at the ALS.

## Soft X-Ray Spectrograph for MERLIN

A soft x-ray emission spectrograph working in the transition-metal M-edge range (photon energy 36–150 eV) has been designed and fabricated. The optical layout is shown on the left in Figure 3. A slitless design is used to increase the acceptance angles. Two optics, a spherical focusing mirror and a 2,000-line/mm VLS plane grating, are used to achieve resolving powers of better than 10,000. A high-quantum-efficiency CCD detector with 13.5-µm square pixels is also used to maximize throughput. The overall length of the spectrograph is around 2 m. Ray tracing results at hv= 49 eV with a source size (in the dispersive direction) of 4 µm are shown on the right in Figure 3. Three photon energies were used: 49.005 eV (top), 49.000 eV (middle) and 48.995 eV (bottom). It is clear that these three curves are well separated, indicating an energy resolution of better than 5 meV.

Preliminary tests were done at Beamline 12.0.1, with straight beam passing through the spectrograph onto the CCD detector. The source size (in the dispersive direction) was measured to be ~6  $\mu$ m. The fully binned (nondispersive-direction) profiles are shown in Figure 4. The beamline slit was set at 10  $\mu$ m. Comparing the full width and the dispersion across the CCD detector, the energy resolution is found to be around 11 meV at 49 eV. The beamline contribution is approximately 10 meV, giving a spectrograph resolution of better than 5 meV.

The spectrograph resolution is also determined at various photon energies. In the bottom panel of Figure 4, the red curve shows the resolution determined from the tests. The brown curve is the beamline resolution corrected for the proper slit size, assuming ideal performance. The cyan curve is the deduced spectrograph resolution assuming a quadratic sum, and the blue



23 Left: Optical layout of the spectrograph. Right: Ray-tracing (SHADOW) results at  $hv = 49 \text{ eV} \pm 5 \text{ meV}$ . Three distinct features are well separated, indicating that the energy resolution is better than 5 meV.





curve is the theoretical spectrograph resolution. Agreement between the experimental and theoretical spectrograph resolutions is quite good below 60 eV. A slight deviation can be seen when the excitation photon energy is above 60 eV. We believe that this is due to the distorted beam profile from the KB mirror producing unwanted shoulders in the CCD image that can be removed by partially masking the beam just before the sample location. Further commissioning of the spectrograph by carrying out initial experiments is underway. This effort is collaboration between CXRO (E. Gullikson, P. Batson, and K. Goldberg), the ALS (Y.-D. Chuang and Z. Hussain) and Princeton University (Z. Hasan).

### Angle-Resolved Photoemission at Beamline 12.0.1

The ARPES branch of Beamline 12.0.1 enjoyed trouble-free user operation this year. Not a single user shift was lost due to endstation malfunction. This, combined with

recent improvements in resolving power (Figure 5) and throughput, has helped to create a stable user community that includes many groups active in the photoemission research of strongly correlated materials. At the moment the core of the photoemission program consists of six groups: D. Dessau (University Colorado, Boulder) studied CMR materials (manganites); Z. Hasan (Princeton University) and H. Ding (Boston College) both studied doped oxides of cobalt, which have emerged as the most intriguing strongly correlated materials of today; K. Smith (Boston University) investigated low-dimensional charge-density wave materials; A. Lanzara (UC Berkeley) looked at the electronic structure of cuprate superconductors; J. Allen (University of Michigan) and J. Denlinger (ALS) have measured Fermi surface maps of rareearth and uranium compounds (Figure 6).

The endstation has received a new low-temperature (down to ~10 K) sample manipulator capable of three independent angular motions (tilt, azimuth, and polar angles) as well as high-precision sample positioning along the x, y, and z axes. All motions are computer-controlled via the LabView program, which is derived from the general beamline control software package developed by E. Domning and B. Smith of the ALS Controls Group. Smith has established a link between the software and the data-acquisition software used with the photoemission spectrometer (Scienta SES 100). This has made it possible to automatically record photoemission spectra during the one- or two-dimensional coordinate scans with the coordinates being any of the three angles; the three x, y, and z coordinates; or the photon energy. Hence, experiments requiring the collection of large numbers of data points, such as the mapping of Fermi surfaces or lateral element distributions, have became feasible. Figure 6 displays an example of a Fermi surface map recently measured at the ARPES endstation of Beamline 12.0.1.

Several instrumentation developments have been planned. D. Dessau, who runs an approved program, has invested funds into improving beamline performance: an order has been placed for ruling a new VLS grating that will extend the useful range of photon



Fermi edge of polycrystalline gold held at ~12 K. This measurement demonstrates an energy resolution of ~6 meV for the ARPES branch of Beamline 12.0.1.



Measured Fermi surface of LaRu<sub>2</sub>Si<sub>2</sub>, obtained at Beamline 12.0.1.

energies down to ~30 eV (two existing highresolution VLS gratings commissioned last year have peak efficiencies at 60 and 120 eV, respectively). Grating delivery is anticipated by the end of 2005. Another beamline improvement involves installation of Mg, Al, Si, and B band-pass filters. The filters cut light originating from the higher diffraction orders of the grating. This in turn will dramatically reduce the background photoemission signal.

The scientific program has resulted in a number of new insights into the physics of strongly correlated materials. For example, it was possible for the first time to visualize the coupling of quasiparticles to phonons in the CMR material  $La_{2:2x}Sr_{1+2x}Mn_2O_7$  (Figure 7). Since phonons play a central role in many theories describing CMR, this result may lead to a major breakthrough in understanding the CMR effect.

## Cluster Research on Beamline 10.0.1

Clusters of atoms or molecules are an intriguing class of materials whose physical



Quasiparticle dispersion relations in the vicinity of the Fermi level in  $La_{2\cdot 2x}Sr_{1+2x}Mn_2O_7$  obtained at Beamline 12.0.1. The arrow indicates the energy of the phonon that couples to the quasiparticles and renormalizes the otherwise nearly parabolic dispersion.

properties differ from those of condensedphase material and from constituent atoms or molecules. For example, small clusters of silicon are predicted to exhibit metallic behavior, an attribute exhibited by neither the atom nor the crystalline material. In collaboration with the research group of N. Berrah (Western Michigan University) and using the suite of instruments available in the High-Resolution Atomic, Molecular, and Optical physics program on Beamline 10.0.1, we have studied a variety of clusters.

