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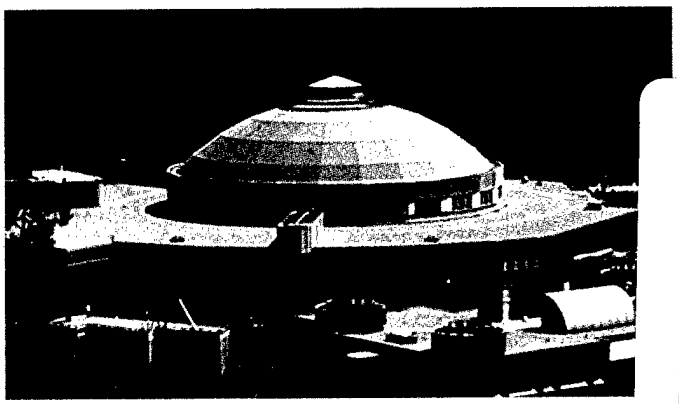

ACTIVITY REPORT 1996/97

SEPTEMBER 1997

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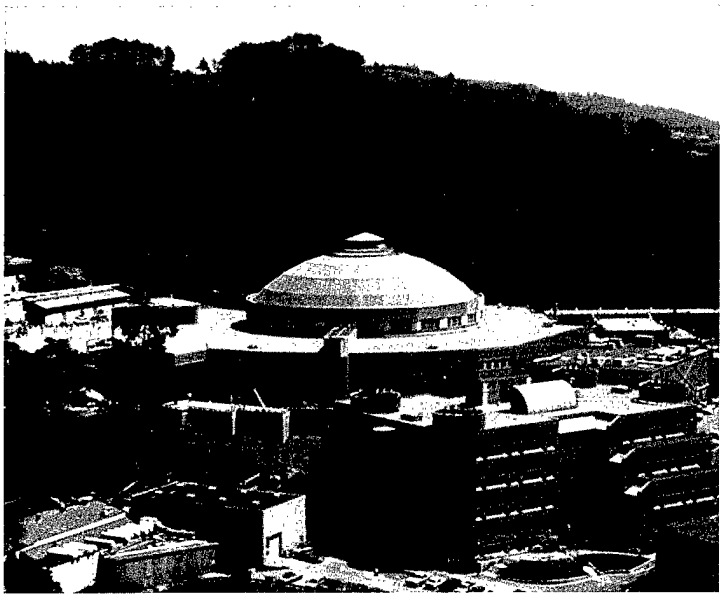

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Ernest Orlando Lawrence Berkeley National Laboratory
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This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Materials Science Division, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

Ten years ago, the Advanced Light Source (ALS) existed as a set of drawings, calculations, and ideas. Four years ago, it stored an electron beam for the first time. Today, the ALS has moved from those ideas and beginnings to a robust, third-generation synchrotron user facility, with eighteen beamlines in use, many more in planning or construction phases, and hundreds of users from around the world.

Progress from concepts to realities is continuous as our scientific program, already strong in many diverse areas, moves in new directions to meet the needs of researchers into the next century. ALS staff members who develop and maintain the infrastructure for this research are similarly unwilling to rest on their laurels. As a result, the quality of the photon beams we deliver, as well as the support we provide to users, continues to improve.

The ALS Activity Report is designed to share the results of these efforts in an accessible form for a broad audience. The Scientific Program section, while not comprehensive, shares the breadth, variety, and interest of recent research at the ALS. (Our *Compendium of User Abstracts and Technical Reports* provides a more comprehensive and more technical view.) The Facility Report highlights progress in operations, ongoing accelerator research and development, and beamline instrumentation efforts. Although these Activity Report sections are separate, in practice the achievements of staff and users at the ALS are inseparable. User-staff collaboration is essential as we strive to meet the needs of the user community and to continue the ALS's success as a premier research facility.

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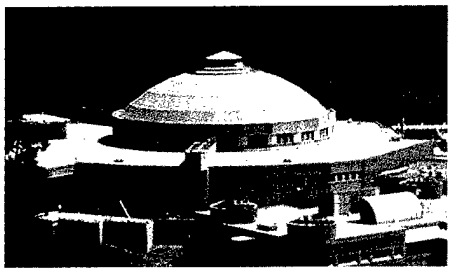
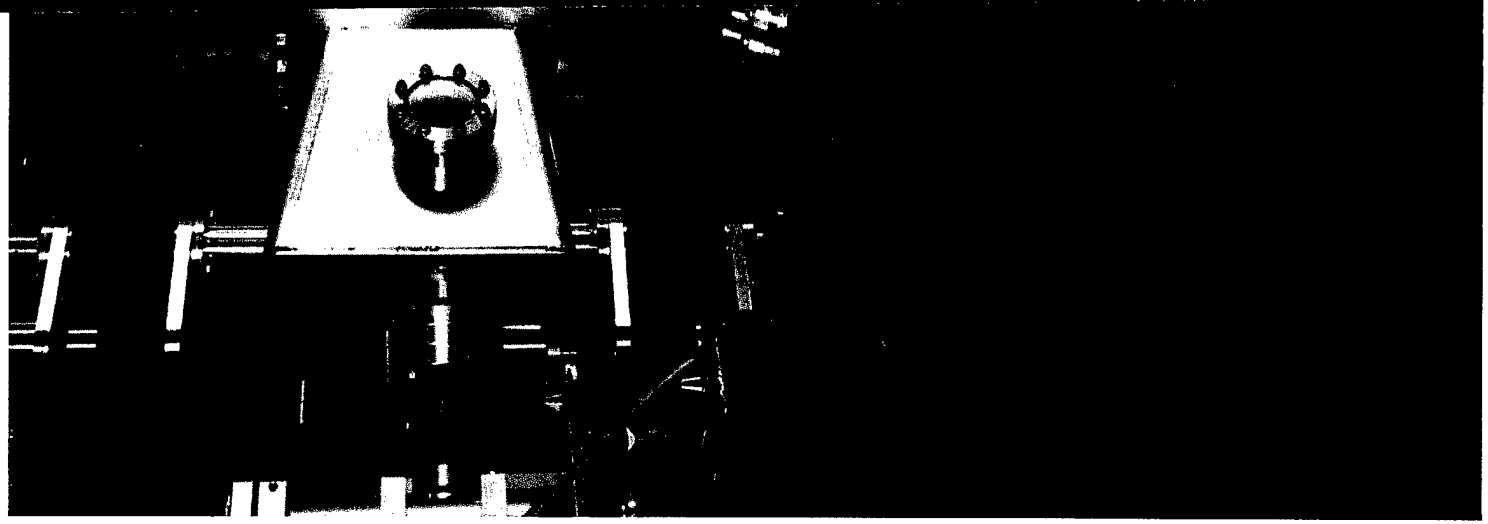
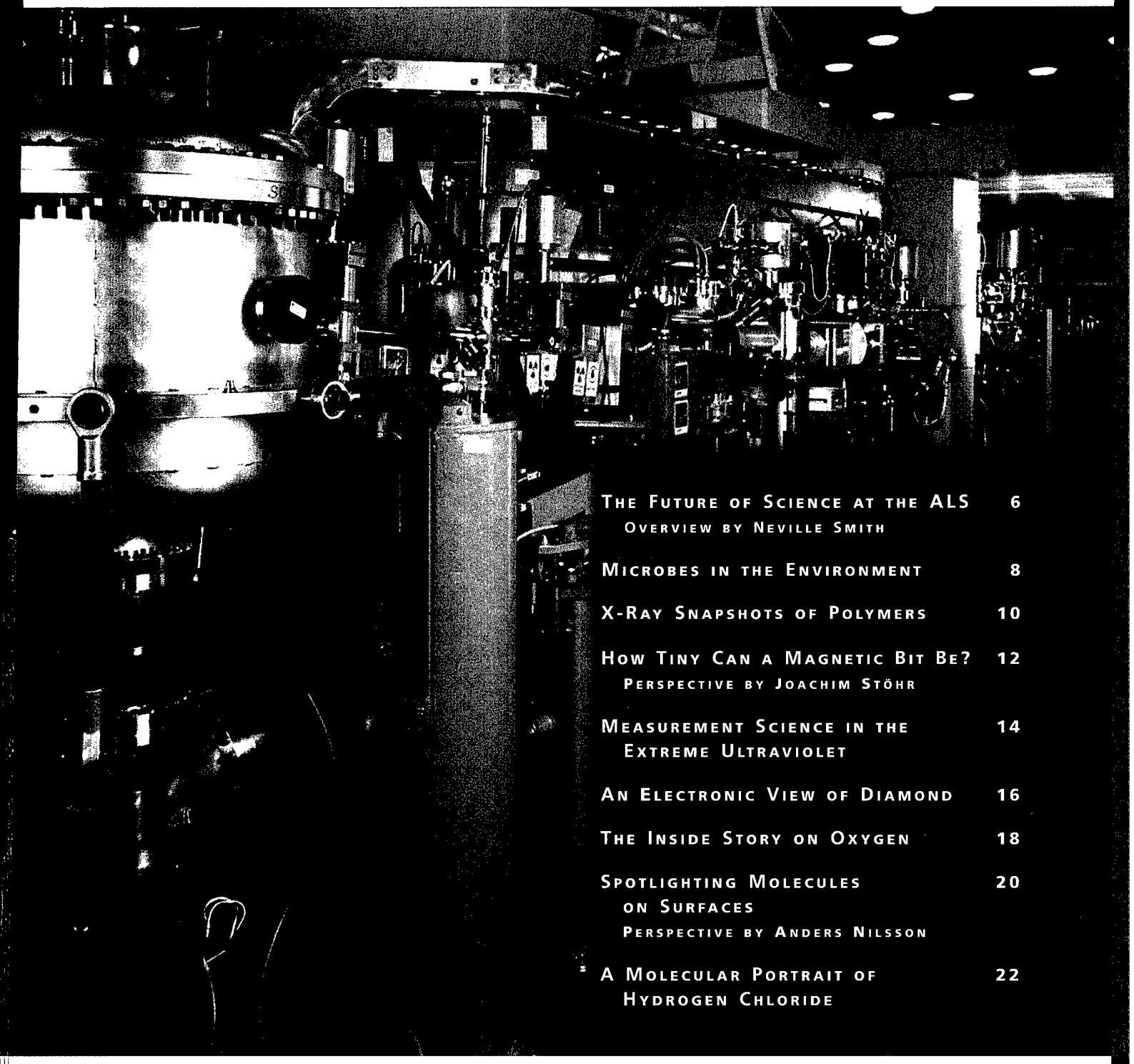


The Advanced Light Source, a national user facility located at Ernest Orlando Lawrence Berkeley National Laboratory of the University of California, is available to researchers from academia, industry, and government. Its building incorporates the dome that once housed the 184-inch Cyclotron built by the Laboratory's founder, E.O. Lawrence.



SCIENTIFIC PROGRAM



THE FUTURE OF SCIENCE AT THE ALS

Developing a Strategic Vision for the 21st Century

Neville V. Smith
Scientific Program Head
Advanced Light Source

What is the strategic scientific vision at the ALS? At our present stage of development, this question comes to the fore. Now that we have brought the ALS into reliable, routine operation that meets or exceeds its design specifications, with users producing a wealth of scientific results, what directions will be most important to this facility over the next 10 to 20 years?

Understanding Complex Systems

We believe that four major scientific areas will be preeminent in the twenty-first century: (1) life science, (2) nanoscience, (3) environmental science, and (4) information science. These choices reflect a shift in emphasis away from the reductionist science that has dominated the twentieth century (e.g., what are the ultimate elementary particles?) and toward the understanding and manipulation of complex systems. These areas are also responsive to societal needs, an important consideration given the changed funding climate in the post–Cold War era. Are the users of the ALS likely to be major players in this new scientific dispensation, and if so, what strategic actions should we be taking now to redirect our emphasis?

In the area of life science, we have growing programs in protein crystallography, x-ray biomicroscopy, and spectroscopy on metallo-organic systems. In nanoscience, we are very strongly positioned. The extremely high brightness of the ALS translates into high spatial resolution, and the various x-ray microprobes and microscopes operating at the micron- and nanometer-length scales at the ALS match the analytical needs of the microelectronics and magnetic recording industries. In environmental science, we have a modest program at present, but we expect this to grow. Recent workshops have exposed a national need for chemical and structural "speciation" spectroscopy and biomicroscopy in the soft x-ray region, and we have pending a major initiative to build out a sector of the ALS storage ring for this purpose. The area of information science is software-dominated, but has a hardware component, specifically semiconductor microelectronics and magnetic recording media. It is in these vital fields that we expect to have considerable impact through our contributions to nanoscience in collaboration with companies such as Intel and IBM.

Basic Research Still a Priority

High brightness also translates into high spectral resolving power, and this is what drives our basic research. Programs in chemical dynamics, atomic

and molecular physics, and condensed-matter physics are already benefiting from the unprecedented energy resolution available at the ALS. Thanks to a much-needed boost from the DOE Scientific Facilities Initiative, approved by Congress for 1996, which funded an increase in both facility operations and user equipment, we are adding new programs, such as spin-resolved photoemission studies of magnetic and highly correlated materials, to our growing portfolio of research.

The following pages highlight a selection of ALS research covering the period from 1996 to mid-1997. We have also added a new feature to this year's Activity Report, two perspectives on growing areas of study by leaders in those fields. Together, the highlights and perspectives demonstrate our intention to exploit the high brightness of the ALS by advancing into the twenty-first-century themes enumerated above while maintaining our commitment to basic research. Of course, highlights never tell the whole story. For a much more complete, and more technical, overview of the ALS scientific program, the interested reader should consult our annual compendium of user abstracts and technical reports.

MICROBES IN THE ENVIRONMENT

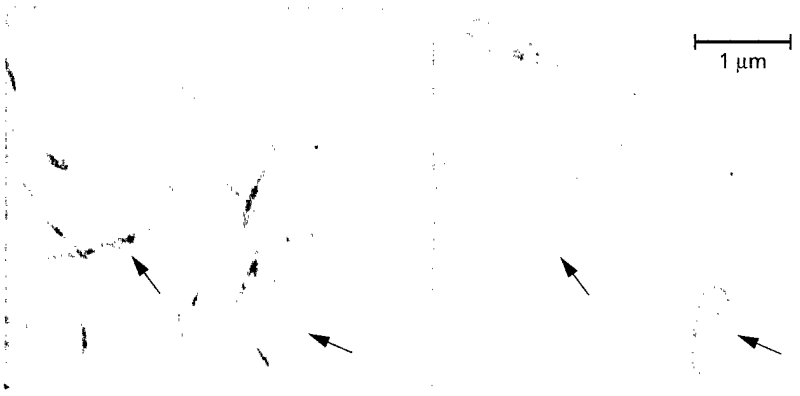
Examining Bioremediation of Contaminants

Cleaning up the environment is a monumental task, now consuming many billions of dollars annually. Based on the belief that effective waste-remediation treatments will come by scrutinizing, at a molecular level, the various chemical compounds that enter the environment as the result of human activity, the new field of molecular environmental science (MES) is emerging. Practitioners of MES investigate the route contaminants take to their final destinations in the environment, including formation of new compounds due to interaction with their surroundings, transport through soils and groundwater, uptake in plant and animal life, and possible immobilization in benign forms. It turns out that bacteria are potentially key players with the ability to purify contaminated soils and water supplies (bioremediation).

Where the Action Is

The complex chemistry taking place in the environment is dominated by reactions in the presence of water. Among other functions, water serves as a medium to transport metal atoms to and from microbes and chemical compounds in the soil. It is known that bacteria can oxidize (remove electrons from) or reduce (add electrons to) metal atoms, such as iron and manganese. Oxidation of iron or manganese that is dissolved in water creates insoluble oxide compounds, such as goethite or manganite (FeOOH or MnOOH), resulting in solid mineral deposits (biomineralization). Conversely, reduction of the metals already in mineral particles causes them to dissolve in the surrounding water.

There are at least two ways biomineralization could help in environmental cleanup. If bacteria



Depending on their species, bacteria can either oxidize metals dissolved in water, thereby causing the formation of metal-oxide particles, or reduce the metal in solid particles, thereby causing it to dissolve. These x-ray microscope images were taken in the same area of a sample, (left) at x-ray wavelengths (photon energies) absorbed by the manganese atoms in needle-shaped particles of manganite (MnOOH), and (right) at wavelengths absorbed by the carbon atoms in microbes. The two arrows in each image indicate the locations of a manganite needle and a bacterium.

could directly mineralize contaminants such as plutonium, uranium, and chromium, this bacterial digestion would immobilize them as insoluble sediment. Alternatively, biomineralized deposits of other metals, manganese for example, could attract contaminants, which would then form insoluble compounds on the surfaces of the mineral deposits. Learning which, if either, of these mechanisms is a potential route to bioremediation involves analyzing the chemical reactions, their products, and where they occur relative to the bacteria and the particle surfaces.

Getting the Picture

X-ray absorption spectra offer researchers much of the information they want because the wavelengths at which a metal atom in a molecule absorbs x rays identify its oxidation state. Owing to the small size of both bacteria and mineral particles, spatial resolution is also necessary to map the distribution of metals and their oxidation states and to probe their local properties rather than averaging over wide areas. At the ALS, the combination of spectroscopy with imaging in an x-ray microscope (spectromicroscopy) fills the bill. However, the watery nature of environmental systems creates a challenge, since water also absorbs many x rays. To work with wet samples, therefore, researchers have had to develop specially designed sample holders that minimize the distance the x rays must travel through water.

The first step in the investigation—now accomplished—is demonstrating the ability to image bacteria and mineral particles in the same wet-sample cell with high resolution. For example, manganese minerals occur as needle-shaped crystals about 1 μm long and 0.1 μm wide. Bacteria that metabolize manganese have a similar length but are a little more rotund. Since the manganese and carbon atoms in the bacteria absorb x rays at different wavelengths, the mineral particles and microbes are easily distinguished by making separate images at the appropriate wavelengths. Because water influences the wavelengths and shapes of x-ray absorption peaks, future absorption measurements to identify chemical species will require detailed examination of model compounds in wet cells to establish characteristic spectral signatures.

Research conducted by B.P. Tonner (principal investigator) and K. Nealson (University of Wisconsin–Milwaukee), and W. Meyer-Ilse and J. Brown (Berkeley Lab's Center for X-Ray Optics), using the x-ray microscope (XM-1) at Beamline 6.1.2. Funding: Office of Biological and Environmental Research of the U.S. Department of Energy, Laboratory for Surface Studies and Center for Great Lakes Studies (University of Wisconsin–Milwaukee), and Office of Basic Energy Sciences of the U.S. Department of Energy.

X-RAY SNAPSHOTS OF POLYMERS

Revealing Structure on a Microscopic Scale

While they may look uniform to the eye, most of the materials that find their way into our high-tech world are actually complicated mixtures when viewed under the right kind of microscope. Polymer materials, such as plastics, are no exception. Moreover, the physical and chemical properties, such as the combination of strength with light weight and the resistance to corrosive substances, that make polymers attractive depend critically on the multiple components making up the mixtures. So does the all-important manufacturing cost.