Using a continuous-beam supersonic gas jet, we have produced van der Waals clusters of rare-gas atoms and studied their photoionization on Beamlines 4.0.2, 9.0.2, and 10.0.1 by high-resolution electron spectroscopy with both a hemispherical electronenergy analyzer and TOF electron spectrometers. Clusters formed by condensation in a supersonic expansion have a wide range of sizes, usually with a distribution equal in width to the average number of atoms in the cluster. This distribution of cluster sizes degrades the resolution of the resulting photoelectron spectra, owing to averaging of the different cluster sizes in the beam (as well as additional low-energy modes). This is illustrated in spectra obtained for argon clusters (Figure 8) with the conditions of the supersonic expansion set to produce clusters of 2, 3, and 4 atoms. The measurements were done in collaboration with E. Poliakoff





Positive photoion product yields of the  $B_n^-$  species indicated in the vicinity of the B K edge obtained at Beamline 10.0.1.

Electron spectra of small argon clusters in the vicinity of the Ar 3p photoelectron lines obtained on Beamline 10.0.1. The average size of the cluster for the three different operating conditions of the continuous beam supersonic gas jet source are indicated.

(Louisiana State University). The spectrum of  $Ar_2$  shows distinct vibrational structure that is subsequently washed out as the average size of the cluster is increased.

To overcome this limitation, we have begun to study size-selected clusters, in collaboration with R. Bilodeau and Berrah (both of Western Michigan University), using the Ion-Photon Beamline endstation and a cesiumsputter negative-ion source to produce beams of negatively charged clusters. The beamline utilizes a sector magnet to momentum-resolve the ion beam produced by the source and thus provides a monodisperse beam of cluster ions. Photoionization of size-selected cluster beams has been performed for several different atomics species. Figure 9 illustrates the results for the different positive-ion products from B<sup>-</sup>, B<sub>2</sub><sup>-</sup>, and B<sub>3</sub><sup>-</sup>. These results illustrate the exciting possibilities of studying the photoionization of

size-selected clusters using the host of techniques available at the ALS and expanding our limited knowledge of the electronic structure of these species at the frontiers of atomic and molecular physics and nanoscience.

### The Electronic Structure Factory at Beamline 7.0.1

The Electronic Structure Factory endstation is dedicated not only to the analysis of the momentum structure of solids over a wide range of k space, but also to the study of a wide variety of in-situ-grown samples with complicated geometries. Commissioned in late 1993, it is one of the oldest running endstations at the ALS, and its continuing popularity owes much to a long-term program of upgrades: low temperature, parallel angular detection, and advanced preparation facilities. As a testament to its ongoing popularity (typically two groups per week share the endstation), current data acquisition of valence band images totals in excess of 30 GB per month. The present data throughput has increased five orders of magnitude since its inception as a core-level spectroscopy machine.

In the last year, we procured and installed a Gammadata SES-R4000 analyzer. Together with a significant vacuum pump upgrade, this increased the useful angular acceptance from 7.5° to greater than 30° and the mean radius of the analyzer from 100 to 200 mm. These improvements promise an order-of-magnitude increase in throughput over the existing end-station and will keep the Electronic Structure Factory a premier facility for the analysis of in-situ-prepared crystalline samples.

With this new upgrade come significant challenges to the user in terms of data analysis and storage. To ensure the continued ability of data visualization to keep pace with data acquisition, a new dual-processor 64-bit workstation was installed at the analysis endstation, together with a new four-dimensional data browser.

### Pulsed-Laser Deposition System for Complex Oxide Materials

As synchrotron scientists continue to study the rich scientific problems posed by strongly correlated electronic materials, the need for high-guality, epitaxial layers continues to increase. Ideal experimental situations would allow in-situ sample growth and transfer under UHV conditions. To address this important need, an ultrahigh-vacuum pulsed-laser deposition (PLD) system has been developed as a prototype for a pulsed-laser molecular-beam epitaxy system that will be attached to an ALS beamline. Recently, work focused on developing the ability to grow complex oxide materials in an ALS sample-preparation laboratory while the beamline-based growth system was being designed. The current PLD system, shown in Figure 10, consists of a 248-nm Lambda Physik excimer laser and a spherical growth chamber ( $P_{base} \sim 1 \times 10^{-10}$  Torr) that accommodates sample load-lock introduction and interchamber transfer. Using this unique synchrotron-based facility, numerous epitaxial perovskite oxides, including ferrites and vanadates, have been grown and characterized. PLD is ideally suited to growing multi-



**10** Ultrahigh-vacuum PLD chamber and transfer suitcase. The PLD chamber is spherical while the vacuum suitcase is formed by a six-direction cross. The excimer laser is positioned on an optical table.

component oxide materials, the class to which many strongly correlated electronic systems belong. The development of in-situ capabilities for the growth and transfer of complex oxides will make it possible to apply the power of the ALS to a broad range of complex physical systems and properties.

# Bioinorganic Research at Beamline 9.3.1

New research on organometallic and bioinorganic compounds is possible on Beamline 9.3.1 because of upgrades and improvements in the beamline's capabilities. The improvements allow x-ray absorption measurements at the S and Cl K edges and the Pd L edge by the observation, with high spectral resolution, of fluorescence radiation from cooled samples. The results are relevant to many physiological processes, including the regulation of blood pressure and neural functions.

Beamline 9.3.1 is a bend-magnet beamline that uses a double-crystal monochromator to select photon energies in the S and the V Kedge range (approximately 2.3–5.4 keV). Beamline operation has been significantly improved in recent years, providing a beam that is stable in position and repeatable in



11 Chlorine K edge (top) and palladium L edge (bottom) of chloropalladium initiators of homogeneous catalytic reactions showing significant electronic structure changes as a function of palladium oxidation state and ligand environment.

energy. Improvements for thermal stability have included water cooling of the first crystal in the double-crystal monochromator. The mechanical system of the boomerang, the mechanical linkage between the first and second crystals, has been improved, and beam-position stabilization by use of feedback has been implemented. An entirely new LabView-based control system brings all invacuum motions under computer control, and encoders allow easy operation of the beamline and good energy repeatability. A new user interface provides a friendly and easy-to-use connection to both the beamline controls and the data-acquisition system. The research group of R.K. Szilagyi (Montana State University) has collected data at the S and CI K edges as well as at the Pd L edge for organometallic compounds and bioinorganic model compounds. Sulfur K-edge measurements of S-nitrosated thiols show unique spectral features (Figure 11) that clearly distinguish the S-nitroso form of a cysteine amino acid from the deprotonated thiolate or protonated sulfhydril forms, as well as from the methionine residue. This suggests that sulfur K-edge XAS can be a sensitive probe for the presence of S-nitrosated proteins in cells that may have roles in controlling blood pressure, neural functions, and cell apoptosis. Measurements were made using samples cooled with liquid nitrogen to eliminate radiation damage, which had been observed with room-temperature samples. Samples can also be heated in the XAS endstation.

Future upgrades to the beamline include improved capabilities for electron emission and absorption measurements with better normalization to photon flux, more userfriendly energy calibration, the application of computer control to additional beamline operations, and possibly the extension of the energy range of the monochromator to both higher and lower energies.

## USER SERVICES Gary Krebs, User Services Group Leader

### Introduction

The User Services Group mission is to provide a friendly and efficient interface to the ALS focusing on safety for users and visitors. The group is made up of four sections: the User Services Office, Beamline Coordination, Material Management, and Technical Information Services. These groups work together to provide the users with a wide range of services.

## User Services Office

The User Services Office is staffed by administrative personnel who help new and continuing users with the registration process. All registered users must carry an electronic identification key card, which allows them access to Berkeley Lab and the ALS experiment floor. About 1900 users accessed the experimental floor in 2004. New users can complete much of the processing before they arrive by preregistering on the ALS Web site (www.als.lbl.gov/4DCGI/WEB\_GetForm/ PGIFormEntry.shtml/Initialize).

General-user proposals for beam time are received through the ALS Web site and are peer reviewed and ranked for scientific merit by the Proposal Study Panel (PSP). The User Services Office provides administrative and logistical support for the PSP. The proposal submission and beam time allocation process is described in greater detail on the ALS Web site (www.als. lbl.gov/als/quickguide/ independinvest.html). In addition, the User Services Office provides administrative support to the UEC. The UEC, elected annually by the users, serves as the voice of that diverse group and represents them in ALS strategic planning.

For out-of-towners, the User Services Office can also help in finding a place to stay while working at the ALS. The office manages the ALS apartments; detailed information can be found on the Web at www.als.lbl.gov/als/ quickguide/housing.html.



User Services Office. Front: Olga Poblete, David Malone, Sharon Fujimura, Marissa Tablan, Barbara Phillips. Back: Jeff Troutman, Valerie Wysinger, Gary Krebs.

The User Services Office is managed by Jeff Troutman and includes Sharon Fujimura, Olga Poblete, Barbara Phillips, Marissa Tablan and Valerie Wysinger (Figure 1).

## Beamline Coordination

The Beamline Coordination section coordinates the safety inspection required for each experiment. All experiments are examined and documented in detail to ensure the safety of users, visitors, and operations personnel. Beamline coordinators work closely with Berkeley Lab safety specialists in the areas of electrical, mechanical, chemical, radiation, seismic, and laser safety. The Beamline Coordination Section is led by Donna Hamamoto and includes John Pruyn and David Malone (Figure 2).

### Material Management

The Material Management section provides shipping, receiving, temporary storage, and endstation setup services. The section main-



Beamline Coordination. John Pruyn, Donna Hamamoto, David Malone.



Commonly needed parts and equipment are available in a user stock room available 24 hours a day by key card.



Material Management. Gary Giangrasso, Todd Anderson, Jason DePont.

tains a stockroom of parts and equipment commonly needed by ALS users and technicians (Figure 3). These supplies are accessible by key-card 24 hours a day. The section is managed by Gary Giangrasso and includes Jason DePont and Todd Anderson (Figure 4).

### **Technical Information**

The Technical Information section is responsible for producing this Activity Report as well as the ALS Web site, newsletter, science highlights, and countless special brochures and posters. The section provides science writing, graphic design, and Web expertise to help keep the ALS scientific and technical community, government officials, and the general public informed about the science carried out at the ALS. The group maintains strong ties to the educational community, both within the state of California, the U.S., and internationally. The section is led by Art Robinson and includes Elizabeth Moxon, Lori Tamura, and Greg Vierra (Figure 5).



Tec

Technical Information. Art Robinson, Elizabeth Moxon, Greg Vierra, Lori Tamura.

# User Demographics in 2004

The User Services Group collects user demographics and publication information. As a national user facility, the ALS is required to report these statistics annually to the U.S. Department of Energy. The ALS continued to grow rapidly in 2004. Figure 6 shows the growth in particular scientific fields and the overall user growth from 1997-2004. The breakdown of different institutions that make up our user base is shown in Figure 7. The growth of the user community over the past 10 years is mirrored by the growth in beamlines and publications, as shown in Figure 8. With new beamlines opening and under construction, the ALS expects continued growth in the ALS user community for the next several years.







Pie chart showing percentages of different types of user institutions.





# Special Events





### ALS Users' Meeting

This year's ALS Users' Meeting combined challenging weather, capacity audiences, stimulating workshops, and a visit from Division Director Daniel Chemla to become the most successful meeting to date. More than 400 users and staff attended a variety of activities that included a welcome from new Berkeley Lab Director Steven Chu, plenary sessions dedicated to recent scientific highlights, an accelerator tutorial, poster sessions, eight focused workshops, and a reception for vendors who support the annual meeting. Vendors endured a surprise storm that rattled the exhibit tent on the meeting's second day, but in the end, nature cooperated and provided a beautiful sunset during the outdoor awards banquet on the ALS patio.