Polyurethane Foams

Among polymers, polyurethanes are particularly versatile because chemical manufacturers can tailor them in several distinct forms with different physical and chemical properties. Among these are both flexible and rigid foams used to make products as diverse as seat cushions, bedding, building insulation, and lightweight structural parts. Polyurethane foams are chemically complex materials formed by the reactions of liquid starting ingredients (isocyanates and polyethers). The foamy structure results from the release of carbon dioxide bubbles generated by a reaction of water with the isocyanate. Other chemical reactions that convert the soup of initial ingredients into a polymer also influence the final structure and physical properties.

On a microscopic scale, polyurethane foam comprises a matrix laced with small particles that either form naturally during the fabrication process or are added deliberately. Since the microstructure (concentration, size distribution, and chemical composition) of the particles can influence the foam's properties, chemical producers often add inexpensive filler materials to yield a material with improved hardness, strength, and "foaminess." Common fillers include styrene acrylonitrile (SAN) and urethane-based polyisocyanate polyaddition (PIPA) particles. Determining the chemical composition of individual filler particles is difficult, owing to their minute size and their sensitivity to radiation damage by x-ray or electron beams, as well as the chemical complexity of the polyurethanes. To address these issues, a team of researchers working at the ALS turned to the x-ray microscope.

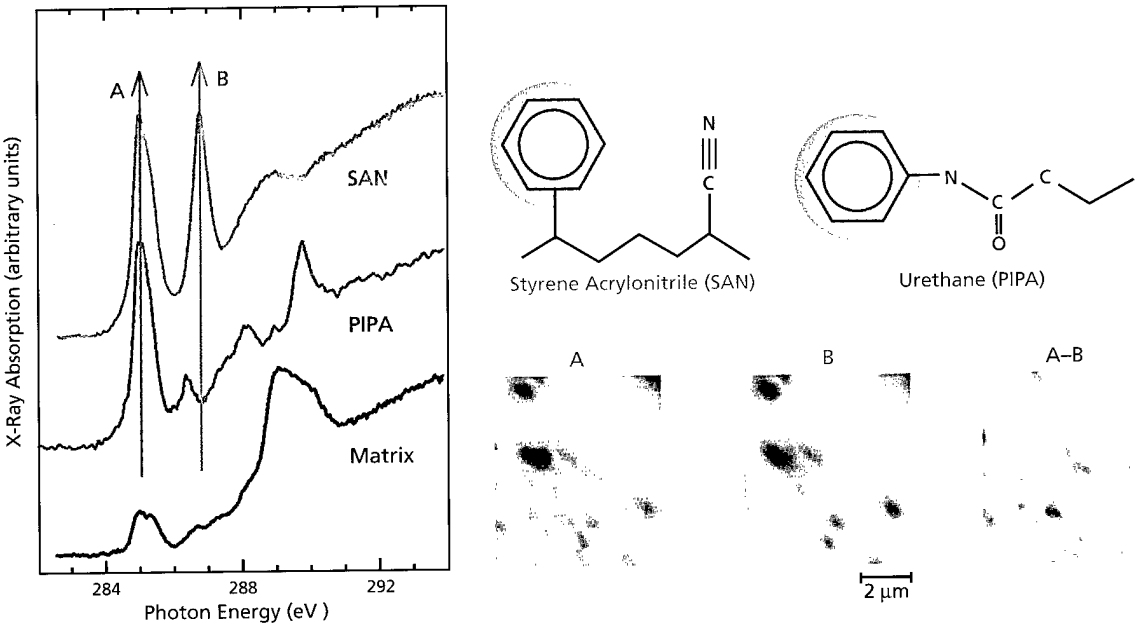
Spectroscopic Imaging

X-ray microscopes at the ALS offer several advantages over conventional instruments. The higher resolution due to the short x-ray wavelength allows smaller structures to be imaged. But more important for dissecting polymers is that x rays are absorbed most strongly at wavelengths (absorption edges) characteristic of the elements present. Subtle differences in the positions of the absorption peaks, called chemical shifts, also indicate the chemical bonding with neighboring atoms, thereby providing a means of distinguishing closely related species in the complex polyurethanes. Moreover, researchers have found that the radiation damage with an x-ray microscope can be about 500 times less than with an electron microscope, giving more flexibility in studying the chemistry of these materials.

Owing to the high brightness of the ALS, researchers can focus an intense x-ray beam to a spot smaller than the filler particles, which can range from 0.3 μm to several microns in diameter, allowing full analysis of each particle separately. Conversely, selecting a wavelength matching an absorption peak and scanning the sample through the focused x-ray beam generates an image mapping the distribution of one chemical compound. This combination of capabilities is called spectroscopic imaging or spectromicroscopy.

A polyurethane foam with SAN and PIPA filler particles provides a case in point. The absorption spectra of these two materials, whose carbon atoms experience distinct chemical surroundings, differ only slightly. The difference is the key to using x-ray microscopy, allowing the researchers to make separate images of SAN and PIPA particles by measuring the transmitted light at wavelengths where the light is selectively absorbed by the components of interest.

Research conducted by E.G. Rightor (principal investigator) and G.E. Mitchell (Dow Chemical); A.P. Hitchcock and S.G. Urquhart (McMaster University); H. Ade, A.P. Smith, and A. Garcia (North Carolina State University); R. Steele, S. Seal, S. Cerasari, and T. Warwick (ALS); and B.P. Tonner (University of Wisconsin–Milwaukee), using the scanning transmission x-ray microscope (STXM) at Beamline 7.0.1. Funding: Dow Chemical, Natural Sciences and Engineering Research Council (Canada), Office of Basic Energy Sciences of the U.S. Department of Energy, and National Science Foundation.



Styrene acrylonitrile (SAN) and urethane-based polyisocyanate polyaddition (PIPA) filler materials are added to customize the physical properties of polyurethane foams. The scanning transmission x-ray microscope at the ALS identifies and maps these components by illuminating the sample with x rays at wavelengths (photon energies) where the light is selectively absorbed by the components of interest. In this example, image A, recorded at a photon energy absorbed by carbon in the phenyl ring (blue), maps both SAN and PIPA. Image B, recorded at a photon energy absorbed by the carbon-nitrogen triple bond (green), shows only the SAN. Image A–B, which is the difference between the two, maps the PIPA component. The spatial resolution in these images is about 150 nm (improved to 80 nm in later experiments).

HOW TINY CAN A MAGNETIC BIT BE?

Advancing Computer-Disk Technology through Miniaturization

Joachim Stöhr
IBM Almaden Research Center

Every year computer users want more and more disk capacity to store data. Staying at the leading edge of data storage means cramming more information on a disk by making the magnetic bits that represent digital data smaller. In the last two years, for example, the bit size decreased by half, thereby doubling the number of bits per square inch to 1.8 billion (280 million bits/cm^2). By 2005, we would like to see that number soar to 50 billion bits per square inch (7.8 billion bits/cm^2), but finding magnetic materials that can store a bit in an area only 2000 nm^2 and materials that can read the minuscule magnetic signal from such a tiny spot poses major technology challenges.

Microstructures Are the Key

Magnetic data-storage devices, such as the hard disk drive in a personal computer, include a spinning disk to hold the information and a set of read/write heads to put the information in and take it out. Underneath protective coatings, the magnetically active part of today's disk is a granular alloy consisting of cobalt-platinum particles believed to be covered with skins of chromium, boron, and tantalum. Each particle is a tiny magnet. To store a bit, the magnetic field from a write head aligns about 1000 of these particle magnets, forming a magnetic domain. Neighboring domains are separated by transition regions (domain walls) about one or two particles (20 nm) wide. In the disk of 2005 the structure of the domain walls will continue to be especially important, since the sharpness of these boundaries determines the magnetic-field flux that the read head senses.

A read head detects the bits by the change in electrical resistance (magnetoresistance) of a nickel-iron alloy as the disk spins rapidly beneath. The next-generation read heads will be based on the more sensitive giant magnetoresistance (GMR) effect in structures comprising alternating magnetic and nonmagnetic metals in layers only a few atoms thick. To design high-performance read heads, we need to know not only the overall response of these layered structures to different magnetic fields but also the magnetism (magnetic moment), chemical bonding, and geometrical arrangement of the atomic elements in each layer. We also need to be sensitive to the interfaces between the layers, since it is the interactions between the layers, not just their separate behaviors, that create the GMR effect.

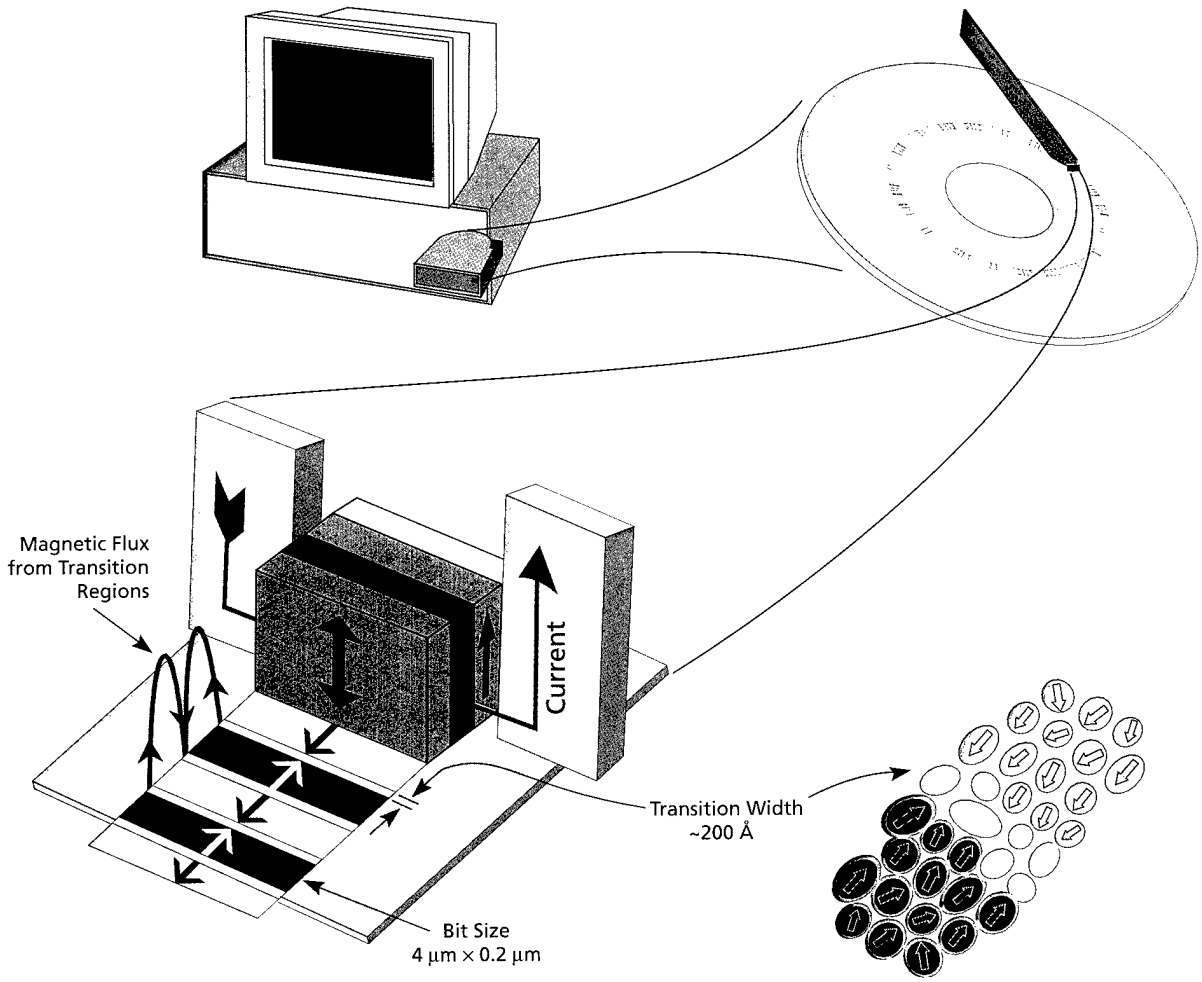
Circular Polarization Beamlines

No single analytical tool can fulfill every requirement, but we are vigorously exploring the use of circularly polarized x-ray synchrotron radiation at the ALS both to visualize the structure of domains and, ultimately, domain walls in disk materials, and to probe GMR structures layer by layer and element by element.

The net magnetic effect in an alloy depends on the magnetic moments of the constituent atoms and the way they interact with each other. The difference between the absorption of left and right circularly polarized x rays by magnetized materials (magnetic circular dichroism or MCD) measures the magnetic moments of the atoms. Since the wavelength at which x rays are absorbed also identifies the atomic elements and their chemical bonding state, we have much of the information we are searching for. By imaging the dichroism at each point on the surface, we can also visualize the domains and their boundaries.

The ALS is an ideal x-ray source for experiments of this type because it can generate extraordinarily bright circularly polarized beams. We are just completing Beamline 7.3.1.1 with a new electron micro-

scope that will image the electrons ejected from the surface of a sample where x rays are absorbed, thereby allowing us to portray magnetic domains with an expected spatial resolution of 30 nm or better. We are also working with the ALS on the even more powerful Beamline 4.0 complex, which will be equipped with stations for MCD measurements and an advanced electron microscope that will push the resolution for imaging to below the size of individual magnetic particles. The first stage of this beamline will be ready in 1998.



Materials challenges in advanced computer disk technology arise both in the disk itself and in the read head that extracts data from the disk. Ultimately, we would like to be able to investigate the structure of the narrow transition regions between magnetic bits on the disk, since the sharpness of these boundaries determines the magnetic flux that the read head senses by a change in the electrical current flowing through the head. The spin-valve version shown here consists of an antiferromagnetic substrate (yellow) on which two ferromagnetic layers (green) are separated by a nonmagnetic layer (brown). In the read head, we would like to measure the contributions of each atomic element in each layer and the way they interact with each other to generate the overall device behavior.

MEASUREMENT SCIENCE IN THE EXTREME ULTRAVIOLET

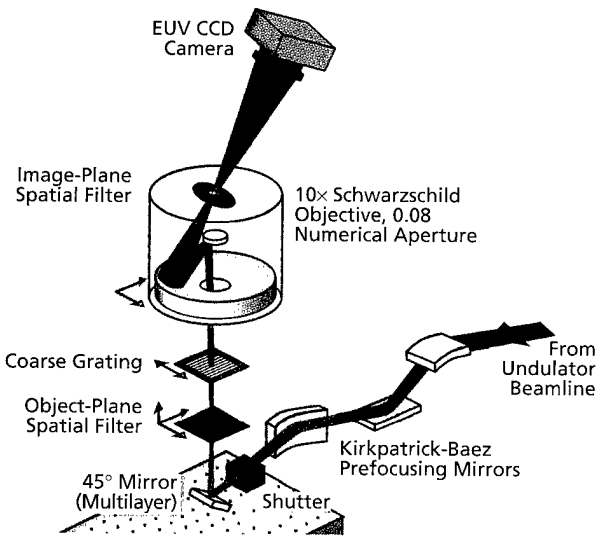
TESTING ADVANCED OPTICS FOR PRINTING INTEGRATED CIRCUITS

Metrology, the science of measurement, plays a key role in new technologies. In order to make something accurately, you have to be able to measure it at least as accurately. Metrology is thus a key issue for the integrated-circuit (IC) industry, which uses ultraviolet light to etch the finely detailed patterns in computer chips in a process called projection lithography. The industry would like to produce chip patterns with smaller features, packing up to ten times more circuits in the same area by 2004, but feature sizes now in mass production are limited by the wavelength of ultraviolet light. This problem could be solved by using extreme ultraviolet (EUV), which has much shorter wavelengths, but there's a catch. Conventional lenses used for UV light are opaque to EUV light. To overcome this difficulty, researchers are developing new imaging optics for EUV light, using curved mirrors coated to increase their reflectivity. These mirrors must be so accurately shaped and have surfaces so smooth that advanced measurement techniques are needed to judge their quality.

EUV INTERFEROMETRY

Researchers at the ALS are addressing this challenge with a new measurement tool that operates at EUV wavelengths. There are three reasons for them to take this "at-wavelength" approach (evaluating an optic using the same wavelength of light with which the optic will be used) rather than using existing visible-light measurement systems. First, the optical flaws they must detect are only 1/2500 the size of a visible light wave. Measurements so fine are beyond present technology. Although visible-light techniques may improve, with EUV light the same flaws are 1/50 of a wavelength in size. Second, visible light reflects off only the outer surface of the mirror coating, which consists of multiple layers only a few atoms thick, and is insensitive to the layered coating structure that is critical for EUV reflection. Third, at-wavelength measurements demonstrate actual mirror performance.

The new instrument, called a phase-shifting, point-diffraction interferometer (PS/PDI), starts with a very bright, narrow beam of EUV light from the ALS, focused through a very small pinhole to produce a uniform spherical wavefront. (Even though pinholes exclude most of the incoming light, the brightness of the beam ensures that enough light passes through to allow rapid data acquisition.) A diffraction grating splits the light into several partially overlapping beams, two of which reflect from the mirrors in the test optic. One beam serves as the test beam and passes through a square window large enough (5 μm on a side) to allow the wave to pass through without distortion, thereby preserving the aberrations it picks up from any flaws in the test optic. A neighboring beam passes through another tiny pinhole, again becoming a uniform spherical reference wavefront. Where the aberrated test wave and the reference wave overlap, they interfere and produce a pattern



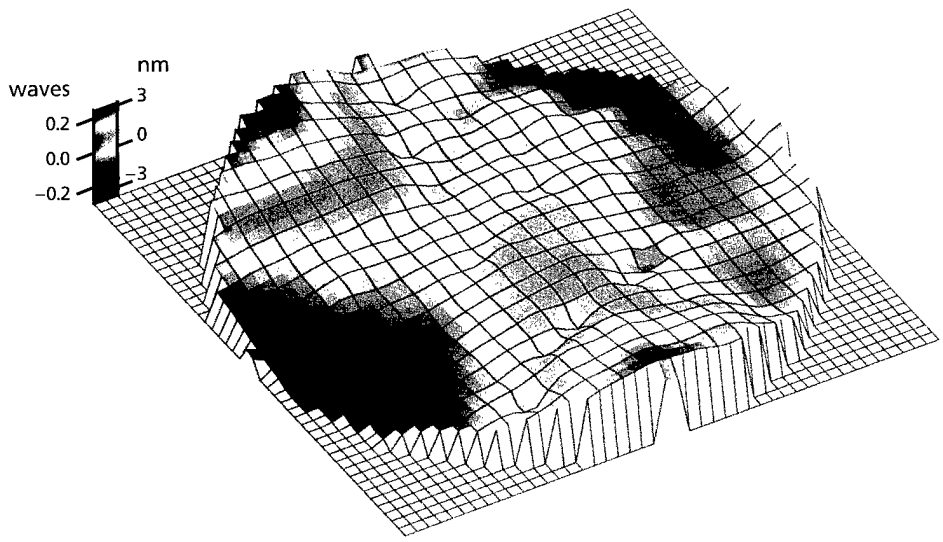
This diagram of the main elements of the phase-shifting, point-diffraction interferometer (PS/PDI) shows how extreme ultraviolet (EUV) light from the ALS is used to analyze a Schwarzschild objective (lens) comprising two spherical mirrors. The EUV light from the ALS is split into two beams that overlap and interfere at the location of an electronic (CCD) camera. The pattern of light and dark fringes recorded by the camera provides the raw data for the analysis.

of light and dark fringes that is recorded on an electronic (CCD) camera. Mathematical analysis of this fringe pattern, including the removal of systematic experimental errors, yields information about flaws in the test optic.