Among those welcoming meeting attendees were, from left, Berkeley Lab Director Steve Chu, Acting ALS Division Director Janos Kirz, and UEC Chair Dennis Lindle.



Berkeley Lab's David Attwood presented Pat Dehmer, Director of Basic Energy Sciences, with original artwork created by a UC Berkeley student during a visit to the ALS.



Science highlight speakers included Berkeley Lab's Andrea Cavalleri (left) on "Using Femtosecond Synchrotron Pulses for Time-Resolved X-Ray Absorption in Photo-Excited VO<sub>2</sub>" and Anne Gorden (right) on "Structure of a Plutonium/Sequestering Agent Complex by Synchrotron X-Ray Diffraction." Uwe Arp (center) of the National Institute of Standards and Technology introduced *lightsources.org*, a one-stop shop of light-source information for everyone from users to the general public.

Vendor exhibits (top) and a busy poster session (center) capped the first day of the meeting. Mandana Veiseh of the University of Washington (bottom) shows her award-winning work, "Direct Bacterial Detection by Single-Cell-Based Sensors and Synchrotron FTIR Spectromicroscopy," during the student poster competition.









A lucky break in the weather allowed the awards banquet to take place on the ALS patio as planned.



During the banquet, the Tim Renner User Service Award was presented to James Holton (Physical Biosciences Division) for "friendly and tireless support of users and for implementation of his ELVES program that optimizes the usage of beam time." The Klaus Halbach Award for Innovative Instrumentation at the ALS went to Frank Ogletree (Materials Sciences Division), Hendrik Bluhm (Chemical Sciences Division), Zahid Hussain (ALS), and Miquel Salmeron (Materials Sciences Division) for "the development of a photoelectron spectrometer that operates in ambient gas pressures of up to tens of torr." And the David A. Shirley Award for Outstanding Scientific Achievement at the ALS went to Andrea Cavalleri (Materials Sciences Division) for "pioneering ultrafast x-ray experiments on the metal-insulator transition." Mandana Veiseh (noted above) won the Student Poster Award. Pausing after the banquet for a photo are, from left, Zahid Hussain, Frank Ogletree, James Holton, Corie Ralston (Users' Meeting Program Co-Chair) Miquel Salmeron, Andrea Cavalleri, Hendrik Bluhm, and Keith Jackson (Users' Meeting Program Co-Chair).



In July, Department of Energy Secretary Spencer Abraham listened as David Attwood (second from left) explained how EUV lithography research at the ALS is contributing to the development of smaller, more powerful semiconductors. Berkeley Lab Director Steve Chu (right) looks on.



For the first time in its history, the Council of University of California Staff Assemblies (CUCSA) met at Berkeley Lab for its annual two-day meeting. Comprising two representatives from each UC institution—including the three labs managed by UC—the Council works to bring a staff perspective to UC policymakers. While on site, ALS staff scientists Eli Rotenberg (above) and John Bozek (right) gave the group an inside view of the facility.




University of California Regent Gary Novak (second from right) talked to Physical Bioscience's Carolyn Larabell about recent developments in x-ray microscopy at the ALS. Mr. Novak was touring Lab facilities with Director Steve Chu (left).

The ALS was again one of the "bright spots" for this year's lab-wide Daughters and Sons to Work Day. Girls and boys ages 9–14 were given tours of the ALS before exploring the properties of light with lenses and lasers (right).



### About the ALS





## ALS STAFF

This is a cumulative list of all those who worked at the ALS during the 2004 calendar year. The list includes visitors, students, as well as staff members from other divisions who were matrixed to the ALS.

#### Division Management

- D. Chemla†
- J. Kirz
- B. Feinberg
- J. Krupnick
- N. Smith

#### Accelerator Physics

- D. Robin, Group Leader
- C. Steier, Deputy Leader
- W. Byrne
- A. Loftsdottir\*
- H. Nishimura
- G. Portmann
- H. Sannibale
- T. Scarvie
- W. Wan
- W. Wittmer\*\*

#### Administration

- C. Cooper
- B. Dixon
- A. Reza
- N. Sallee
- E. Saucier
- L. Senft

#### **Budget**

- J. Coyne
- J. Kekos
- M. Lewis

#### Computer Protection

About the ALS / ALS Staff

E. Williams

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#### Controls

- A. Biocca, Group LeaderC. Timossi, Deputy Leader
- E. Domning
- H. Huang
- C. Ikami
- S. Jacobson
- T. Kellog
- A. Robb
- B. Smith
- J. Spring
- R. Steele
- J. Turner
- M. Urashka
- E. Williams

#### Electrical Engineering

- W. Barry, Group Leader G. Stover, Deputy Leader
- B. Bailey
- M. Balagot
- K. Baptiste
- M. Bell R. Candelario
- P. Casey
- ......
- M. Chin
- R. Colston
- S. Cooper
- P. Cull
- J. Elkins
- M. Fahmie
- R. Gassaway
- R. Gervasoni
- A. Geyer L. Holzer
- J. Julian
- B. Kelius
- P. Kozy

I. Kuneli
5. Kwiatkowski
E. Lee
N. Mattson
? Molinari
R. Mueller
J. Nomura
. Ottens
S. Rogoff
? Rosado
VI. Sawada
A. Sippio
R. Slater
VI. Szajbler
R. Valasco
D. Vandyke
M. Vinco
J. Weber

K. Woolfe

#### Environment, Safety, and Health

- R. Baker
- B. Fairchild
- T. Kuneli
- G. Perdue

#### Experimental Systems

- H. Padmore, Group Leader
- A. Warwick, Deputy Leader
- A. Bartelt\*\*
- R. Celestre
- M. Church
- S. Clark
- A. Doran
- S. Fakra
- J. Feng
- J. Glossinger

J. Hao P. Heimann M. Howells S. Irick T. Kellog A. MacDowell M. Marcus W. McKinney G. Morrison S. Morton J. Nasiatka K. Opachich A. Scholl N. Tamura B. Valek V. Yashchuck

E. Glover

#### Mechanical Engineering

- R. Schlueter, Acting Group Leader
- R. Duarte, Acting Deputy Leader
- N. Andresen

A. Young

- R. Beggs
- D. Calais
- A. Catalano
- M. Coleman
- D. Colomb
- C. Cummings
- M. Decool
- A. DeMello
- S. Dimaggio
- D. Ellis
- D. Fritz A. Gavidia

D. Gibson

J. Haugrud

C. Hernikl

- C. Hopkins D. Horler D. Hull D. Jones J.-Y. Jung N. Kelez S. Klingler M. Kritscher K. Krueger A. Lim A. Lobodovsky R. Low D. MacGill S. Marks P. McKean H. Meyer T. Miller V. Moroz G. Morrison D. Munson W. Ogelsby M. Omerbashich J. Osborn E. Palmerston J. Pepper K. Peterman P. Pipersky D. Plate S. Prestemon A. Rawlins D. Shuman K. Sihler A. Smith T. Stevens M. Thomas W. Thur M. Wingert
- E. Wong
- F. Zucca

#### Operations

J. Pusina, Group Leader W. Byrne, Deputy Leader

- M. Beaudrow
- D. Brothers
- K. Osborne
- A. Pearson
- D. Richardson
- D. Riley-Cole
- S. Stricklin
- M. Wolfe

#### Procedure Center

R. Jones

#### Project Management

- A. Catalano
- S. Rossi

#### **Quality Assurance**

D. Richardson

#### Scientific Support

Z. Hussain, Group Leader J. Bozek, Deputy Leader G. Ackerman E. Arenholz W. Bates A. Bostwick K. Chesnel\*\* Y.-D. Chuang\*\* J. Denlinger A. Federov J. Guo A. Guy C. Hauck D. Kilcoyne G. Lebedev M. Martin S. Mun J. Pepper M. Pfeifer\*\* E. Rotenberg B. Rude F. Schlachter J. Spear

#### **User Services**

- G. Krebs, Group LeaderA. Robinson, Deputy Leader
- T. Anderson
- J. De Ponte
- S. Fujimura G. Giangrasso
- D. Hamamoto
- D. Malone
- E. Moxon
- B. Phillips
- O. Poblete
- J. Pruyn
- J. Troutman
- M. Tablan
- L. Tamura
- G. Vierra
- V. Wysinger

### Visitors and Students

T. Araki\*\* B. Batterman F. Baumberger\*\* R. Bilodeau\*\* A. Budiman S. Caldwell A. Chakmatov S. Chourou A. Comin\*\* C. Cui\*\* A. Das P. Dietrich B. Freelon\*\* P. Glans\*\* A. Gleason M. Greaves Z. Hao\* F. Himpsel M. Hindi S. Kashtanov

S. Kevan

A. Kouprine

- K. Smith J. Soderstrom\*\* J. Spence M. Van Hove D. Walker M. Watanabe M. Watanabe M. Water C. Won\* A. Wu W. Yang J. Zaanen X. Zhou ALS Docto

M. Kunz

D. Lacy

M. Liberati\*\*

A. MacPhee

N. Mannella\*\*

J. McChesney

G. Meyer

B. Nellis

H. Ohldag

K. Opachich\*

G. Paranthaman

T. Ohta\*

J. Patel

M. Perri\*\*

M. Rossi

D. Shiraki

M. Nip

#### ALS Doctoral Fellows

C. Cappa\*
Y. Chen\*
H. Fu\*
J. Holroyd\*
T. Learmonth\*
P. Strachan\*
F. Wang\*
M. Weinberger\*
\*fOn leave
\*Graduate Student Research Assistant
\*\*Postdoc

## ALS ADVISORY PANELS

#### Scientific Advisory Committee

- Neil Ashcroft, Cornell University
- Samuel Bader (chair), Argonne National Laboratory
- Phil Bucksbaum, University of Michigan
- Dennis Lindle (ex-officio), University of Nevada, Las Vegas
- Jennifer Doudna, Berkeley Lab
- Wolfgang Eberhardt, BESSY GmbH, Germany
- Pascal Elleaume, European Synchrotron Radiation Facility
- Yves Idzerda (ex-officio), Montana State University
- Stephen D. Kevan (past chair), University of Oregon
- Miquel Salmeron, Berkeley Lab
- Sunil Sinha, University of California, San Diego
- Donald L. Sparks, University of Delaware
- John Spence, Arizona State University
- Anthony Starace, University of Nebraska-Lincoln
- J. Friso van der Veen, Paul Scherrer Institut
- Linda Young, Argonne National Laboratory

#### Users' Executive Committee

- John Bozek, Advanced Light Source, Berkeley Lab
- Sophie Canton (student), University of Western Michigan
- Greg Denbeaux (vice chair), University at Albany, State University of New York
- Jennifer Doudna (past chair), University of California, Berkeley
- Dan Dessau, University of Colorado
- Clemens Heske, University of Nevada, Las Vegas
- Keith Jackson, Center for X-Ray Optics, Berkeley Lab
- Dennis W. Lindle (chair), University of Nevada, Las Vegas
- Gary E. Mitchell, Dow Chemical Company
- Alexander Moewes, University of Saskatchewan
- Yasuji Muramatsu, Japan Atomic Energy Research Institute
- Corie Ralston, Physical Biosciences Division, Berkeley Lab
- Eli Rotenberg, Advanced Light Source, Berkeley Lab
- Ed Westbrook, Molecular Biology Consortium

#### Science Policy Board

Massimo Altarelli, Elettra Sincrotone Trieste

- Samuel Bader, Argonne National Laboratory
- Paul Fleury, Yale University
- Franz J. Himpsel, University of Wisconsin, Madison
- Walter Kohn, University of California, Santa Barbara
- Yuan T. Lee, Academia Sinica, Taiwan
- Albert Narath, Lockheed Martin Corporation (retired)
- Yves Petroff, European Synchrotron Radiation Facility
- Alan Schriesheim, Argonne National Laboratory
- Robert Tjian, University of California, Berkeley
- Eberhard Umbach, University of Würzburg, Germany



Members of the Users' Executive Committee attending an ALS strategic planning retreat at the UC Berkeley Faculty Club. First row: Sophie Canton, Corie Ralston, Gary Mitchell. Second row: Ed Westbrook, Keith Jackson, Dennis Lindle, Dan Dessau. Third row: Greg Denbeaux, John Bozek, Alexander Moewes, Eli Rotenberg.