First Test Results

In a prototype EUV projection lithography system now being tested, a Schwarzschild objective (a pair of nested spherical mirrors) produces a demagnified image of the pattern in a mask, transferring it to a computer chip that is 10 times smaller than the mask pattern. Recent experiments to evaluate such a 10× Schwarzschild objective have enabled researchers to characterize the PS/PDI's precision. Repeating the same measurements in many ways, each time completely realigning the instrument, the researchers have established an excellent repeatability in the measured aberrations, which were the same to within ± 1/125 wavelength (rms). The tougher job of verifying high accuracy by identifying systematic measurement errors is still under way. Some systematic errors can already be subtracted, and a so-called null-test procedure should reduce several more. Moreover, projection lithography experiments with the Schwarzschild objective produced results consistent with predictions based on PS/PDI measurements, suggesting that the remaining errors are small.

Research conducted by J. Bokor (principal investigator), K.A. Goldberg, E. Tejnil, S.H. Lee, and D.T. Attwood (University of California at Berkeley and Berkeley Lab's Center for X-Ray Optics) and H. Medecki and K.H. Jackson (Berkeley Lab's Center for X-Ray Optics), using the at-wavelength EUV interferometry endstation at Beamline 12.0.1.2. Funding: Intel Corporation, Extreme Ultraviolet Limited Liability Corporation, Semiconductor Research Corporation, Defense Advanced Research Projects Agency of the U.S. Department of Defense, and Office of Basic Energy Sciences of the U.S. Department of Energy.



From the fringe patterns formed at the intersection of the test and reference waves from the phase-shifting, point-diffraction interferometer, researchers can calculate a wavefront-aberration phase map, above, that yields information about flaws in the test optic. The height (measured in wavelengths of the extreme ultraviolet light, about 13.4 nm in these experiments) is a measure of the optic's deviation from perfect shape.

AN ELECTRONIC VIEW OF DIAMOND

Achieving a Match between Theory and Experiment

The foundation for calculating many of the large-scale properties of a solid, whether a structural steel alloy or a semiconductor computer chip, consists of a theoretical model for the behavior of electrons, particularly the valence electrons, whose accuracy can be validated experimentally. Rather than being localized around the atomic nuclei, the valence electrons in the chemical bonds that hold solid materials together travel throughout the volume of a sample. Theorists label each of the delocalized electrons with a momentum (technically, crystal momentum) and an energy. When plotted on a graph, the closely spaced momentum and energy values form continuous structures called valence bands.

The Valence Band Width

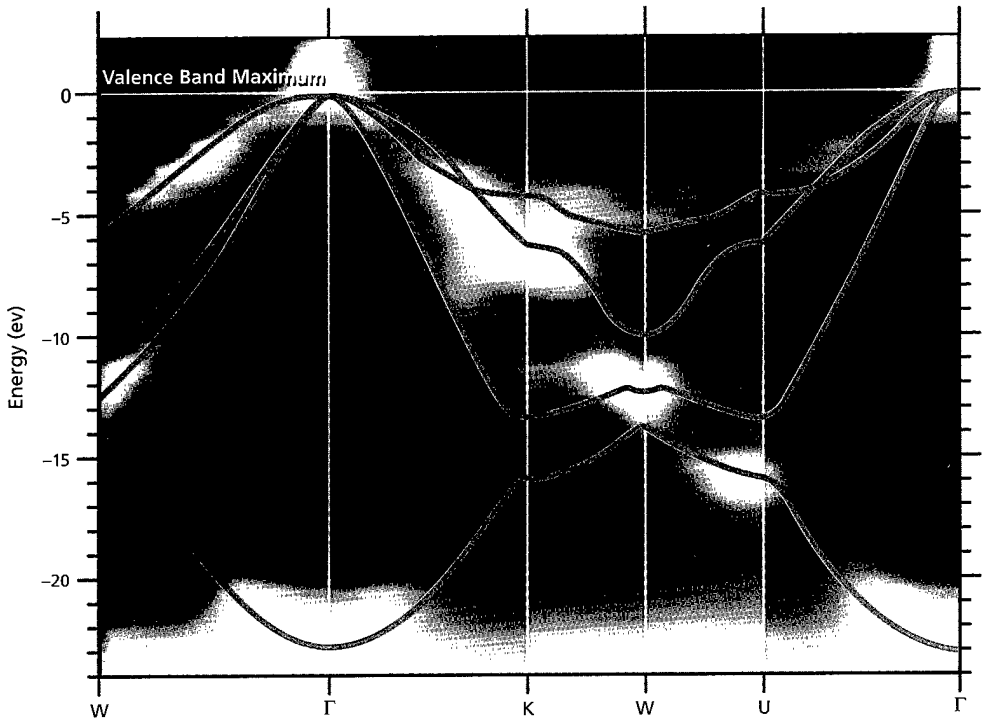
The difference between the maximum and minimum electron energies in the valence band (band width) may be the single most important energy band parameter. For example, when the band width is small compared to the energy associated with electrostatic repulsion between neighboring negatively charged electrons, each electron tends to localize around one atom, because this is the easiest way for the electrons to avoid each other. Some of the most interesting materials today, including magnetic materials that are candidates for use in future computer data storage systems, fall in this category and have electrons that straddle the boundary between localized and delocalized behavior. The theory for such materials is not well established, and its development will require reliable experimental methods to measure key parameters.

One such tool is photoelectron spectroscopy, which uses ultraviolet and long-wavelength (soft) x rays to excite valence electrons to higher energy bands from which they can travel to the surface and escape. By varying the wavelength (energy) of the light, experimenters can selectively sample valence electrons with different energies (constant-final-state photoelectron spectroscopy). The direction of the photoelectrons (angle-resolved photoelectron spectroscopy) provides information about their momentum distributions. Combining this information displays the energy-momentum relationship (band structure).

Quasi-Particles

In the conventional band model, theorists regard each electron as behaving independently of other electrons. This is called the one-electron approximation. While often useful, this approximation breaks down in many cases in which electrons appear to act in concert. Angle-resolved photoemission is a case in point. The problem is that the excitation of a valence electron leaves an empty state or hole in the valence band, which is effectively positively charged relative to the filled band. The resulting redistribution of electrons around the hole and the excited electron forms a "quasi-particle" which affects the energy of all electronic states and must be considered to make accurate calculations. A quasi-particle is an example of a many-body effect in which electrons do not act independently. It is the quasi-particle energies rather than the one-electron energies that photoelectron spectroscopy measures.

With this point in mind, researchers at the ALS using angle-resolved photoelectron spectroscopy have reported the first quantitative experimental verification of the valence-band structure of diamond. The experiments confirmed the quasi-particle model for diamond. In particular, they showed that the energy band width agreed with quasi-particle calculations by two different research groups but disagreed with one-electron calculations, which predicted band widths significantly smaller than measured.



The diagram shows the valence-band structure for diamond for different momentum directions, designated by letters at the bottom representing points of symmetry. The energy scale is relative to the top of the valence band. The calculated quasi-particle band structure is shown in green; the angle-resolved photoelectron spectroscopy data are shown in shades of orange and white, with lighter colors representing higher detected electron intensities. The horizontal axis shows crystal momentum. The experimental and theoretical data shown here are in excellent agreement for the characteristics modeled by the theory.

Collecting the large quantity of data required for accurate band mapping was aided by the use of a large area detector (display analyzer or ellipsoidal mirror analyzer). This device images photoelectrons emitted into an 84-degree cone around the sample on an electronic channel-plate detector, thereby preserving angular information while recording the electrons emerging from the surface. This approach, combined with the high brightness of the ALS, allows momentum distributions to be recorded in only a few seconds for each energy.

Research conducted by I. Jiménez, L.J. Terminello (co-principal investigator), D.G.J. Sutherland, and J.A. Carlisle (Lawrence Livermore National Laboratory); E.L. Shirley (National Institute of Standards and Technology); and F.J. Himpsel (co-principal investigator, University of Wisconsin at Madison), using the display analyzer station at Beamline 8.0.1. Funding: Office of Basic Energy Science of the U.S. Department of Energy, National Science Foundation, and the Spanish Ministerio de Educación y Ciencia.

THE INSIDE STORY ON OXYGEN

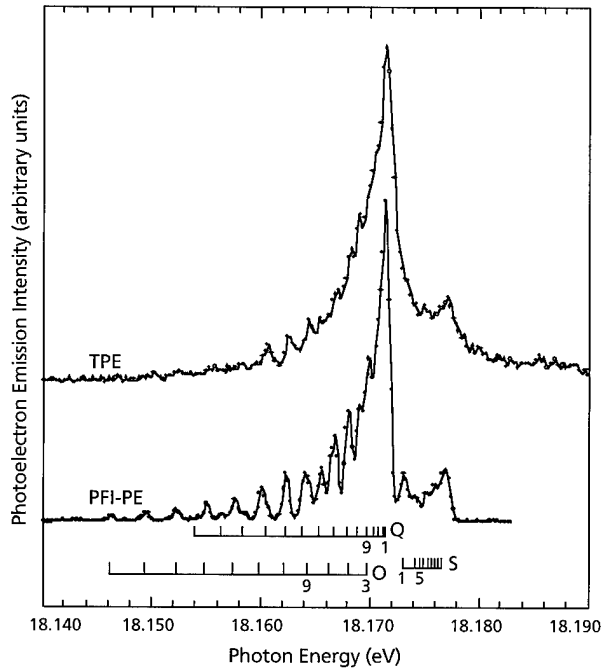
A New Way to Look at This Atmospheric Molecule

Oxygen molecules, which make up about 20 percent of the earth's atmosphere, serve as a shield (along with nitrogen, ozone, and other molecules) against ultraviolet radiation from the sun by absorbing the radiation before it reaches the earth's surface. Therefore, understanding the absorption process and the lengthy cycle of subsequent chemical reactions that may lead to the regeneration of oxygen is of deep interest to atmospheric chemists. A key absorption process is photoionization. Upon absorption of a short-wavelength ultraviolet ray (vacuum ultraviolet or VUV) that cannot penetrate through air, an oxygen molecule ejects an electron, thereby becoming a positively charged ion (cation). The ultimate fate of the oxygen depends on the distribution of energy in the cation as the result of photoionization (the internal state of the cation), because this state determines the result when the cation collides with an electron or with another atmospheric molecule.

The Role of Spectroscopy

Understanding the internal state of the oxygen cation (O_2^+) comes down to unraveling its electronic structure. In an atom, the outer shell (valence) electrons contribute to the chemical bonding that turns a group of atoms into a molecule. The bonding electrons form orbitals associated with the molecule as a whole rather than the individual constituent atoms. In addition, the atoms in the molecule may vibrate and rotate. Overall, the molecule has a spectrum of energies that depends on the orbitals, with small contributions from the vibrations and smaller ones still from the rotations. This is the electronic structure.

Chemists use VUV spectroscopy to study the electronic structure of molecules. Measuring the wavelengths at which electrons in the molecular orbitals receive just enough energy to escape but no more (threshold photoelectron spectroscopy) is a sensitive method of probing the molecular electronic structure. Sensitivity is essential, since absorption peaks for molecules that differ only in their rotational motions are very closely spaced and tend to overlap. One big problem is finding a VUV source that provides an intense beam in a narrow wavelength band that can be tuned to the absorption



The advantage of the pulsed-field ionization photoelectron spectroscopy (PFI-PE) technique, as compared to the more conventional threshold photoelectron spectroscopy (TPE), is its ability to resolve spectral peaks due to different rotations in photoionized molecules in excited states. Here the comparison of spectra for molecular oxygen cation (O_2^+) shows that the pulsed-field ionization method results in clearly resolved rotational structure that is obscured in the traditional technique. The marks on the Q, S, and O scales indicate where theory says the peaks should be. Comparison of measured spectra with theoretical calculations yields information about the inner workings of the molecule; for example, which electrons and molecular orbitals make dominant contributions to the creation of excited states.

peak of interest. Another is limiting the detection to only the threshold electrons with just enough energy to escape, since electrons in other orbitals that need less energy to escape are also ejected.

Pushing Spectroscopy to New Limits

At the ALS, researchers have successfully attacked these issues by adapting a laser technique to synchrotron radiation. The basic idea is to use VUV light from the ALS to give target electrons almost enough energy to escape, but not quite (exciting them to high-*n* Rydberg states). A voltage pulse applied a few nanoseconds later then adds the extra energy needed to escape from the Rydberg states, but in the meantime, all the higher-energy electrons have moved out of the area. The researchers call this technique pulsed-field ionization photoelectron spectroscopy.

After an electron escapes from the oxygen molecule, the resulting cation may be left in a variety of internal states with different energies specified by the molecular orbitals and the vibrations and rotations. The ALS provides bright beams of VUV light over a wide range of wavelengths, which scientists can use to probe molecules with electrons in high-energy orbitals (excited electronic states) that are inaccessible to lasers because of the limited VUV-wavelength range they cover. However, switching light sources creates a new challenge. In the laser version, the time delay between light and voltage pulses is a few microseconds, but light pulses at the ALS come much faster. To meet this challenge, the researchers designed a special photoelectron spectrometer that can reduce the delay to nanosecond intervals.

Researchers have now demonstrated this high-speed, high-resolution capability at the ALS with the molecular oxygen cation. Their results exceed the highest spectral resolving power ever achieved for molecular photoelectron spectroscopy using synchrotron radiation. And the researchers were able, for the first time, to obtain spectra with clearly resolved peaks for the different rotational states of the cation in excited states at energies above those accessible with lasers.

Research conducted by C.Y. Ng (principal investigator), M. Evans, and S. Stimson (Ames Laboratory and Iowa State University); C.-W. Hsu (Berkeley Lab); and P. Heimann (ALS), using the photoionization endstation at Beamline 9.0.2.2. Funding: Office of Basic Energy Sciences of the U.S. Department of Energy.

SPOTLIGHTING MOLECULES ON SURFACES

Looking at Chemical Bonding Atom by Atom

Anders Nilsson
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Uppsala University

Chemical reactions at surfaces play central roles in such economically important processes as the catalysis of chemical production, corrosion, the fabrication of computer chips, the behavior of biomaterials, and the fate of contaminants in the environment. Chemical bonding of atoms and molecules to the surface (adsorption)—the first step in many such reactions—occurs when some of the electrons that are less tightly bound to atomic nuclei (valence electrons) rearrange themselves. Because of this loose binding, the valence electrons can be shared by several atoms, forming molecular orbitals. How these orbitals are distributed, on the atoms and along different bond directions, and what energies the electrons in the orbitals can have are some of the details that we would like to know.

X-Ray Emission Spectroscopy

To observe the orbitals involved in the surface chemical bond is an experimental challenge because of the much larger number of atoms in the solid below the surface (substrate). What we need is a method that allows us not only to separate out the orbitals on the adsorbed entity (adsorbate) but also to spotlight one atom at a time. This tall order can be filled by using x-ray emission spectroscopy (XES), also called x-ray fluorescence spectroscopy, in which the absorption of an x ray is followed by the emission of a fluorescence x ray at a different wavelength.

Though simple sounding, x-ray emission yields the information we seek. The wavelength of the incoming x ray identifies which atom is absorbing, since atoms of different elements (or the same element in distinct chemical-bonding environments) absorb at characteristic wavelengths. Similarly, the wavelength of the fluorescence x ray identifies the molecular orbital, and the intensity of the fluorescence indicates how much of the orbital is around the absorbing atom. Additional information about the orientation (symmetry) of the orbitals comes from measurements made at various angles relative to the surface of the incoming and fluorescence x rays. Finally, since the fluorescence comes only from the adsorbate, there is no obscuring signal from below the surface.

XES applied to surfaces is extremely demanding owing to the considerable inefficiencies associated with the creation and detection of fluorescence x rays and with the low adsorbate concentration. It is only recently that the field has begun to be exploited, thanks to the appearance of third-generation synchrotron radiation sources, such as the ALS, whose high brightness makes it possible to overcome these limitations.

Adsorbates on Metal Surfaces

In experiments at Beamline 8.0.1, our group has used XES to examine a sequence of increasingly complex molecules on metal surfaces, beginning with molecular nitrogen (N_2) and carbon monoxide (CO) on nickel and copper. We have discovered new details about the bonding between these molecules and the surface, which show that surface bonding involves not only new orbitals derived from both the adsorbate and the substrate, but also rearrangements within the orbital structure of the molecule itself. We are now moving on to large molecules of the type that are common in biological materials and in the environment.

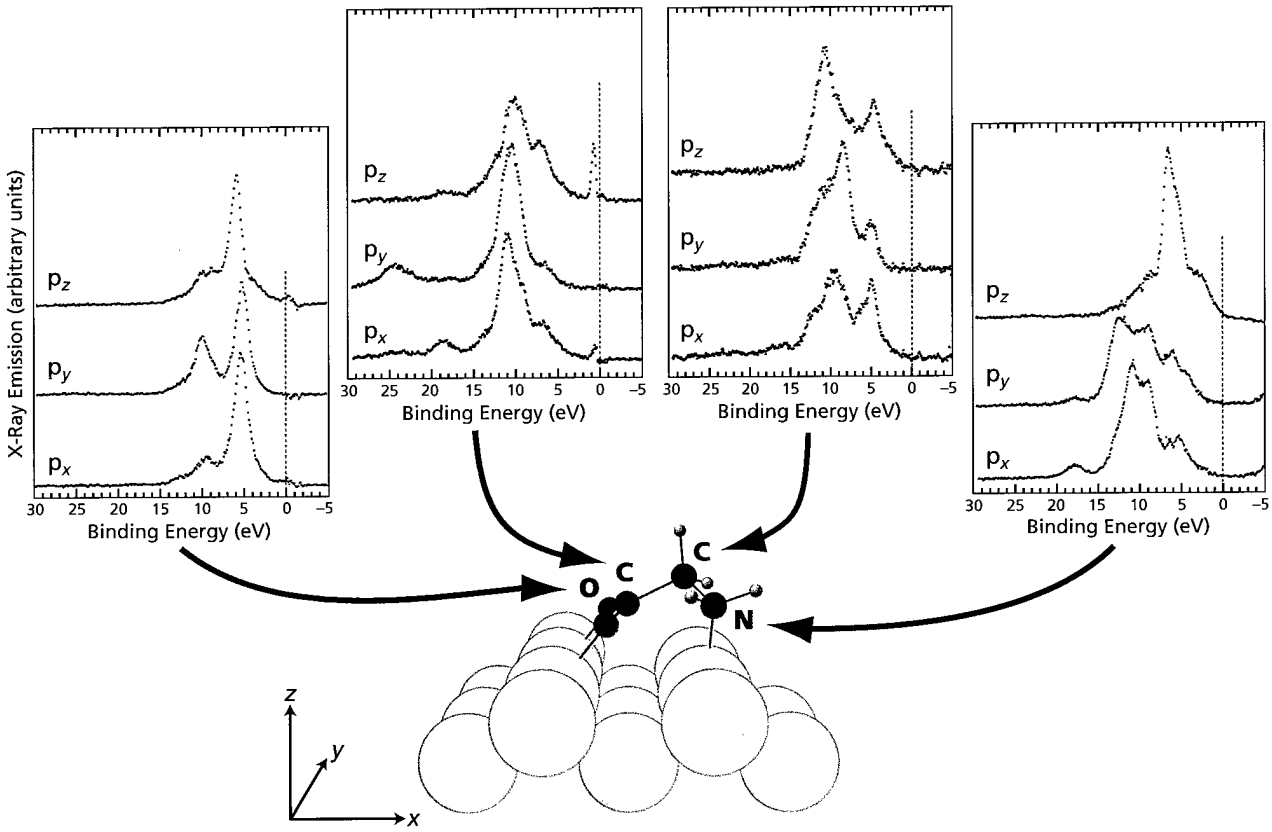
Adsorption of a simple amino acid, such as glycine (NH_2CH_2COOH), on copper [specifically, the Cu(110) surface] provides a simple example. The Cu(110) surface has twofold symmetry, in which the surface atoms are lined up in rows and the glycine molecule adsorbs in an orientation perpendicular to these rows with both ends of the molecule bonding

to the surface. Combining experiment with theoretical calculations, we can now study how molecular orbitals of a specific symmetry are distributed over different atomic sites in a complicated molecular adsorption complex.