## FACTS AND FIGURES

### Using the Advanced Light Source

The ALS, a Department of Energy national user facility, welcomes researchers from universities, industry, and government laboratories. There are three principal modes of access to the ALS: general users, approved programs, and participating research teams. In all cases, access is through a proposal that has been peer reviewed by one of our advisory bodies, the Scientific Advisory Committee and/or one of the Proposal Study Panels. The ALS does not charge users for beam access if their research is nonproprietary. Users performing proprietary research are charged a fee based on full cost recovery. All users are responsible for the day-today costs of research (e.g., supplies, phone calls, technical support).

The nominal operating energy of the ALS storage ring is 1.9 GeV, although it can run from 1.0 to 1.9 GeV, allowing flexibility for user operations. At 1.9 GeV, the normal maximum operating current is 400 mA in multibunch operation. The spectral range of undulator and wiggler beamlines extends from photon energies of roughly 5 eV to 21 keV, on superbend beamlines the range is between 2.4 and 60 keV. Bend magnets produce radiation from the infrared to about 20 keV.

The ALS is capable of accommodating approximately 50 beamlines and more than 100 endstations. The first user beamlines began operation in October 1993, and there were 37 simultaneously operating beamlines, with several more under construction, by the end of fiscal year 2004.



#### ALS Beamlines<sup>a</sup>

Beamline	Source	Areas of Research/Techniques	Monochromator	Energy Range	Operational
1.4.3	Bend	Infrared spectromicroscopy Interferometer		0.05-1.2 eV (600-10,000 cm <sup>-1</sup> )	Now
1.4.4	Bend	Infrared spectromicroscopy	Interferometer	0.05-1.5 eV (400-12,000 cm <sup>-1</sup> )	Now
3.1	Bend	Diagnostic beamline	Mirror/filter	1-2 keV	Now
3.2.1	Bend	Commercial LIGA	None	3-12 keV	Now
3.3.1	Bend	LIGA	None	3-12 keV	Now
3.3.2	Bend	LIGA	None	3-12 keV	Now
4.0.1	EPU9	MERLIN	SGM	10-130 eV	2006
4.0.2	EPU5	Magnetic spectroscopy			
		Advanced photoelectron spectrometer/diffractometer	Variable-included-angle PGM	52-1900 eV	Now
		L-edge chamber with superconducting spectrometer	Variable-included-angle PGM	52-1900 eV	Now
		XMCD chamber (6 T, 2 K)	Variable-included-angle PGM	52-1900 eV	Now
		Eight-pole electromagnet	Variable-included-angle PGM	52-1900 eV	Now
4.2.2	SB	MAD and monochromatic PX	Double crystal	5-17 keV	Now
5.0.1	W11	Monochromatic PX	Curved crystal	12.4 keV	Now
5.0.2	W11	MAD and monochromatic PX	Double crystal	3.5-14 keV	Now
5.0.3	W11	Monochromatic PX	Curved crystal	12.4 keV	Now
5.3.1	Bend	Femtosecond phenomena	Double crystal	1.8-12 keV	Now
5.3.2	Bend	Polymer STXM	SGM	250-700 eV	Now
6.0.1	U3	Femtosecond phenomena	Double crystal	2.2-10 keV	2006
6.0.2	U3	Femtosecond phenomena	VLS-PGM	130-1800 eV	2005
6.1.2	Bend	High-resolution zone-plate microscopy	Zone-plate linear	300-1300 eV	Now
6.3.1	Bend	Calibration and standards, EUV/soft x-ray optics testing, solid-state chemistry	VLS-PGM	300-2000 eV	Now
6.3.2	Bend	Calibration and standards; EUV optics testing; atomic, molecular, and materials science	VLS-PGM	50-1300 eV	Now
7.0.1	U5	Surface and materials science, spectromicroscopy			
		Scanning photoemission microscope	SGM	100-800 eV	Now
		Electronic Structure Factory	SGM	60-1200 eV	Now
		Advanced x-ray inelastic scattering	SGM	80-1200 eV	Now
7.2	Bend	Diagnostic beamline	Filter/none	Far IR-17 keV	Now
7.3.1.1	Bend	Magnetic microscopy, spectromicroscopy	SGM	175-1500 eV	Now
7.3.1.2	Bend	Surface and materials science, micro x-ray photoelectron spectroscopy	SGM	175-1500 eV	Now
7.3.3	Bend	X-ray microdiffraction	White light, two or four crystal	6-12 keV	Now
8.0.1	U5	Surface and materials science, imaging photoelectron spectroscopy, soft x-ray fluorescen	ce		
		Ellipsoidal-mirror electron energy analyzer	SGM	65-1400 eV	Now
		Soft x-ray fluorescence spectrometer	SGM	65-1400 eV	Now
8.2.1	SB	MAD and monochromatic PX	Double crystal	5-17 keV	Now
8.2.2	SB	MAD and monochromatic PX	Double crystal	5-17 keV	Now
8.3.1	SB	MAD and monochromatic PX	Double crystal	2.4-18 keV	Now
8.3.2	SB	Tomography	Double crystal	3-60 keV	Now
9.0.1	U10	Coherent optics/scattering experiments	None or off-axis zone plate	10-800 eV	Now
9.0.2	U10	Chemical dynamics			
		Crossed molecular beam	White light, Off-plane Eagle	5–30 eV	Now
		Molecular-beam photoelectron/photoion spectroscopy	White light, Off-plane Eagle	5-30 eV	Now
		Molecular-beam photoelectron/photoion imaging and spectroscopy	White light, Off-plane Eagle	5-30 eV	Now
		Flame chamber	White light, Off-plane Eagle	5-30 eV	Now
		Ablation chamber	White light, Off-plane Eagle	5-30 eV	Now
		Aerosol and free nanoparticle chamber	White light, Off-plane Eagle	5-30 eV	Now
		Kinetics machine	White light, Off-plane Eagle	5-30 eV	Now

Beamline	Source	Areas of Research/Techniques	Monochromator	Energy Range	Operational
9.3.1	Bend	Atomic, molecular, and materials science			
		Angle-resolved time-of-flight electron spectrometer	Double crystal	2.2-5.5 keV	Now
		Ion time-of-flight spectrometer	Double crystal	2.2-5.5 keV	Now
		Magnetic mass analyzer	Double crystal	2.2-5.5 keV	Now
		Polarized-x-ray emission spectrometer	Double crystal	2.2-5.5 keV	Now
		X-ray absorption cell	Double crystal	2.2-5.5 keV	Now
		XAFS station	Double crystal	2.2-5.5 keV	Now
9.3.2	Bend	Chemical and materials science, circular dichroism, spin resolution			
		Advanced materials chamber	SGM	30-1400 eV	Now
		Ambient pressure photoemission	SGM	30-1400 eV	Now
10.0.1	U10	Photoemission of highly correlated materials; high-resolution atomic, molecular, and op	tical physics		
		High energy resolution spectrometer	SGM	17-340 eV	Now
		HIRAMES	SGM	17-340 eV	Now
		Ion-photon beamline	SGM	17-340 eV	Now
		Electron spin polarization	SGM	17-340 eV	Now
10.3.1	Bend	X-ray fluorescence microprobe	White light, multilayer mirrors	3-20 keV	Now
10.3.2	Bend	Environmental and materials science, micro x-ray absorption spectroscopy	White light, two crystal	2.5-17 keV	Now
11.0.1	EPU5	PEEM-3	VLS-PGM	100-2000 eV	2005
11.0.2	EPU5	Molecular environmental science			
		Wet spectroscopy	Variable-included-angle PGM	95–2000 eV	Now
		High-pressure photoemission spectroscopy	Variable-included-angle PGM	95-2000 eV	Now
		STXM	Variable-included-angle PGM	130-2000 eV	Now
11.3.1	Bend	Small-molecule crystallography	Channel-cut Si(111)	6-17 keV	Now
11.3.2	Bend	Inspection of EUV lithography masks	VLS-PGM	50-1000 eV	Now
12.0.1	U8	EUV optics testing and interferometry, angle- and spin-resolved photoemission			
		EUV interferometer (2 available)	VLS-PGM	60-320 eV	Now
		Angle- and spin-resolved photoemission	VLS-PGM	20-320 eV	Now
12.0.2	U8	Coherent soft x-ray science			
		Coherent optics	VLS-PGM	200-1000 eV	Now
		Coherent scattering	VLS-PGM	200-1000 eV	Now
12.2.2	SB	CALIPSO			
		Nanoscience/materials chemistry	Double crystal	6-40 keV	Now
		Solid-state physics/geoscience	Double crystal	6-40 keV	Now
12.3.1	SB	SIBYLS	Double crystal and double multilayer	5.5-17 keV	Now
BTF	Linac	Beam Test Facility	None	50-MeV electrons	Now

aThe information in this table is valid as of May 2005. The most current information about ALS beamlines is available on the Web at www-als.lbl.gov/als/als\_users\_bl/bl\_table.html.Bend = bend magnetEPUx = x-cm-period EPUUx = x-cm-period undulatorWx = x-cm-period wiggler

#### ALS Insertion Device Parameters<sup>a</sup>

Device	Beamline	Status	Energy Range at 1.5 GeV (eV)	Energy Range at 1.9 GeV (eV)	Period (cm)	No. of Periods	Operating Gap Range (cm)	Effective Field Range (T)
U3	6.0.1	Installed	73-3100	120–5000 4000–11000 <sup>b</sup>	3.0	50	0.55-2.7	1.5-0.13
U5	8.0.1	Operational	50-1900	80-3000	5.0	89	1.4-4.5	0.85-0.10
U5	7.0.1	Operational	50-1900	80-3000	5.0	89	1.4-4.5	0.85-0.10
U8	12.0.1	Operational	18-1200	20-1900	8.0	55	2.47-8.3	0.80-0.07
U10	9.0.1	Operational	5-950	8-1500	10.0	43	2.27-11.6	0.98-0.05
U10	10.0.1	Operational	8-950	12-1500	10.0	43	2.31-11.6	0.80-0.05
EPU5	4.0.2	Operational	47-1000 <sup>c</sup>	75–3000 <sup>c</sup>	5.0	37	1.40-5.5	0.86–0.10 <sup>d</sup> 0.58–0.10 <sup>e</sup>
EPU5	11.0.1	Operational	50-1000 <sup>c</sup>	80-3000 <sup>c</sup>	5.0	36.5	1.44-5.5	0.85–0.10 <sup>d</sup> 0.57–0.10 <sup>e</sup>
EPU5	11.0.2	Operational	47-1000 <sup>c</sup>	75–3000 <sup>c</sup>	5.0	37	1.38-5.5	0.86–0.10 <sup>d</sup> 0.58–0.10 <sup>e</sup>
W11	5.0.2	Operational	6000-13000 <sup>b</sup>	6000-21000 <sup>b</sup>	11.4	29	1.25-18.0	1.94-0.03

<sup>a</sup> The information in this table is valid as of May 2005.

<sup>b</sup>Wiggler mode. <sup>c</sup>Elliptical polarization mode. <sup>d</sup>Vertical field.

<sup>e</sup>Horizontal field.

#### ALS Storage Ring Parameters<sup>a</sup>

Parameter	Value
Beam particle	Electron
Beam energy	1.0-1.9 GeV
Injection energy	1.0-1.5 GeV
Beam current	
Multibunch mode	400 mA
Two-bunch mode	2 × 25 mA
Filling pattern (multibunch mode)	276 to 320 bunches, possibility of 10-mA "camshaft" bunch in filling gap
Bunch spacing	
Multibunch mode	2 ns
Two-bunch mode	328 ns
Circumference	196.8 m
Number of straight sections	12
Current number of insertion devices	10
Radio frequency	499.642 MHz
Beam size in straight sections, rms (1.9 GeV multibunch mode)	310 microns horiz. × 16 microns vert.