Liquid Interfaces

With the successful development of XES for surfaces and interfaces, we see a unique opportunity for a new application of these methods to liquid interfaces, since x-ray-in/x-ray-out spectroscopies do not require samples to be in a vacuum. For example, a new interdisciplinary field, referred to as molecular environmental science, has emerged in the last few years in response to the need for basic research to underpin long-term solutions to environmental problems. It is clear that many of the reactions involving contaminants take place at liquid-solid interfaces, and we expect that XES will make a major contribution to understanding some of these important processes.

Research conducted by A. Nilsson (principal investigator), J. Hasselström, O. Karis, M. Weinelt, and N. Wassdahl (Uppsala University); M. Nyberg and L.G.M. Pettersson (University of Stockholm); and J. Stöhr and M. Samant (IBM Almaden Research Center), using the soft x-ray emission endstation at Beamline 8.0.1. Funding: Swedish Natural Science Research Council and Göran Gustafssons Foundation for Research in Natural Science and Medicine.



X-ray emission spectra from the amino acid glycine (NH_2CH_2COOH) adsorbed on copper [specifically, the Cu(110) surface] were taken at different angles relative to the surface. These spectra were combined to decompose the molecular orbitals associated with the oxygen atoms, each of the two carbon atoms (which have different chemical environments), and the nitrogen atom into the components labeled p_x, p_y, and p_z, which have different symmetries and energies. For a complete understanding of the molecular orbitals for complicated adsorbates of this type, experimental data must be compared to theoretical calculations.

A MOLECULAR PORTRAIT OF HYDROGEN CHLORIDE

Data in Two Dimensions Paint a Detailed Picture

The high brightness of the ALS makes it possible to generate data much more rapidly than at older synchrotron facilities. This capability certainly boosts scientific productivity by increasing the number of experiments that researchers can do in their time at the facility. But just as important is the ability to record much more detailed sets of data. The detail comes in several forms. It may be more closely spaced wavelength intervals in spectroscopy experiments (high spectral resolution); it may be small areas of a sample (high spatial resolution or imaging); or it may be two or more variables, such as wavelength and electron energy (two-dimensional measurements). The bottom line is that, with more data, researchers can paint a finer portrait of whatever physical, chemical, or biological process they are investigating.

Two-Dimensional Maps

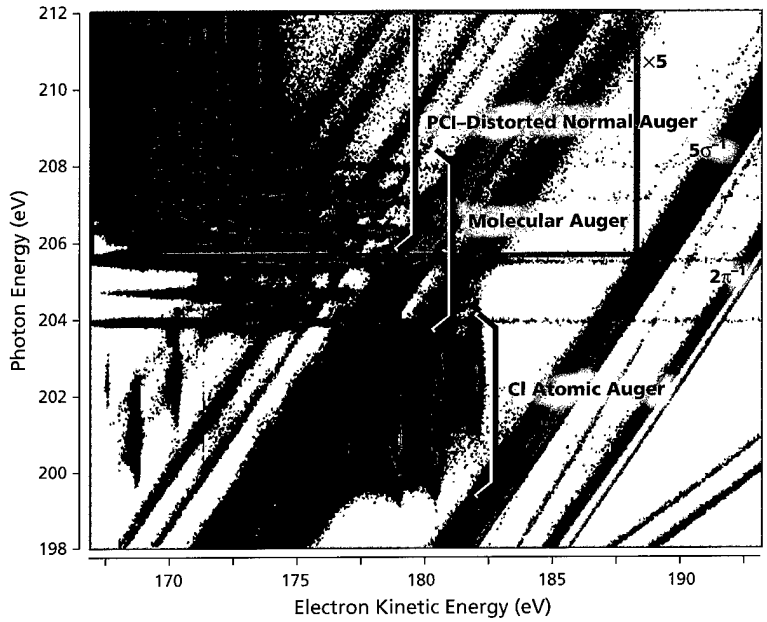
A case in point is two-dimensional electron spectroscopy of the hydrogen chloride molecule (HCl). As a comparatively simple molecule with just two atoms, hydrogen (only one electron) and chlorine (17 electrons), HCl is a natural step up in complexity from atoms to molecules and therefore serves as a model system to investigate fundamental aspects of molecular behavior that ultimately affect chemical bonding in reactions. For example, researchers want to understand internal processes in which two or more electrons act in concert rather than independently (electron correlation and many-body effects). With the understanding gained from studies of simpler molecules, scientists can advance to larger, more complex assemblies of many atoms, which would otherwise be too difficult to address.

Absorption of an ultraviolet ray or x ray by a molecule usually results in the emission of one or more electrons (and sometimes molecular fragments) that provide the data for the experiment. The emitted electrons have a spectrum of possible kinetic energies, with peaks at energies where a large number of electrons are detected. The energy spectrum reflects the behavior of the electrons in the molecule. The spectrum also depends on the wavelength of the x rays, since this determines how much energy is available to eject the electrons. Although much useful information comes from measurements at one or a few x-ray wavelengths, a more complete picture emerges from a two-dimensional map of peak positions and intensities with both electron kinetic energy and x-ray wavelength as axes. Measurement of the direction the emitted electrons take relative to the incoming x-ray beam provides still more detail.

Inner-Shell Ionization

At the ALS, researchers have combined the high brightness of the ALS with advanced data-acquisition equipment and a rotatable experimental chamber to obtain two-dimensional electron spectra of HCl at several angles. In these experiments, HCl molecules absorb x rays with wavelengths blanketing an energy range above and below that sufficient to eject a tightly bound electron in an orbital associated mainly with the chlorine atom (ionization threshold). This absorption stimulates several processes that show up on the two-dimensional map. In general, the inner-shell chlorine electron (Cl 2*p*) can use the x-ray energy to move up into a less tightly bound molecular orbital or out of the molecule altogether (becoming a photoelectron). What happens next sheds light on other orbitals in the molecule, including those responsible for chemical bonding, and on the way the molecule reacts to a sudden increase in its energy.

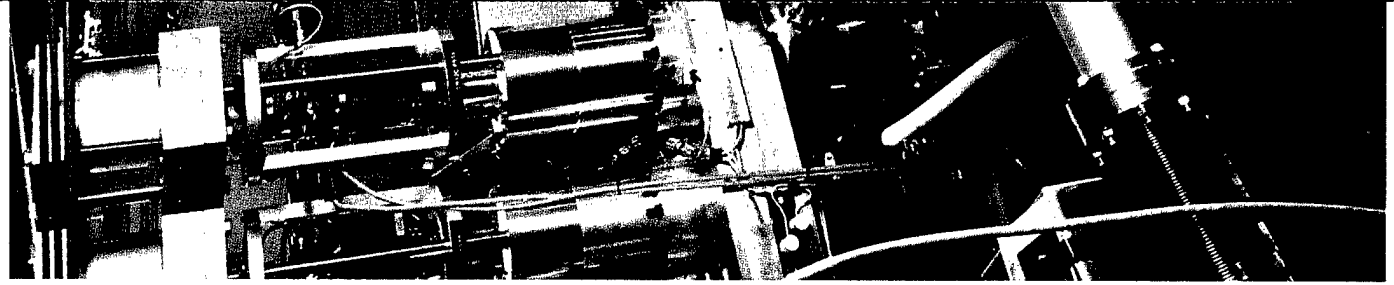
After the initial x-ray absorption, another electron in a molecular orbital may "drop down" and fill the empty chlorine orbital. In so doing, it usually



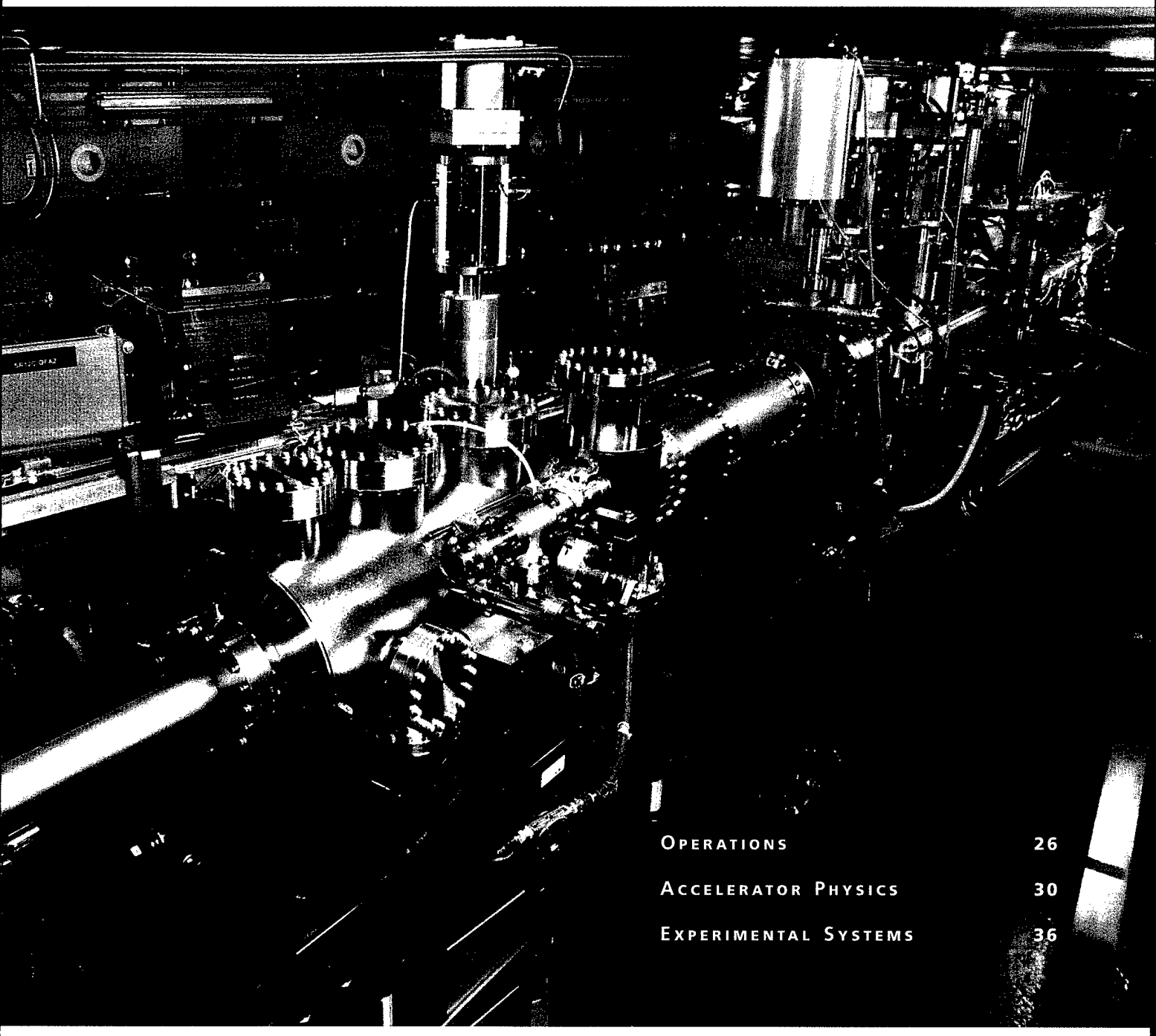
Owing to the high brightness of the ALS and to advanced data-acquisition technology, researchers have been able to record two-dimensional electron spectra for the hydrogen chloride (HCl) molecule in the wavelength (photon energy) range near the threshold for ionization of a tightly bound inner-shell electron associated with the chlorine atom (Cl 2*p*). With the energy of the incoming photons and the kinetic energy of the ejected electrons as the two axes, the peak positions and their intensities identify numerous processes such as the chlorine atomic Auger, molecular resonant Auger, and normal Auger transitions distorted by post-collision interactions (PCI) labeled in the figure. (To make the latter more visible, the signal in the green box is shown at five times its actual value.) The diagonal lines, such as those labeled $5\sigma^{-1}$ and $2\pi^{-1}$, refer to the absorption of x rays by electrons in outer (valence) molecular orbitals rather than deep inside the chlorine atom, so that the electrons are ejected with high kinetic energy. Following these lines, one can study the interplay between the photoemission and Auger processes.

gives energy to a third electron, which then escapes from the molecule (molecular Auger electron). At some x-ray wavelengths, however, the chlorine electron jumps to an "antibonding" molecular orbital, which makes the molecule unstable, so that it dissociates into hydrogen and chlorine atoms. Auger electrons generated after the dissociation are then called atomic Auger electrons. These and other processes, such as slowing down or even recapture of electrons by the molecule (post-collision interactions), have been accurately tracked at the ALS using the positions and intensities of electron peaks in the two-dimensional map.

Research conducted by N. Berrah (principal investigator), A. Wills, E. Kukk, and B. Langer (Western Michigan University), and J.D. Bozek (ALS), using the high-resolution atomic and molecular spectroscopy endstation at Beamline 9.0.1. Funding: Office of Basic Energy Sciences of the U.S. Department of Energy.



FACILITY REPORT



OPERATIONS

Operations at a synchrotron light source are key to the success of the scientific endeavors conducted there. Researchers need high-quality photon beams delivered on a reliable schedule in the context of a safe, efficient work environment. Over the years, researchers have come to expect first-rate operations and continuing technological progress at the ALS. In 1996/97, they were not disappointed.

During this period, we increased the beam time available to users, offered a broader range of operating conditions, achieved smaller-than-ever electron beam dimensions (and therefore lower emittance) for routine operations, and enhanced the beam's stability so that users could capitalize on the excellent spatial and spectral resolution that a very-low-emittance beam affords. Moreover, we installed a 2-tesla wiggler to serve as the source for a macromolecular crystallography beamline, installed this beamline and other new beamlines, and completed new facilities to support research in structural biology.

Increased User Access

Since late 1995, when the Scientific Facilities Initiative boosted FY96 funding for the ALS and other DOE national user facilities, we have been able to serve more experiments than ever before. The total number of hours of beam delivered to ALS users in FY96 amounted to 4,461—up 73% from 2,580 hours in FY95.

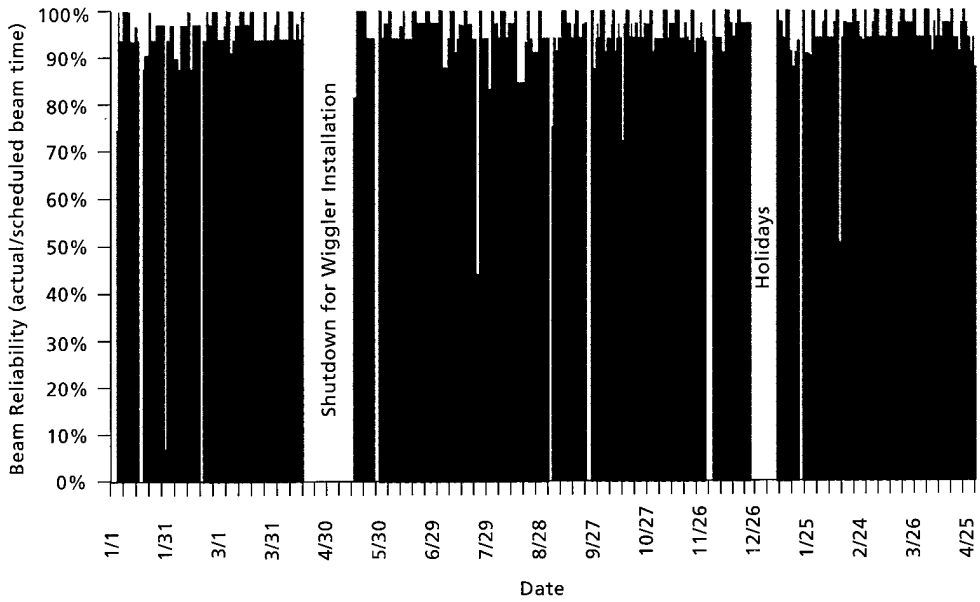
Sixteen 8-hour shifts per week are dedicated to users. Of the five remaining shifts per week, three are assigned to accelerator physics, one is for maintenance and installation activities, and one is for start-up and testing. Other scheduled down time consisted of one two-day period per month for minor maintenance and installation activities and one five-week period in April–May 1996, during which the wiggler was installed. We had no significant unplanned beam outages that resulted in loss of user beam time. Thus, for the period from January 1, 1996, to April 25, 1997, we can boast 89.6% beam reliability (actual/scheduled beam time) during user shifts. If injection periods were included in the users' actual beam time, beam reliability would amount to 94%.

When it comes to scheduling beam time, ALS users have a substantial voice. Scheduling is done at least six months in advance by the users, the Users' Executive Committee, and ALS management; and each week, the schedule for the following two weeks is fine-tuned.

"Customized" Operating Conditions

With its increasing number of beamlines and the concomitant diversity of its scientific program, the ALS is subject to requests for a wide variety of operating conditions. In 1996/97, ALS users had a greater choice than ever before. Operations were conducted at electron beam energies of 1.1, 1.3, 1.5, and 1.9 GeV; however, 1.9-GeV mode was the most common operating mode, as it increases the variety of experiments that can be performed efficiently by providing more usable photon flux at high photon energies. In spring 1997, photon flux was further enhanced when the ALS began operations at 1.9 GeV with the full current of 400 mA.

The ALS also offers several options when it comes to fill pattern (the number and distribution of electron bunches circulating in the storage ring). These include 320 bunch, 304 bunch, 287 bunch, and 2 bunch. In addition, we provide a "camshaft" option, which is a 20-mA spike inserted at the middle of the gap in the 287-bunch fill pattern. The camshaft allows users to synchronize lasers or other instruments with the spike, but does not diminish the photon flux for those using the multibunch fill pattern.