Parameter	Value at 1.5 GeV	Value at 1.9 GeV
Beam lifetime		
Multibunch mode	~3.5 hours at 400 mA	~8.0 hours at 400 mA
Two-bunch mode	not used	~60 min. at 40 mA
Horizontal emittance	4.2 nm-rad	6.3 nm-rad
Vertical emittance <sup>b</sup>	0.2 nm-rad	0.13 nm-rad
Energy spread ( $\Delta E/E$ , rms)	$8 \times 10^{-4}$	1 × 10 <sup>-3 c</sup>
Pulse length (FWHM)	65 ps	70 ps

<sup>a</sup> The information in this table is valid as of May 2005.

<sup>b</sup> Vertical emittance is deliberately increased to improve beam lifetime.

<sup>c</sup>Above 8 mA per bunch in two-bunch mode, the energy spread increases because of the microwave instability.

### 2004 PUBLICATIONS

Listed below are publications (e.g., journal articles, conference papers, theses, and book chapters) that were published in calendar year 2004 and are based on data obtained in whole or in part at the ALS as well as publications containing descriptions of experiment, beamline, or accelerator systems developed at the ALS.

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## ACRONYMS AND ABBREVIATIONS

1D one dimensional
2D two dimensional
3D three dimensional
AFM atomic-force microscopy
AFRD Accelerator and Fusion Research
Division, Berkeley Lab
APS Advanced Photon Source
ARPES angle-resolved photoemission spec-
troscopy
AT Accelerator Toolbox
ATP adenosinetriphosphate
BCS Bardeen-Cooper-Schrieffer (theory of
superconductivity)
BER Biological and Environmental
Research, DOE Office of
BES Basic Energy Sciences, DOE Office of
BOA Born-Oppenheimer approximation
BPM beam position monitor
CAD computer-aided design
CALIPSO California High-Pressure Science
Observatory
CBP Center for Beam Physics
CCD charge-coupled device
CDR conceptual design report
CIRCE Coherent Infrared Center
CMR colossal magnetoresistance
CNT clostridal neurotoxin
COLTRIMS cold-target recoil-ion momentum
spectrometry
CSR coherent synchrotron radiation
CUCSA Council of University of California
Staff Assemblies
CXRO Center for X-Ray Optics
DE double exchange
DOE Department of Energy
EPAC European Particle Accelerator
Conference
EPICS Experimental Physics and Industrial Control System
EPU elliptically polarizing undulator
ESG Experimental Systems Group
ESRF European Synchrotron Radiation
Facility
EUV extreme ultraviolet

EXAFS	. extended x-ray absorbtion fine structure
FF	. feedforward
FTIR	. Fourier transform infrared
FWHM	. full-width half-maximum
FY	. fiscal year
GMR	. giant magnetoresistance
HDV	. hepatitis delta virus
HIRAMES	High-Resolution Atomic and
	Molecular Electron Spectrometer
НОМ	. higher-order mode
HTSC	. high-temperature superconductor
ICFA	. International Committee for Future
	Accelerators
ID	. insertion device
IDP	. interplanetary dust particle
IXS	. inelastic x-ray scattering
КВ	. Kirkpatrick-Baez
LCLS	. Linac Coherent Light Source
LFB	. longitudinal feedback
LIGA	. German acronym for lithography,
	electroplating, and molding
LLNL	. Lawrence Livermore National
	Laboratory
LMS0	. La <sub>0.7</sub> Sr <sub>0.3</sub> MnO <sub>3</sub>
LOCO	. Linear Optics from Closed Orbits
MAD	. multiple-wavelength anomalous dif-
	fraction
MERLIN	. meV-resolution beamline
ML	. monolayer
MRAM	. magnetic random-access memory
MRI	. magnetic resonance imaging
NanoSIMS	. nano secondary ion mass spec-
	trometry
NASA	. National Aeronautics and Space
	Administration
NEXAFS	. near-edge x-ray absorption fine-
	structure spectroscopy
NGF	. nerve growth factor
NIH	. National Institutes of Health
NSF	. National Science Foundation
NSLS	. National Synchrotron Light Source
NSRC	. Nanoscale Science Research Center
OML	. Optical Metrology Laboratory

	PEEM photoemission electron microscope
	PGMplane grating monochromator
	PIE photoionization efficiency
	PLD pulsed-laser deposition
	PSD power spectral density
	PSP Proposal Study Panel
	PX protein crystallography
	QERLIN q-resolved inelastic scattering beamline
ter	RAM random-access memory
	rf radiofrequency
tor	rms root-mean-square
iture	SAC Scientific Advisory Committee
	SAXS small-angle x-ray scattering
	SB superconducting bend (magnet)
	SGM spherical grating monochromator
	SIBYLS Structurally Integrated Biology for
	Life Sciences
	SLAC Stanford Linear Accelerator Center
۱y,	SNARE soluble N-ethylmaleimide-sensitive factor attachment protein receptor
	SPPS Sub-Picosecond Pulse Source
	SRT spin reorientation transition
	SSG Scientific Support Group
	SSRL Stanford Synchrotron Radiation
its	Laboratory
s dif-	STXM scanning transmission x-ray microscopy
	THC third-harmonic cavity
	TOF time-of-flight
ory	UC University of California
	UEC Users' Executive Committee
C-	UHV ultrahigh vacuum
	UK United Kingdom
ce	VLS variable line spacing
	VUV vacuum ultraviolet
<u>}-</u>	XAFSx-ray absorption fine structure
	XASx-ray absorption spectroscopy
	XMCD x-ray magnetic circular dichroism
	XMLDx-ray magnetic linear dichroism
e	XMLDx-ray magnetic linear dichroism XRSx-ray scattering

![](_page_138_Picture_0.jpeg)

![](_page_138_Picture_1.jpeg)

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![](_page_139_Picture_2.jpeg)

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