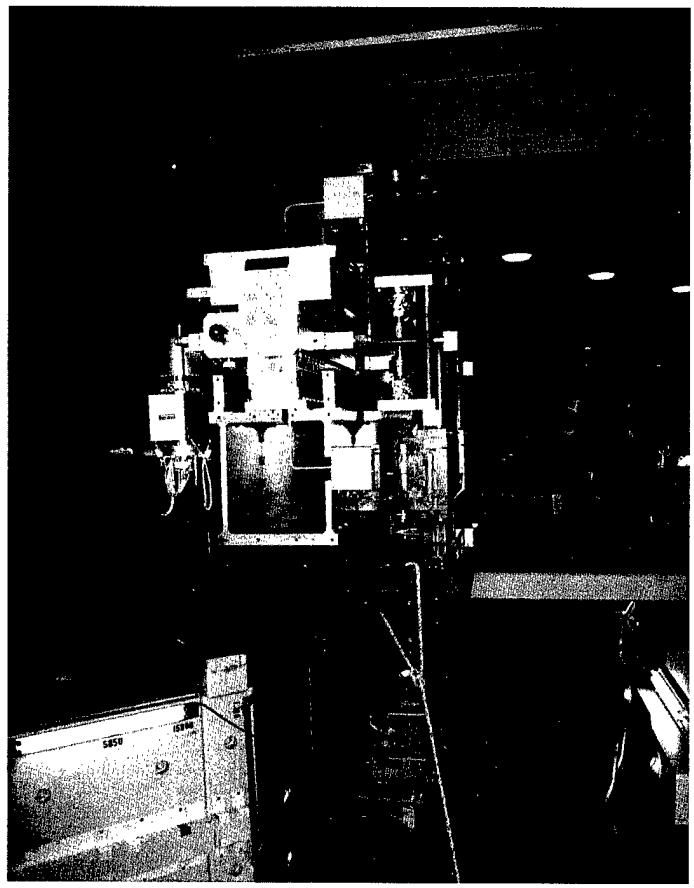


During the period from January 1, 1996, to April 25, 1997, ALS beam reliability (actual/scheduled beam time) was 89.6% during user shifts and 90.0% overall. (If injection periods were included in the users' actual beam time, beam reliability would be 94%.)

Improvements Yield Dividends for Users

We made several hardware and software improvements that benefited the stability and quality of the electron beam and thus the quality of the photon beams delivered to ALS users. In 1995, we had discovered that variations in the temperature of the ALS's low-conductivity water (LCW) supply were the cause of a periodic deviation in the electron-beam orbit. Although we corrected this problem when it was discovered, an overhaul of the LCW system to avoid recurrences became one of our priorities. In 1996, we replaced several components with counterparts that offer better performance. In addition, a cathodic protection system to prevent corrosion was installed on all the LCW water lines connected to the cooling tower.

Also in 1996, we brought our new transverse and longitudinal multibunch feedback systems into routine operation, an improvement that resulted in the smallest electron beam ever available at the ALS for production runs. However, the decreased beam size magnified the importance of some remaining instabilities in the beam's orbit. A task force of physicists and engineers succeeded in identifying the sources of these instabilities. A major source was found to be the temperature regulation of the chilled water supplying the air-conditioning system for the storage ring. Now that this problem has been corrected, we can boast an orbit so stable that its standard deviation is less than one-fourth that stated in the design specifications (see "The Quest to Improve Orbit Stability," p. 34). Among the tools that contributed to this success are new, highly reliable beam position monitors that were installed in eleven of the twelve straight sections around the storage ring.



The 2-tesla wiggler being lowered into position in the ALS storage ring. Its installation was completed in April 1996. The wiggler delivers photons with energies in the 3.5–14 keV range to the new macromolecular crystallography beamline.

A Growing Facility

Only one major shutdown was scheduled during 1996, primarily for the purpose of installing a 2-tesla wiggler into Sector 5 of the storage ring. The fifth insertion device to be added to the ring, the wiggler serves as the source of photons for the ALS's new macromolecular crystallography beamline.

The spectrum and flux of radiation produced by a wiggler depend on the peak field strength of the magnets used in the device. With 38 poles, this wiggler has a peak field strength of 2.1 tesla—more than double that of the ALS bend magnets. Operating the ALS storage ring at 1.9 GeV improves the flux and brightness even more. For example, at 1 Å (the wavelength conventionally used for macromolecular crystallography), operation at 1.9 GeV yields x rays three times brighter than those produced during 1.5-GeV operation.

The Macromolecular Crystallography Facility is now served by Beamline 5.0, one of four new beamlines that became operational during 1996/97. Researchers who use this beamline benefit not only from the bright x rays generated by the wiggler but also from the new Structural Biology Support Facilities (SBSF) adjacent to the ALS. Completed in

October 1996, these facilities include laboratories, computers for data reduction and visualization, and office space.

Also new is Beamline 7.3.1.2, which delivers x rays with energies in the range 260–1500 eV from a bend magnet. Researchers use it to perform micro x-ray photoelectron spectroscopy studies on materials (see "Micro X-Ray Photoelectron Spectroscopy," p. 40). An infrared microscopy beamline, 1.4, was recently completed for use in chemical mapping studies, including some that could benefit the environment. The fourth new beamline, 12.0.1, delivers x rays from the U8 undulator via two branches. One, which delivers x rays in the energy range 95–130 eV, is designed for conducting spectromicroscopy studies on materials. The other is used in detecting and measuring flaws in reflective optics intended for use in extreme ultraviolet (EUV) projection lithography. The work conducted at this beamline may play a major role in enabling the further miniaturization of integrated circuits, a continuing quest in the electronics industry.

The Structural Biology Support Facilities (SBSF) adjacent to the ALS were completed in 1996. Among the instrumentation at the SBSF is an electron paramagnetic resonance (EPR) spectrometer (left) equipped with a computer console (right). This instrument is used to confirm that samples of metal-containing proteins remain active before and after their exposure to x rays from an ALS beamline. Scientists using the EPR spectrometer want to avoid "doing good physics on bad samples."

ACCELERATOR PHYSICS

For researchers at the ALS, 1996/97 was a period of achieving new milestones in resolution. A major factor in this progress was the work of the Accelerator Physics Group, which advanced the properties of the electron beam to the theoretically expected levels and sent higher-quality photon beams down the beamlines. Each step forward in performance, however, has side effects that influence the behavior of the electron beam and introduce new challenges. In meeting each challenge, we build up our understanding of the way the accelerators behave. As our fund of knowledge accrues, so does our ability to carry out our mission of ensuring reliable, ever-improving performance for users.

Among our activities in 1996/97, three characterize the scope of our work. The first improved the operational capabilities of the ALS. The second enhanced the measurement-based modeling tools being used to improve accelerator performance. The third led to unambiguous identification of the "fast-ion instability," a previously unproven effect associated with ions interacting with the electron beam. This research pushed the boundaries of accelerator physics toward the domain of next-generation storage rings, which will be more susceptible to such ion effects.

The Challenge of a Better Beam

One of our major achievements was to bring the multibunch feedback systems (commissioned in 1995) into routine operation. These systems monitor the longitudinal, horizontal, and vertical motion of each electron bunch in the storage ring and feed back correction signals to minimize the motion. As a result of this work, the natural emittance and energy spread of the beam reached their theoretically predicted values of 4 nm-rad and 0.08%, respectively. Furthermore, we achieved an extraordinarily low vertical emittance of less than 0.1 nm-rad at 1.5-GeV beam energy—a particularly successful outcome. However, this step forward in performance posed more challenges for the accelerator physicists.

With such low emittance, the lifetime of the densely packed electron bunches is severely reduced because of the Touschek effect (collisions of electrons within the bunches that transfer transverse momentum to the longitudinal direction). To accommodate our user community, we made the compromise of accepting a slightly larger vertical emittance in return for a longer beam lifetime. We increased the vertical emittance by using skew quadrupole fields (a capability designed into the storage ring's sextupole magnets) to redirect some of the energy of the oscillating electrons from the horizontal to the vertical transverse plane. This transfer of energy is termed "betatron coupling."

Having exploited betatron coupling to improve the beam's lifetime, we then had to determine the most effective way of controlling this phenomenon, since it is highly sensitive to changes in the betatron tune (or number of oscillations by the electrons in one turn around the storage ring). Without such control, the beam size would fluctuate whenever users change an undulator gap, a routine operation that alters the betatron tune. We successfully identified magnet settings at which vertical-focusing changes caused by the undulators have an insignificant effect on electron-beam size.

Another consequence of our progress became evident when users began to take advantage of the better resolution they could attain with the higher-quality electron beam. To fulfill their higher expectations, it was necessary to improve the the beam's positional stability. We achieved a satisfactory state of stability without resorting to the usual practice of global orbit feedback (see "The Quest to Improve Orbit Stability," p. 34).

Machine Modeling Pays Off

One phenomenon that the accerator physicists constantly battle is beta beat or irregularity in the storage ring's beta function, a parameter that is a determinant of the size of the electron beam. Beta beat causes serious problems such as variations in the dimensions of the beam from point to point around the ring, decreased injection efficiency, and reduced beam lifetime. Our major weapon in this battle is a model of the storage ring, which enables us to measure the effects of beta beat and compensate for them. Initiated before the ALS started operations, this "machine model" evolved over the years as an increasingly valuable tool.

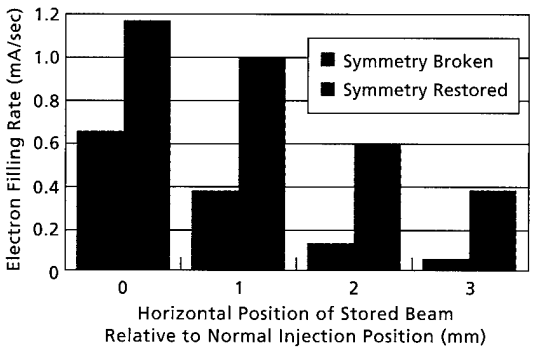
The current version was built by fitting measurement such as betatron tune, chromaticity, dispersion function, and the orbit response matrix. [An orbit response matrix consists of changes in the orbit, as measured at the beam-position monitors (BPMs), resulting from changes in the strength of the steering magnets.] In order to fit the response matrix data (over 15,000 data points), we vary more than 500 parameters in the storage-ring model and thereby achieve a more accurate model. Using this,

In the ALS control room, members of the Accelerator Physics and Electrical Engineering Groups examine plots depicting the variation in the size of the electron beam with changes in the betatron tunes. These plots indicate the outcome of restoring the twelvefold symmetry of the storage ring's magnetic lattice. Focusing errors result in broken symmetry, allowing resonances to become excited, an effect that increases the beam size at certain tunes (as demonstrated in the upper plot on the screen to the right). A model of the storage ring's magnetic lattice allows these scientists to predict quadrupole magnet settings that will restore symmetry. Resonance excitation is thereby reduced, and the betatron tune can be varied with little change in beam size. The lower plot on the right-hand screen demonstrates the effects of restored symmetry. The plot on the left-hand screen shows a scan over a larger area of the lattice with restored symmetry.

we can then predict which parameters should be changed to improve the ring's performance. Throughout 1996/97, we continued to refine the model and improved our measurement technique by increasing the sensitivity of the BPM system.

Our efforts led to better injection efficiency, a measure of the number of electrons actually captured in orbit when injected into the storage ring. It was known that focusing errors (related to the quadrupole magnets around the storage ring) perturb the ring's symmetry, and this condition gives rise to stronger excitation of resonances, which may lead to high electron losses, especially of freshly injected electrons. We used our machine model to conduct studies demonstrating the relation between broken symmetry and injection efficiency. Moreover, fitting the model enabled us to measure the focusing errors and to predict the corrections to the quadrupole field strengths needed to restore symmetry.

Our model also proved its worth by helping us to overcome a focusing effect caused by the 2-tesla wiggler, which was installed in Sector 5 in April 1996. Whenever the wiggler gap was closed, we observed beta beat that resulted in an unacceptable variation in beam size. Although we knew that a solution lay in adjusting the power supplies of the quadrupole magnets, we had to identify the most efficient quadrupoles and determine power supply settings that would correct the focusing over a range of gap widths. The machine model enabled us to select the target magnets and obtain set values that corrected the problem.



Comparison of injection efficiency at various injection-offset distances with symmetry broken (lower efficiency) and with symmetry restored (higher efficiency).

Getting the Jump on Future Challenges

Because of its small transverse beam size, the ALS is one of the first storage rings in the world to be in a position to study the transient regime of ion instabilities. These arise when the electron beam interacts with ions generated by collisions of the electrons with gas molecules. The ions are known to have several deleterious effects, including a reduction in beam lifetime. Such effects become more noticeable with advanced operating conditions—higher beam current, a greater number of electron bunches, and smaller beam dimensions.

One effect, the "fast-ion instability," was first proposed to explain growth in beam emittance observed at Japan's Photon Factory; however, experiments there failed to show any of the predicted parameter-dependent effects. At the ALS, we collaborated with accelerator physicists from Stanford Linear Accelerator Center in conducting a well-controlled series of experiments that unambiguously identified the instability for the first time. Our success has taken us one step ahead in meeting challenges that will inevitably arise from advanced operating conditions at storage rings of the next generation.

Ongoing Initiatives in Accelerator Physics
Refinement of the "machine model"—an interactive computer simulation code for demonstrating the behavior of the ALS storage ring. Application of the model to solve problems, for example, to find sources of beta beat or to create local bumps (offsets) in the beam to test our monitoring system.
Improvement of the feed-forward system, which functions proactively to minimize electron-beam movement as insertion-device gaps are closed.
Further compensation for beta beat in the storage ring, especially when new insertion devices (e.g., the elliptically polarizing undulator) are installed.
Semi-automatic generation of ramping tables for lattice magnets and correctors. (These are tables of settings for raising and lowering the storage ring energy without beam loss or orbit changes.)
Indexing of beam-position monitors to the magnetic centers of quadrupole magnets.
Investigation of readout anomalies from the beam-position monitors in the arc sectors of the storage ring.
Investigation of the relation between electron-beam size and lifetime. (The lifetime of the beam becomes shorter as its dimensions grow smaller.) Our goal is to be able to adjust the degree of trade-off in response to users' needs.
Elimination of parasitic electron bunches when the ALS runs in two-bunch fill mode.
Investigation of the advantages to be gained through a 1.5-gigahertz (third-harmonic) rf cavity—lengthening of the electron bunches in the storage ring with a concomitant increase in the Touschek lifetime.
Investigation of the use of straight sections in which a reduced vertical beta function (i.e., smaller vertical beam dimension) permits the vertical dimension of the vacuum aperture to be reduced, thereby allowing smaller-gap, shorter-period undulators.

THE QUEST TO IMPROVE ORBIT STABILITY

Routine operation of our transverse and longitudinal multibunch feedback systems reduced the electron beam to smaller dimensions than we have ever before achieved for ALS production runs. This feat gave promise of higher-than-ever spectral and spatial resolution for experimental results; but before researchers could capitalize on this promise, the stability of the beam's orbit had to be restored to design specifications. Our design tolerance for deviations in the orbit is stringent, 10% of the nominal beam size. Thus, as the beam grows smaller, so must the distance it is allowed to wander.

Starting in mid-1996, we installed new, highly sensitive beam-position monitors (BPMs) in eleven of the twelve straight sections of the storage ring. Because these BPMs are much more reliable than their predecessors, we began the continuous display of their signals covering a 12-hour period. From these displays, we gained improved insight into distortions of the beam's orbit and were able to recognize systematic trends.

To overcome these distortions, we reconvened an interdisciplinary task force that, in 1995, had successfully identified and eradicated a beam perturbation caused by oscillations in the temperature of the ALS's low-conductivity water supply. This time, the task force was given the mission to bring the orbit's stability to design specifications in the shortest time possible. Time and serious technical constraints precluded working on a closed-orbit feedback system, the standard solution, so we decided to attack the causes of beam motion at their sources.

Since the construction of the storage ring, we have been aware that deviations of a few degrees centigrade in the ambient air temperature cause changes in the shape of the storage-ring girders. As a result, the lattice magnets mounted on the girders become misaligned. For this reason, the ALS building had been air-conditioned to a precision of 1°C. The task force reviewed this effect by applying our machine modeling code and by conducting experiments with the storage ring itself. We discovered that changes in the girder temperature of only 0.2°C were enough to cause magnet misalignments of about 50 μm and, consequently, 300-μm orbit deviations; therefore, more stringent temperature stabilization appeared to be a good solution to improving orbit stability. After two months of testing and analyzing, we established a scenario that led to a dramatic improvement. Our correction strategies included keeping the temperature in the storage ring tunnel lower than that of the ALS building, moving the nine temperature-controlling sensors within the accelerator enclosures away from the air outlets, using the average of the sensor readings around the tunnel as the basis for temperature control, and placing four large fans around the storage ring to move the air in the tunnel in a spiral fashion. The new temperature-stabilization scenario reduced the typical peak-to-peak perturbations in the orbit to 20 μm horizontally and 5 μm vertically—well under the design specifications.

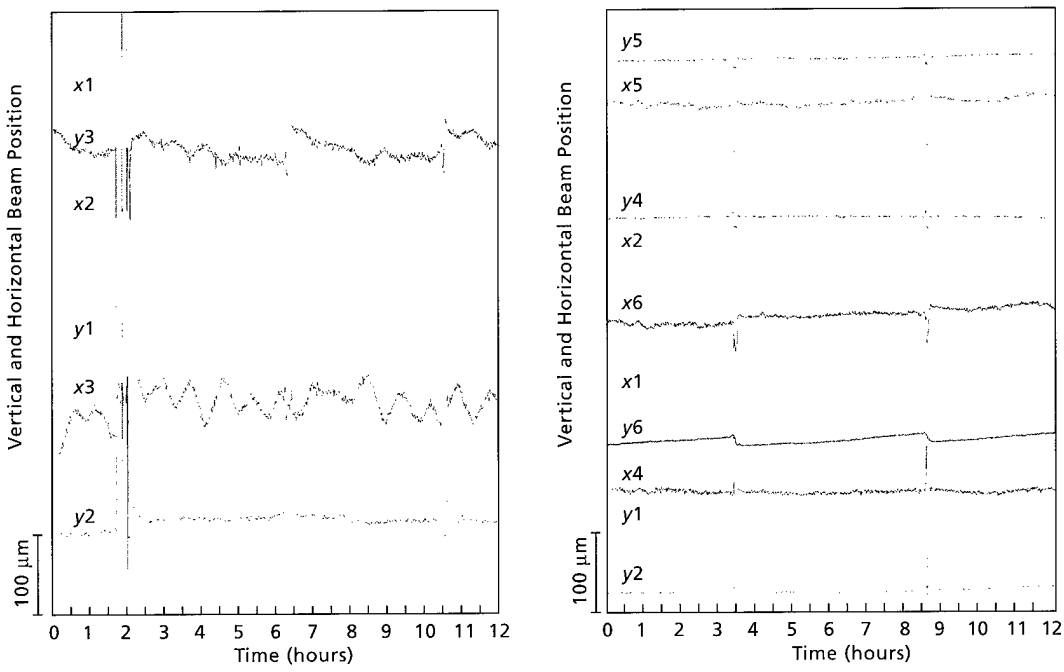
One of the last remaining thermal effects we observed was the "10 o'clock hump," an offset of the orbit that began daily around 10 A.M. and lasted for several hours. We determined its cause to be cross talk between the specialized system for cooling the storage ring and the temperature-control system serving the building. Before 10 A.M., the storage ring relied for cooling on chilled water from the specialized system; however, at that hour, the building system would switch from heating or neutral mode to cooling mode and mix its not-yet-chilled water with that of the storage ring system. The increased water temperature caused the shape of the girders to change and brought on the hump. This effect reversed itself once all the water was

sufficiently chilled; thus, our solution was to maintain the water in both systems at an appropriately cool temperature.

Besides the temperature-related perturbations, the task force analyzed and controlled others from two different sources. One anticipated perturbation occurs whenever the gap of an undulator or wiggler is changed. The problem is due to small imbalances in the magnetic fields of these devices. We are compensating for this effect by applying steerer fields proactively (in a feed-forward mode) and by restoring the gap to its previous width when we start operations after a refill of the storage ring.

Another perturbation had a more surprising cause. It was discovered by researchers who noticed abrupt changes in the intensity of their photon beam when one of the two large cranes in the ALS building was moved past their beamline. A subsequent study demonstrated that any change in the cranes' position from their normal parking places, but not the actual motion of the cranes, was responsible for the perturbation. The obvious solution was adminstrative—to avoid moving the cranes while researchers are using their beamlines.

Our solutions for controlling these perturbations proved to be highly effective. BPM plots taken in early 1997, after the solutions were implemented, indicate a highly satisfactory state of beam stability in contrast to plots taken in mid-1996.



x = Horizontal Position *y* = Vertical Position □= Refill Period

Signals taken over 12-hour periods from beam-position monitors (BPMs) located in the straight sections of the storage ring upstream or downstream from an insertion device. The plots on the left (from three BPMs) were recorded in August 1996. They show strong excursions in the second hour marking an event that would be typical of a crane movement. Most of the plots on the left also show major oscillations with a one-hour period, which proved to be related to variations in the air temperature in the storage ring tunnel. The plots on the right, taken from five BPMs in April 1997, show a dramatic improvement in the stability of the orbit compared with the earlier plots.

EXPERIMENTAL SYSTEMS

The ALS floor bustles with the activity of scientific discovery, as our beamlines and branchlines grow in number. Eighteen were operating as of mid-1997, each delivering synchrotron radiation with unique qualities tailored to the users' specific research goals. The needs of our users, present and potential, drive the efforts of the Experimental Systems Group. In conjunction with the Mechanical and Electrical Engineering Groups, we develop insertion devices and beamline instrumentation to keep ALS users on the leading edge of synchrotron radiation research.

Macromolecular Crystallography Facilities

Among the beamlines completed during 1996/97 was Beamline 5.0, the first at the ALS dedicated to macromolecular crystallography. This technology, which requires a high flux of high-energy photons, is made possible by the beamline's source, a 38-pole wiggler, also new to the ALS. Built by the Mechanical Engineering Group and installed in April 1996, it is the fifth ALS insertion device and the first wiggler. We have been operating the wiggler at full power (1.9 GeV, 400 mA, 2.1 tesla). The beamline, which was built in conjunction with Berkeley Lab's Structural Biology Division, is currently being commissioned.

Spectromicroscopy Options

Also proliferating is our spectromicroscopy program, which boasts several new facilities. The scanning transmission x-ray microscope (STXM) on undulator Beamline 7.0.1 has now been complemented with an ultra-high-vacuum zone-plate microscope known as SPEM (scanning photoemission microscope). Like STXM, SPEM features micro zone-plate focusing, but uses an electron energy analyzer as a detector. Placing the zone-plate scanning stage in ultra-high vacuum and close to the analyzer was a real engineering challenge, but results indicate 0.3-μm resolution as expected, and initial studies on interface formation have yielded spectacular data.

Another spectromicroscopy beamline, bend-magnet Beamline 7.3.1, is now complete and in use. This beamline has two branches, one wide-aperture branch (7.3.1.1) for a photoelectron emission microscope (PEEM) and a second branch (7.3.1.2) for microfocused x-ray photoelectron spectroscopy (μ-XPS). The μ-XPS focusing system uses a pair of elliptically shaped grazing-incidence mirrors, produced by controlled bending within the ultra-high vacuum of the beamline. The microscope is designed to perform scanning XPS on semiconductor wafers with 1-μm-spatial-resolution. (To date, we have achieved 2-μm resolution in preliminary tests.) A co-development with Intel Corporation and Applied Materials, μ-XPS has many features especially designed for wafer samples, such as *in situ* optical fiducialization.

The photoelectron emission microscopy branchline (7.3.1.1) is essentially complete, and the PEEM system itself has a completion date of October 1997. The PEEM operates at high voltage (30 kV) and has two projector stages, a stigmator and several deflectors to keep the beam passing through the center of the lenses, and a directly coupled phosphor-fiber CCD detector. The branchline also offers *in situ* sample preparation and sophisticated sample-manipulation capabilities. A thorough theoretical study has shown that the system should be capable of 30-nm resolution. This instrument is being developed with IBM as part of a cooperative research and development agreement. We are also developing plans for another PEEM that will compensate for spherical and chromatic aberrations of the electron optics and should be capable of 3-nm resolution. This project is a joint effort with teams at IBM and Arizona State University. The system will ultimately use Beamline 4.0.3-4, which will receive light from an elliptical polarization undulator. Operation is scheduled for early 1999.

Infrared Microscopy System

The infrared microscopy beamline (Beamline 1.4) has recently been completed, and commissioning is under way. The system consists of plane and ellipsoidal mirrors inside the storage ring shield wall to focus the radiation through a diamond isolation window, a system of collimating mirrors, and a commercial Nicolet interferometer and microscope. The light it delivers has a wavelength range of 2–35 μm, corresponding to the chemical fingerprinting range for organic species. This beamline will be used for a variety of chemical mapping studies, from identification of particles on silicon wafers to environmental studies of humic material.

Delivery System for Elliptically Polarized X Rays

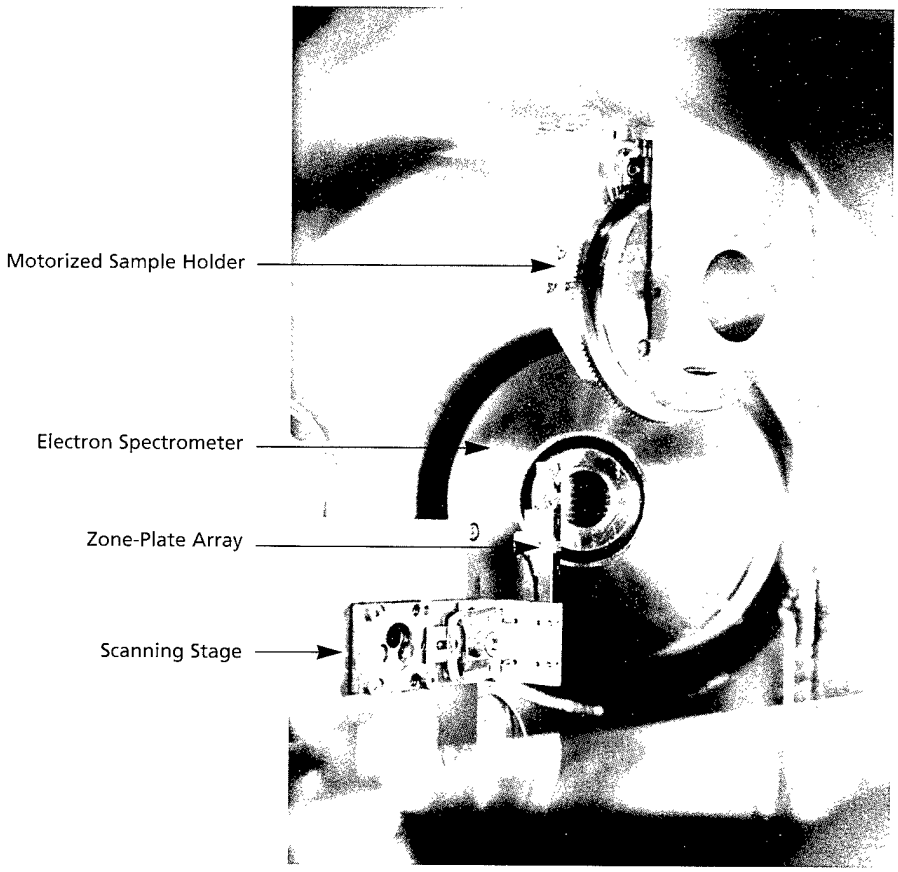
Beamline 4.0.1-2, the first of the beamlines designed to deliver x rays from the elliptical polarization undulator, is now taking shape, and we have contracted for construction of its high-power monochromator. Designed to deliver x rays with energies from 20 eV to 1600 eV, this beamline is expected to start operations during the summer of 1998. It will offer very high resolving power for studies on magnetic systems. We have now begun the optical design of a second monochromator, which will be optimized for high-spatial-resolution microscopy.

Ongoing Activities in Beamline Instrumentation and Engineering
Development of advanced photoelectron emission microscopes (PEEMs) for high-resolution studies of materials such as polymers and thin carbon films (used in computer disk drives).
Commissioning of Beamline 1.4 for infrared microscopy. Potential uses range from chemical fingerprinting studies to investigations of surface adsorption and semiconductor defects.
Design and construction of the elliptical polarization undulators and the associated beamline (4.0) for microscopy and spectroscopy of magnetic materials.
Commissioning of Beamline 5.0 for macromolecular crystallography studies, such as determining the structures of proteins (see "Macromolecular Crystallography," p. 42).
Development of spectromicroscopy, including refinement of the new scanning photoemission microscope (SPEM) on Beamline 7.0.1 and μ-XPS on Beamline 7.3.1.2 (see "Scanning Photoemission Microscopy," p. 38, and "Micro X-Ray Photoelectron Spectroscopy," p. 40).
Design and construction of Beamline 7.3.3 for thin-film strain measurements and spatially resolved x-ray absorption near-edge spectroscopy (XANES).
Optics research for the development of optical metrology, holographic imaging, optical design, switching optics, bendable mirrors, and microfocusing systems.
Development of instrumentation for femtosecond x-ray diffraction studies.
Design and construction of a high-energy-resolution spectrometer (HERS) for photoemission studies of highly correlated systems.
Design and construction of a bend-magnet beamline for scanning transmission x-ray microscopy.
Commissioning and refinement of a system for Fourier transform interferometric spectroscopy at ultra-high resolution (Beamline 9.3.2).

SCANNING PHOTOEMISSION MICROSCOPY

A new high-resolution scanning photoemission microscope (SPEM) began operation at the ALS in March 1997. This instrument opens new avenues for spectromicroscopy research at the ALS. It combines the features of the scanning transmission x-ray microscope—which uses a Fresnel zone-plate lens to produce a microfocus for spectromicroscopy studies—with an electron energy analyzer in an ultra-high-vacuum environment. In designing and building such a system, our aim was to combine these attributes with 0.1-μm spatial resolution.

The new system has a unique method of scanning samples. Unlike other photoemission microscopes, in which the sample is moved in order to form a scanned image, SPEM forms images by moving the focused x-ray beam over a stationary sample surface. It is the first zone-plate photoemission microscope to operate in this way. Keeping the sample stationary makes it possible to use a large, conventional sample manipulator. Thus, researchers using the SPEM will be able to study samples that are cryogenically cooled or heated or to examine



Inside the scanning photoemission microscope, the sample sits on a motorized assembly that lowers it into position in front of the zone-plate array. This array contains three different zone plates, with their corresponding order-sorting apertures, arranged stepwise so that each is correctly positioned for its focal length. The zone-plate array attaches to a scanning stage, which moves the x-ray beam across the stationary sample.

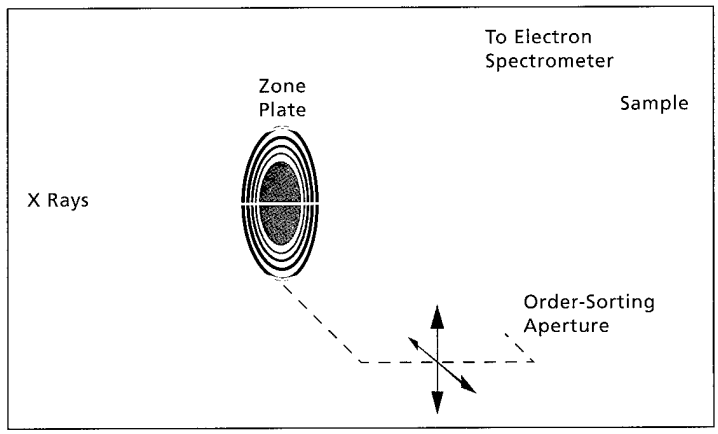
small regions of large (25-mm) samples without having to cut the sample apart. SPEM features a 16-channel electron energy analyzer, which allows detailed spectroscopic analyses to be performed at points on the surface where the photoelectron image shows interesting features.

The new SPEM uses Fresnel zone-plate lenses a quarter of a millimeter in diameter to focus the x-ray beam. These lenses are made by electron-beam lithography and plated with gold to form a diffracting ring structure. The SPEM scans the lens in a raster pattern half a millimeter in front of the sample, moving the focused x-ray beam across the surface. Each lens is accompanied by an order-sorting aperture, which prevents zero-order light from reaching the sample. The aperture must move with the lens and is therefore built into the same assembly at a fixed focal length. Since the appropriate focal length varies with photon energy, we have designed the instrument to accept different assemblies for the various photon energy ranges of interest. The photon energy used in the SPEM can vary from about 200 eV to 900 eV, offering researchers the flexibility of studying microscopic changes in valence band structure as well as performing more traditional core-level spectroscopy.

Early studies with SPEM have focused on problems in composite materials, imaging features a few microns across. In addition, metallurgical problems are particularly amenable to the scanning photoemission technique, as the samples are electrically conducting and can be polished. Electrically insulating samples from the semiconductor industry have been studied as well.

In its commissioning period, SPEM has demonstrated an x-ray spot size of about 0.3 μm. Spatial resolution of 0.2 μm is expected from the zone plates in use now, with improvements of a factor of 2 or more as finer zone plates become available. The instrument's commissioning continues, and we expect it to be fully operational by the end of 1997.

Funding: Office of Basic Energy Sciences of the U.S. Department of Energy, National Science Foundation, University of Wisconsin at Milwaukee, and Lawrence Livermore National Laboratory.

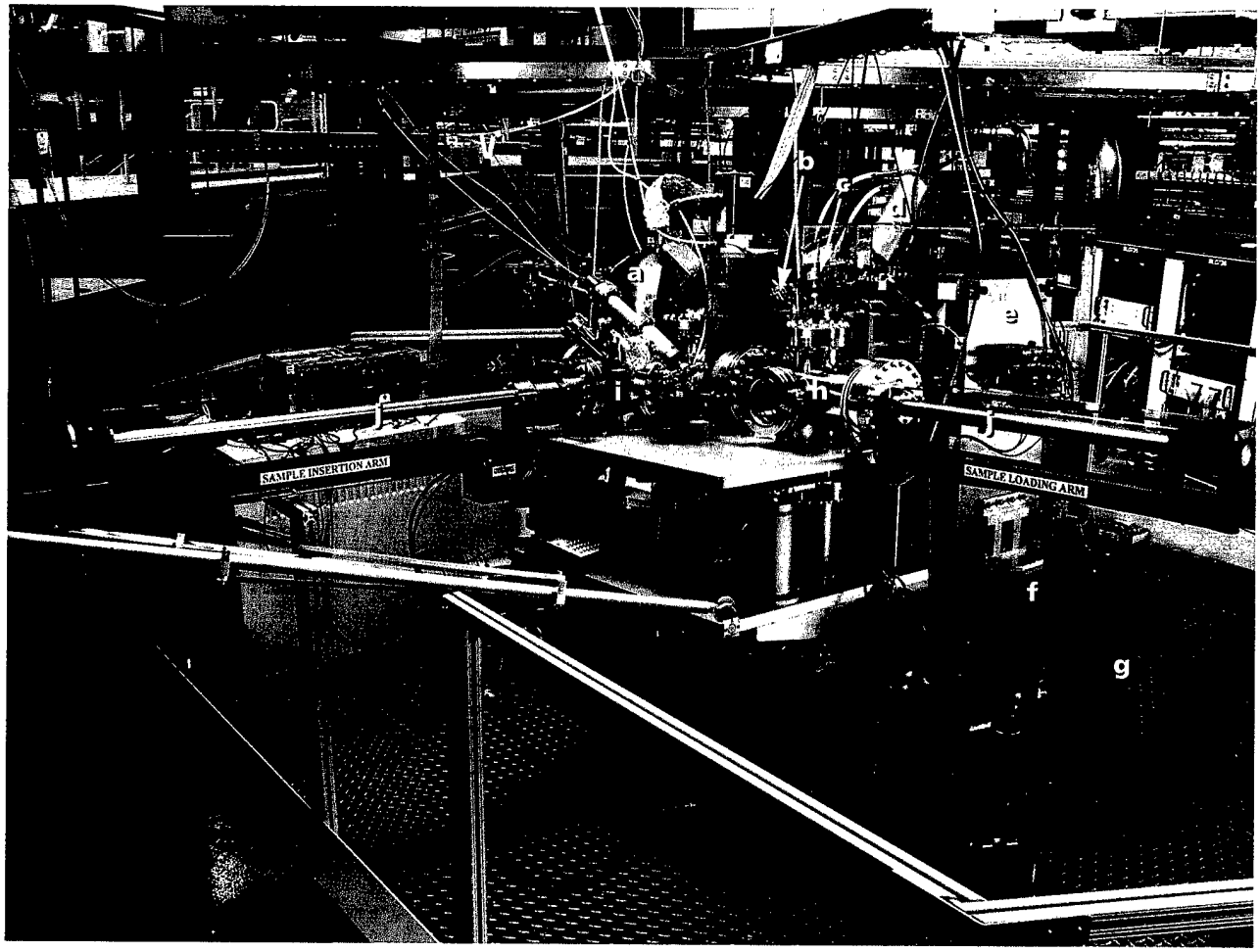


Schematic layout of the scanning photoemission microscope. The zone plate and the order-sorting aperture move in tandem to raster the x-ray beam over a stationary sample.

MICRO X-RAY PHOTOELECTRON SPECTROSCOPY

On January 23, 1997, the new micro x-ray photoelectron spectroscopy (μ-XPS) beamline reached a significant milestone: seeing its first synchrotron light. A joint development with Intel Corporation and Applied Materials, the μ-XPS project grew out of the need, identified in the Semiconductor Industry Association Roadmap, for a technique capable of surface chemical mapping at high spatial resolution. The project was conceived as an XPS system capable of 1-μm spatial resolution on a bend-magnet source.

Achieving such high spatial resolution for surface chemical studies has not been possible with existing laboratory techniques. Infrared spectromicroscopy has limited sensitivity and spatial resolution but good selectivity for organic species. Scanning Auger microscopy (SAM) has excellent spatial resolution (0.1 μm), but the chemical information that can be obtained is extremely limited. Sophisticated laboratory systems for scanning XPS exist, but though the best offer 10-μm resolution, imaging times are very long because of the limited



The micro x-ray photoelectron spectroscopy endstation, showing (a) electron energy analyzer, (b) partial-electron-yield detector, (c) sputtering gun, (d) laboratory hard-x-ray source, (e) precision *x-y* sample manipulator, (f) six-strut chamber support, (g) independently supported "people platform," (h) sample introduction and parking area, (i) sample preparation and transfer area, and (j) magnetic sample transfer arms.

brightness of the source. Our goal, therefore, was to design a micron-resolution system with short image-acquisition times that would take full advantage of the tunability of synchrotron radiation. The selection of photon energy is important in two respects: first, it allows the cross section of the element of interest to be maximized; and second, it allows us to vary the kinetic energy of the photoemitted electrons and hence their escape depth. In this way, we can alter the surface sensitivity and minimize radiation damage.

The μ-XPS system uses a branchline off an existing monochromator in order to reduce the total system cost. This monochromator, together with a spherical, horizontally deflecting branching mirror, delivers a monochromatic focus to an adjustable pinhole, which is the object for the μ-XPS imaging system. The microfocusing is produced by orthogonal elliptical mirrors in a Kirkpatrick-Baez arrangement. These mirrors have to be nearly perfect to produce the desired micron-sized focus and are made by the controlled bending of flats. They must be bent to extreme curvature and therefore are made of high-strength steel. Because of the high demagnification, which requires a mirror-to-sample distance of 0.1 m, the whole optical system for the endstation is in ultra-high vacuum and very close to the sample stage. This unusual space constraint added another dimension to the engineering challenge.

Another key design issue is sample positioning. The patterned wafer samples to be studied are first examined elsewhere by conventional techniques, the areas of interest are identified with reference to fiducial points, and then the samples are transferred to the ALS. Here the samples pass through a fast-entry load lock, through a prep chamber, and into the analysis chamber, in which a high-resolution *in situ* optical microscope is used to find the fiducial points. From these, the system can locate the previously identified areas of interest. The sample holder can accept up to 2-inch × 2-inch wafer sections, and designs are being assessed for a future system capable of handling full 12-inch wafers.

The μ-XPS project was completed and began its initial commissioning only ten months after construction started. Meeting this very tight manufacturing and commissioning goal was of key importance for our industrial partners. With minor adjustments to the system, we have achieved 2-μm × 2-μm resolution at full aperture. With further adjustment, possibly using the new higher-quality mirror substrates we now have available, we are confident of reaching our 1-μm target. Since the diffraction limit of these mirrors at a photon energy of 1 keV is less than 0.1 μm, we can expect, with improved optics and a smaller pinhole, to achieve submicron resolution (given adequate photon flux). The ultimate goal is to build a system providing resolution that is a small fraction of next-generation microcircuit line widths (0.18 μm). If the return on investment for the present system is adequate, we could meet this challenge with an undulator-based system capable of 0.1-μm resolution.

Funding: Office of Basic Energy Sciences of the U.S. Department of Energy, Intel Corporation, and Applied Materials.

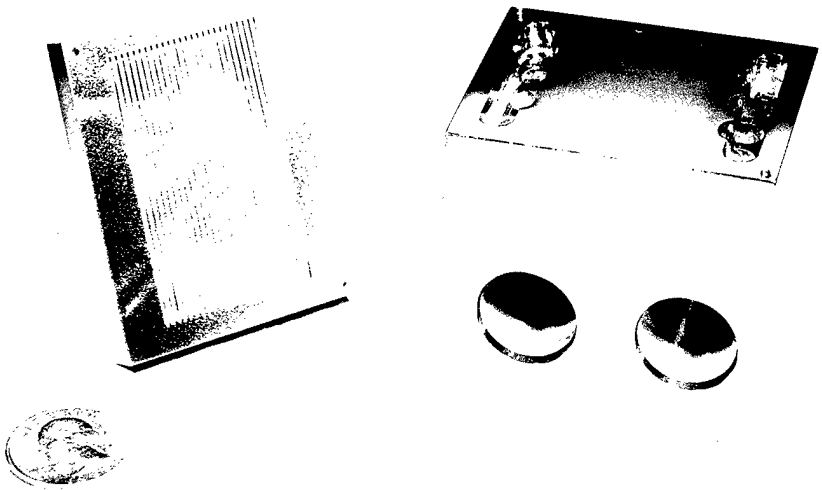
MACROMOLECULAR CRYSTALLOGRAPHY

The end of 1996 marked an important achievement for the Experimental Systems Group, with the December delivery of first light to the macromolecular crystallography beamline. Developed in collaboration with Berkeley Lab's Structural Biology Division, the beamline forms the heart of the new Macromolecular Crystallography Facility at the ALS, which offers structural biologists from industry, government, and academia a choice of crystallographic techniques with semi-automated operation and rapid sample turnaround.

The light source for the beamline is a 38-pole, 2.1-tesla wiggler, emitting 8.4 kW at 1.9 GeV, 400 mA. Engineering a beamline to handle the heat load from such a powerful wiggler source has required several tactics. First, the soft x rays emitted by the wiggler are absorbed by a series of thin carbon filters. These reduce the power falling on the first optical elements substantially. Second, the optics themselves have been designed to handle a high flux of hard x rays.

The focusing arrangement for the completed central branchline is conventional in that a remotely adjustable mirror upstream of the monochromator (inside the storage ring shield wall) provides vertical collimation, the monochromator is a double-crystal arrangement with a fixed exit height, and a toroidal mirror downstream focuses the light to a small spot in the hutch. Because of problems at the optics vendor contracted to make these mirrors, we decided to install temporary mirrors of reduced aperture while new full-size replacement mirrors are fabricated. The first temporary mirror is a silicon flat with simple internal cooling, and the second is a silicon toroid. This arrangement has allowed us to proceed with commissioning the beamline, but with a temporary decrease of about a factor of 2 in energy resolution and about a factor of 3 in flux.

Like the first mirror, the double-crystal monochromator requires cooling. In fact, its first crystal receives the highest power density of any optical component in the beamline, absorbing approximately 700 W/mrad^2 (up to 2.5 W/mm^2 at a Bragg angle of 30°). To preserve spectral resolution, any thermal distortion must be kept to a small fraction of the crystal rocking width (roughly 40 μrad for silicon at 10 keV). In order to achieve this under extreme power loading, the crystal is internally water-cooled



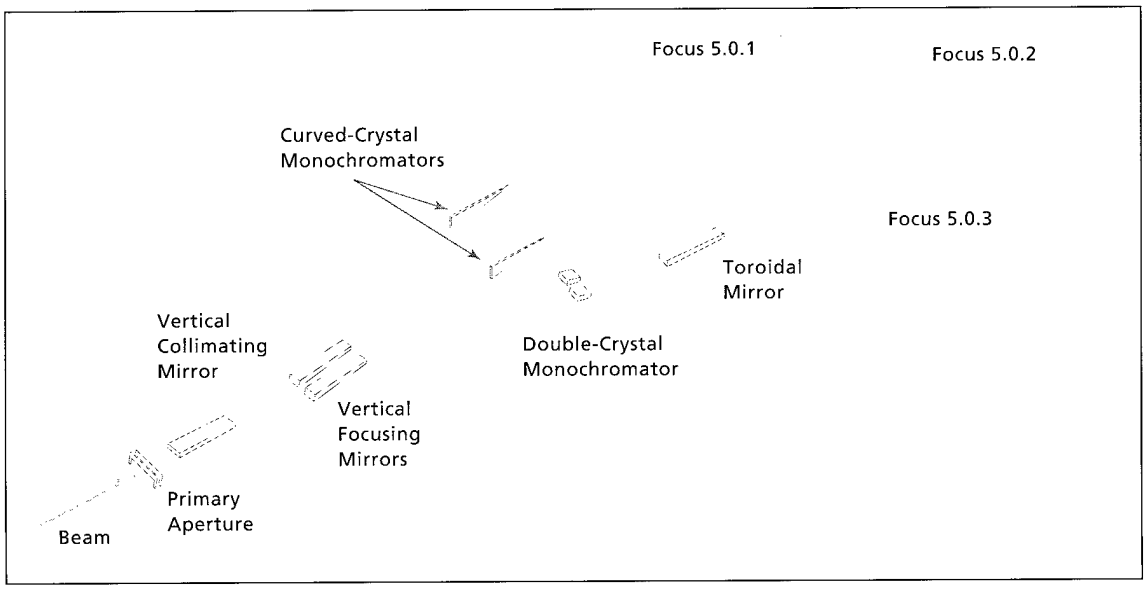
The water-cooled first crystal of the central branchline's monochromator is made up of two pieces of silicon. The thinner piece, one side of which serves as the diffracting surface, has 1-mm water channels machined into the reverse side (left). This piece is then frit-bonded, channel side down, to the second silicon block (right).

through 1-mm-wide channels machined into the crystal within 1 mm of the diffracting surface. In contrast to undulator beamlines at third-generation hard-x-ray sources, where liquid-nitrogen cooling is used, we chose to use water cooling because the monochromator receives a much lower power density even though it absorbs more total power.

The beam focused into the central branchline's hutch passes through an aperture, a flux monitor, an anti-scatter collimator, and a transport tube—all helium-filled to minimize x-ray absorption—before intercepting the crystal to be measured. Diffracted x rays are detected by a 2 × 2–matrix CCD detector that is mounted on a slideway so that users can vary its distance from the sample. The slideway can also be rotated in order to collect the very high-resolution data sometimes available from exceptional crystal samples.

We are now developing up to two side stations that will have asymmetrically cut, curved-crystal monochromators. The wiggler has been run at full power (14 mm gap, 2.1 tesla, 1.9 GeV, 400 mA), and the beamline has transported monochromatic light into the central branchline's hutch under these conditions. In the summer of 1997, we started the detailed characterization of the system, measuring resolution, flux, spot size, and stability. From our initial measurements, the existing beamline appears to be performing to specification. The combination of functioning beamline, state-of-the-art CCD detector, and accompanying crystallography support laboratories means that, overall, we now have one of the best facilities for biological crystallography in the world, and we can look forward to many years of successful operation.

Funding: Office of Biological and Environmental Research of the U.S. Department of Energy, Amgen, Roche Biosciences, University of California at Berkeley, and Berkeley Lab.



Optical layout of the macromolecular crystallography beamline (Beamline 5.0). Light in the central 1.5 mrad of the wiggler beam is reflected by a vertical collimating mirror toward the double-crystal monochromator and hence to the rest of Branchline 5.0.2. When the proposed side branchlines are completed, each one will take 3 mrad of light to one side of the beam's central area. This light will be reflected upward by a vertical focusing mirror to reach the corresponding branchline optics (Branchline 5.0.1 or 5.0.3).

Annual Meeting
of the
Advanced Light Source Users' Association

An Invitation To

Adventures In Light & Science

A Free Workshop for Teachers at the Advanced Light Source – America's Brightest Source of Soft X Rays – sponsored by Lawrence Berkeley National Laboratory and organized in cooperation with local teachers.

August's INTERACTIVE BIOGRAPHY from the People at the ALS

Annette Greiner

When she is not busy coding ALS documents for the WWW, researchers seek her out to decode their scientific mumbo-jumbo for the rest of the world to understand.

AT THE ALS

What does she do at the ALS?
What does her job involve?
What is she doing now?
What is a typical day at the ALS like for her?
What are the highs and lows of her job?

PERSONAL

What is she really like?
How did she get here?
What is very important to her?
What does she do in her spare time?
What else is cool?
What, if anything else, could she have done?

Click here see something cool that she has worked with!

MY TURN

Click here to send your own questions to Annette Greiner.

PUZZLER CHALLENGE

Click here to be the first to enter your solution to Annette Greiner's PUZZLER!

ANNETTE GREINER'S PUZZLER:

Annette Greiner's favorite quote is "Simplify, simplify," from Henry David Thoreau. She finds that it works for writing editing, and life. Can you simplify this sentence into just four words?

The canine under our legal responsibility in case of fault to penalties is harbouring on the external limitine layer of flexible cover and supplying food for vertically moving, parasitic crustaceans.

BLAST FROM THE PAST

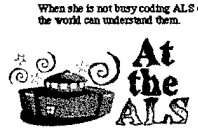
Click here to see past biographies with student questions and interviews or answers!

The Bright & The Busy

Interactive biographies of people at Berkeley Lab's Advanced Light Source

Annette Greiner

When she is not busy coding ALS documents for the Web, she is decoding scientific texts so that the rest of the world can understand them.



What does she do at the ALS?

- What does her job involve?
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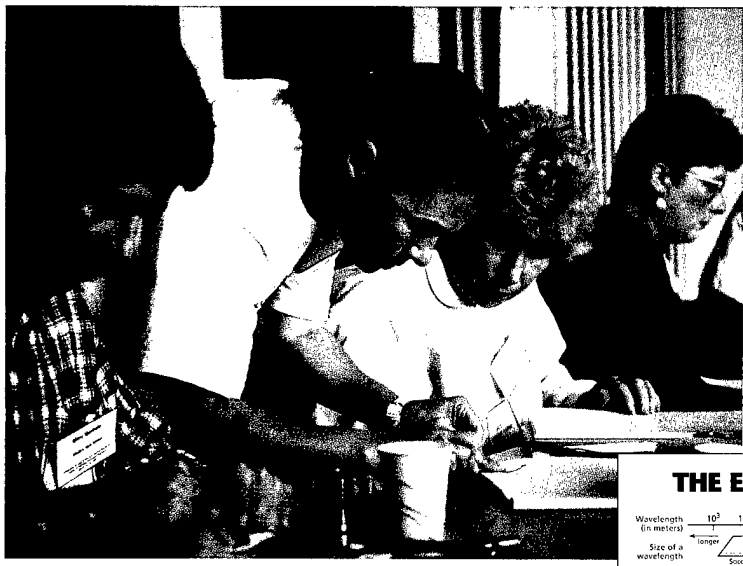
What is she really like?

- How did she get here?
- What is very important to her?
- What does she do in her spare time?
- What is something else cool she has done?

Click here to see Annette's answers to student questions!

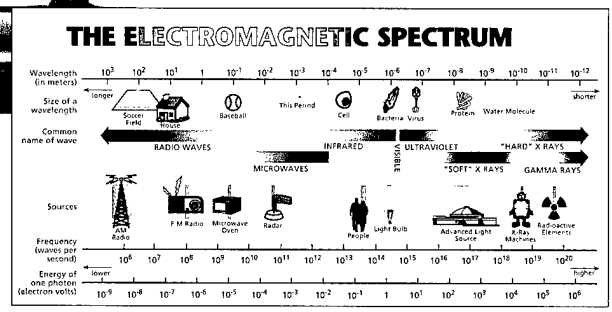
Click here to see something cool she has worked with!

EDUCATIONAL OUTREACH



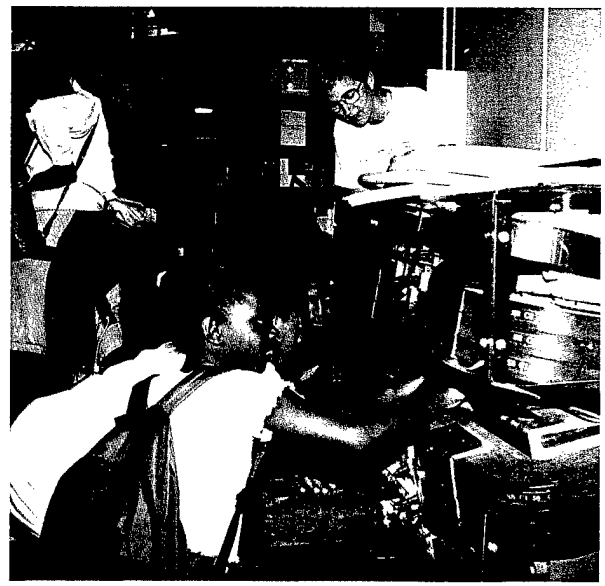
Teachers' Workshop

In March 1996, the ALS followed up on interest generated at the Lab-wide Open House in 1995 by holding a workshop for teachers from the San Francisco Bay Area and beyond. Teachers explored the ALS and related science topics through tours, presentations, and hands-on activities designed to take back to their classrooms. Several teachers from the workshop have prepared their classes for visits to the ALS using these activities and the popular *Inside the ALS* and *Electromagnetic Spectrum* posters.



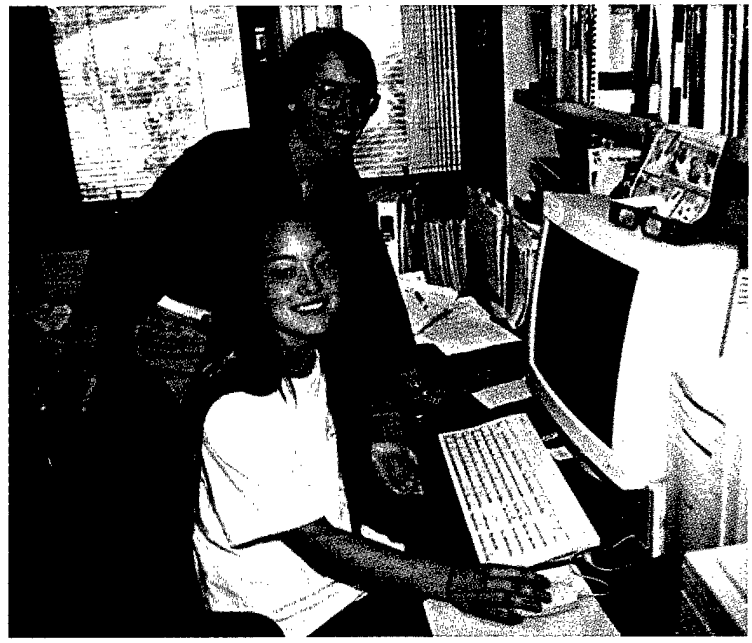
School Visits

Student visits to the ALS don't stop with a tour of the machine; opportunities abound to put this huge research tool in context. Above, students explore the behavior of polarized light and its interaction with materials. At right, getting friendly with a 4000-kg (8800-lb) bend magnet gives students an appreciation for the scale and precision of the ALS.



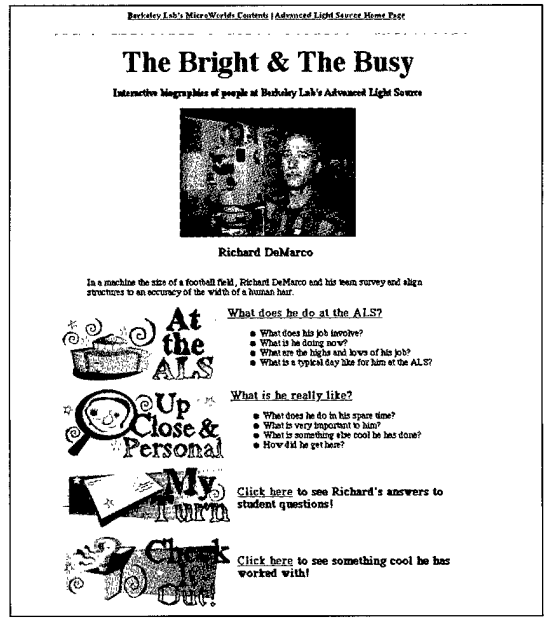
Reaching People Close to Home...

Cal Day in April 1997 provided opportunities for members of the local community to learn more about the ALS. During the Cal Day Open House, organized by the University of California at Berkeley, ALS staff gave crowd-pleasing "Cool Science" demonstrations with liquid nitrogen, vacuum pumps, and other scientific tools used at the ALS.



...and Around the World

Student intern Andrea Macfie spent the summer before her senior year in high school at the ALS, creating a fresh new section for the Microworlds Web magazine. "The Bright and the Busy" tells a worldwide student audience about the variety of jobs at a scientific facility and the people doing those jobs. It features profiles of ALS staff members describing what they do at the ALS and their interests off the job. Microworlds (http://www.lbl.gov/MicroWorlds/) makes ALS science accessible to students and teachers by presenting articles with integrated activities to teach the basic concepts involved.

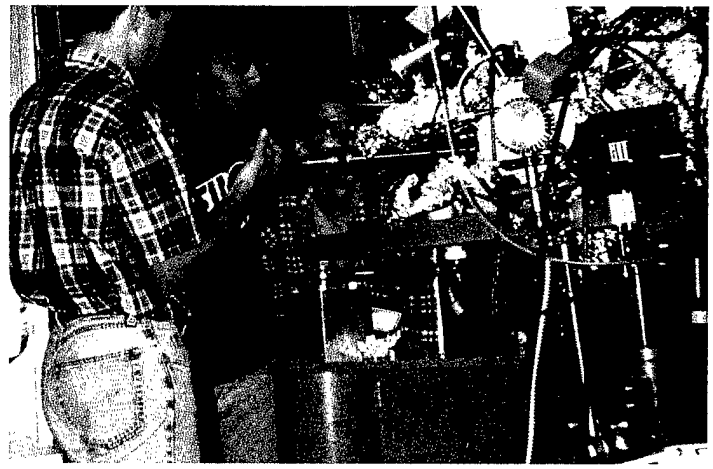


Science Bowl Winners Participate in Research

When choosing their prize for prevailing over 1,700 other teams in the U.S. Department of Energy–sponsored Science Bowl, the team from Venice (California) High School passed up a trip to Alaska's North Slope for a chance to visit the ALS. Team members received a crash course on the ALS for a week in August 1996, from survey and alignment of beamline components to residual gas analysis in ultra-high-vacuum systems and computer-aided design. They then became the first high-school students to participate in experiments on beamlines at the ALS.

Above, the team (clockwise from upper left): Candice Kamachi, My Le Hoang, Richard Erdman (coach), Chris Mayor, Noah Bray-Ali, and David Dickinson.

Above and at right, the team members at work, imaging malaria-infected red blood cells with the x-ray transmission microscope at Beamline 6.1.2, and using photoemission spectroscopy at Beamline 9.3.2 to probe the surface and bulk properties of various materials.



ALS A FOCUS OF COOPERATIVE EFFORT

Industrial Collaboration a Success

Representatives from Intel and Applied Materials joined ALS scientists, engineers, and shops staff on March 5, 1997, to celebrate the on-schedule completion of the first application-specific beamline. Beamline 7.3.1.2 delivers light to a micro x-ray photoelectron spectroscopy endstation (see p. 40) constructed with funding from the two companies and the U.S. Department of Energy and designed to analyze the microstructures and small-area interfaces in integrated circuits (ICs) and the silicon wafers from which ICs are made.

A Visit from Thailand

In May 1997, 23 visitors from the Parliament of Thailand, including six Parliament members, visited Berkeley Lab and the ALS. Led by Pavena Hongsakul (sixth from left, standing), member of Parliament and chair of the House Committee on Science and Technology, the group made a world-wide tour to explore the contributions that high-technology companies and facilities make to the science, technology, and economies of their home countries. A new synchrotron light source, the Siam Photon Project, is under construction in Khorat, Thailand.

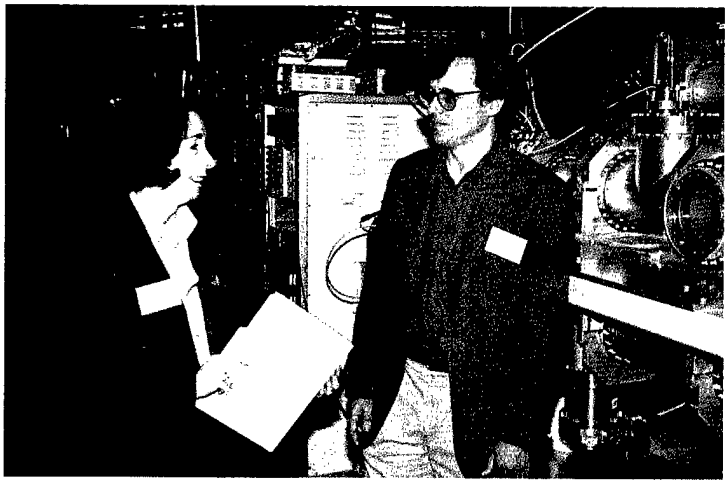
New Links with China

Yang Fujia (left), President of Fudan University in Shanghai and Director of the Shanghai Institute of Nuclear Research (SINR), visited Berkeley Lab in July 1996 to formalize an agreement between SINR and Berkeley Lab on cooperation in synchrotron research. A dinner in Berkeley and an exchange of gifts with Brian Kincaid on behalf of the ALS marked the occasion.

ALS USERS' ASSOCIATION MEETING

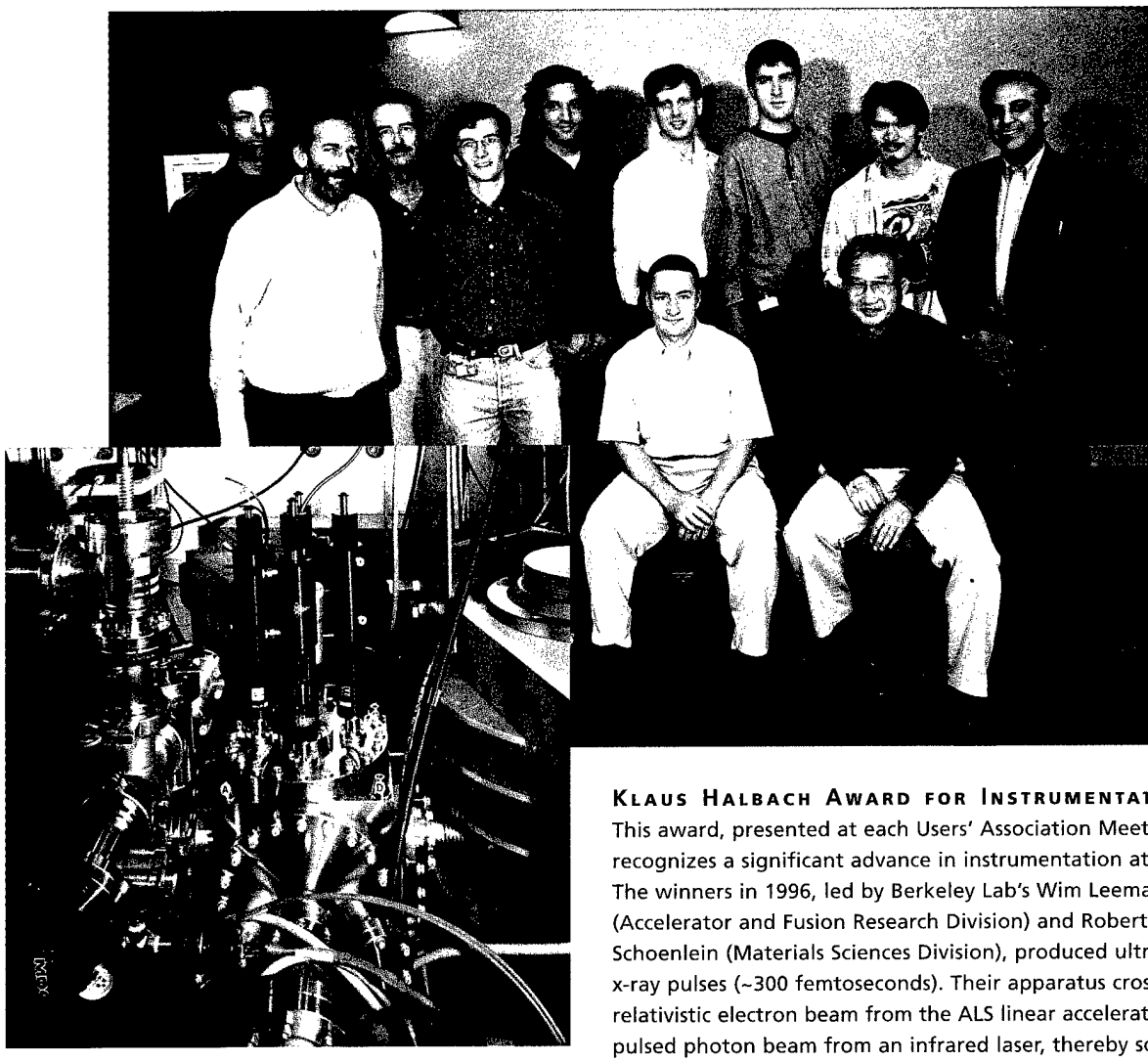
Users' Meeting Draws a Crowd

The October 1996 meeting of the ALS Users' Association attracted 220 participants from 12 countries for talks, workshops, and a chance to view the ever-increasing number of beamlines. At the poster session, held in conjunction with vendor exhibits, participants could discuss their work and see the latest offerings in beamline and endstation components.



Patricia Dehmer, head of the Office for Basic Energy Sciences at the U.S. Department of Energy, gave a talk and also came to the experiment floor (left) to talk with scientists about their work.

A banquet (below) gave participants and family members a chance to relax, enjoy each other's company, and witness the presentation of awards.



KLAUS HALBACH AWARD FOR INSTRUMENTATION
This award, presented at each Users' Association Meeting, recognizes a significant advance in instrumentation at the ALS. The winners in 1996, led by Berkeley Lab's Wim Leemans (Accelerator and Fusion Research Division) and Robert Schoenlein (Materials Sciences Division), produced ultrashort x-ray pulses (~300 femtoseconds). Their apparatus crosses the relativistic electron beam from the ALS linear accelerator with a pulsed photon beam from an infrared laser, thereby scattering the photons up to x-ray energies. Above, the group. Standing, left to right: Jim Dougherty, Max Zolotorev, Leon Archambault, Wim Leemans, T. Ernest Glover, Robert Schoenlein, Peter Balling, Alan Chin, Swapan Chattopadhyay. Seated: Paul Volfbeyn, Kwang-Je Kim. Not pictured: Charles Shank.

ALS-SPONSORED WORKSHOPS

Adventures in Light and Science Teachers' Workshop
March 4 and 16, 1996

High-Resolution Computed Microtomography
August 12–13, 1996

ALS Users' Association Annual Meeting and Workshops
October 21–23, 1996

Molecular Environmental Science at the ALS
March 27–28, 1997

ALS ADVISORY PANELS

Program Advisory Committee

Advises the Director of Berkeley Lab on the ALS scientific program through the ALS Director.

1996

Franco Cerrina
University of Wisconsin

Roger Falcone
University of California at Berkeley

Keith O. Hodgson
Stanford Synchrotron Radiation Laboratory

Christof Kunz
European Synchrotron Radiation Facility

Robert C. McDonald
Intel Corporation

David A. Shirley
Pennsylvania State University

Neville V. Smith
Berkeley Lab *(ex officio)*

Joachim Stöhr
IBM Almaden Research Center (chair)

Robert Stroud
University of California at San Francisco

François Wuilleumier
University of Paris-South, France

1997

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Berkeley Lab

Chien-Te Chen
Synchrotron Radiation Research Center, Taiwan

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University of California at Berkeley

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Berkeley Lab

Neville V. Smith
Berkeley Lab *(ex officio)*

Joachim Stöhr
IBM Almaden Research Center (chair)

Robert Stroud
University of California at San Francisco

Users' Executive Committee

Elected by the members of the Advanced Light Source Users' Association to act as the official voice of the user community in its interactions with ALS management.

1996

Harald Ade
North Carolina State University

Nora Berrah
Western Michigan University

Jeffrey Bokor
University of California at Berkeley (chair)

Richard Brundle
C.R. Brundle & Associates

Thomas A. Callcott
University of Tennessee (past chair)

Werner Meyer-Ilse
Berkeley Lab

Marjorie Olmstead
University of Washington

Eli Rotenberg
Berkeley Lab

Mahesh G. Samant
IBM Almaden Research Center

Arthur Suits
Berkeley Lab

Louis J. Terminello
Lawrence Livermore National Laboratory (vice-chair)

1997

Left to right: Werner Meyer-Ilse, Berkeley Lab (vice-chair); Duane H. Jaecks, University of Nebraska at Lincoln; Stephen D. Kevan, University of Oregon; Jeffrey Bokor, University of California at Berkeley (past chair); Eli Rotenberg, Berkeley Lab; Louis J. Terminello, Lawrence Livermore National Laboratory (chair); Bengt Jörgen Larsson, Berkeley Lab; Mahesh G. Samant, IBM Almaden Research Center; Adam P. Hitchcock, McMaster University, Canada; Thomas Earnest, Berkeley Lab. Not pictured: Arthur Suits, Berkeley Lab.

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FACTS AND FIGURES

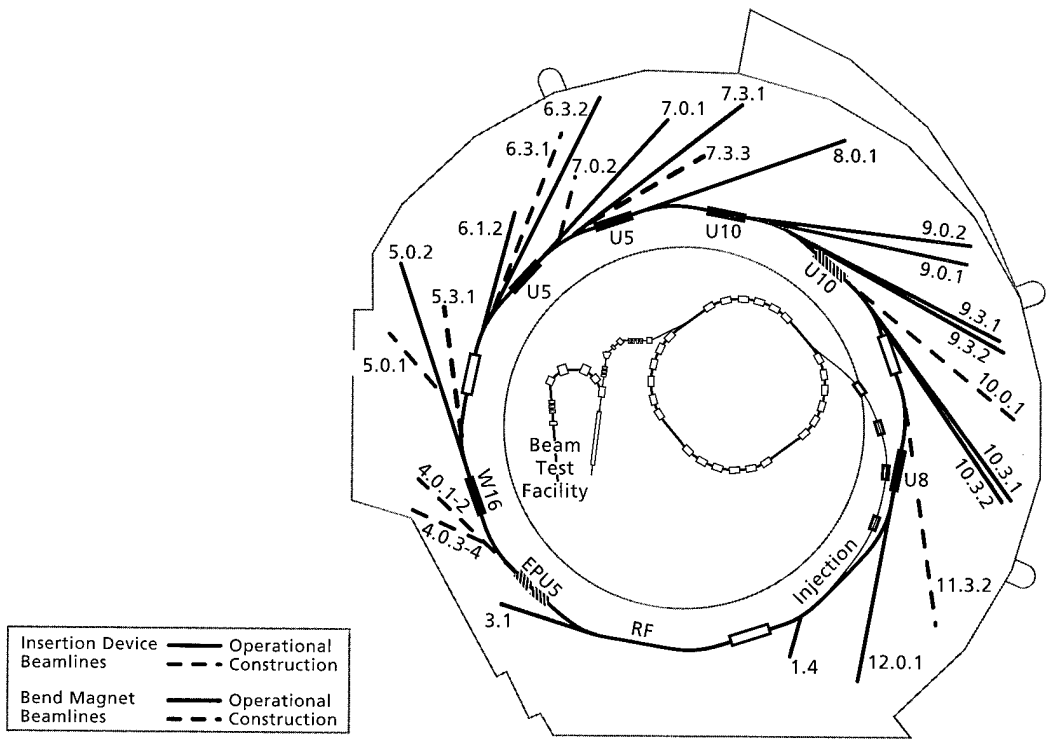
USING THE ADVANCED LIGHT SOURCE

The ALS, a Department of Energy national user facility, welcomes researchers from universities, industry, and government laboratories. Qualified users have access either as members of participating research teams (PRTs) or as independent investigators. PRTs (groups of researchers with related interests from one or more institutions) construct and operate beamlines and have primary responsibility for experiment endstation equipment. They are entitled to a certain percentage of their beamline's operating time according to the resources contributed by the PRT. Through a proposal process, the remaining beamtime is granted to independent investigators, who may provide their own endstation or negotiate access to a PRT-owned endstation.

The ALS does not charge users for beam access if their research is non-proprietary. Users performing proprietary research are charged a fee based on cost recovery for ALS usage. All users are responsible for the day-to-day costs of research (e.g., supplies, phone calls, technical support).

The ALS storage ring is designed to run at energies within the range from 1.0 GeV to 1.9 GeV, allowing flexibility for user operations. 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 10 keV. Bend magnets produce radiation from the infrared to about 12 keV.

The ALS is capable of accommodating approximately 46 beamlines and more than 100 endstations. The first user beamlines began operation in October 1993, and there were 18 operating beamlines with several more under construction by the summer of 1997.



BEAMLINES 1997–1998*

Beamline	Source	Areas of Research	Energy Range	Monochromator	Available
BTF	ALS linac	Beam Test Facility	50 MeV electrons	None	Now
1.4	Bend magnet	Infrared spectromicroscopy, surface science, pump-probe experiments	0.05–1 eV	FTIR	Now
3.1	Bend magnet	Diagnostic beamline	200–280 eV	Mirror/filter	Now
4.0.1-2	EPU5 elliptical polarization undulator(s)	Magnetic spectroscopy	100–2000 eV	PGM	1998
4.0.3-4		Magnetic microscopy	100–1600 eV	SGM	1998
5.0.1	W16 wiggler	Monochromatic protein crystallography	7–14 keV	Curved crystal	1998
5.0.2	W16 wiggler	Multiple-wavelength (MAD) and monochromatic protein crystallography	3.5–14 keV	Double crystal	Now
5.3.1	Bend magnet	Scanning transmission x-ray microscopy	250–750 eV	SGM	1998
6.1.2	Bend magnet	High-resolution zone-plate microscopy	500–800 eV	Zone plate linear	Now
6.3.1	Bend magnet	Calibration and standards, EUV/soft x-ray optics testing, solid-state chemistry	100–2000 eV	VLS-PGM	1998
6.3.2	Bend magnet	Calibration and standards; EUV optics testing; atomic, molecular, and materials science	50–1300 eV	VLS-PGM	Now
7.0.1	U5 undulator	Surface and materials science, spectromicroscopy, spin resolution, photon-polarization dichroism	60–1000 eV	SGM	Now
7.0.2	U5 undulator	Coherent optics experiments	200–650 eV	None	1997
7.3.1.1	Bend magnet	Magnetic spectromicroscopy	260–1500 eV	SGM	1997
7.3.1.2	Bend magnet	Surface and materials science, micro x-ray photoelectron spectroscopy	260–1500 eV	SGM	Now
7.3.3	Bend magnet	Materials science, x-ray microdiffraction, x-ray absorption spectroscopy, sub-picosecond time-resolved x-ray diffraction, deep-etch x-ray lithography (LIGA)	3–12 keV	White light, four crystal	1997
8.0.1	U5 undulator	Surface and materials science, spectromicroscopy, imaging photoelectron spectroscopy	60–1000 eV	SGM	Now
9.0.1	U10 undulator	Atomic, molecular, and optical physics; high-resolution gas-phase spectroscopy**	20–320 eV	SGM	Now
9.0.2.1	U10 undulator	Chemical reaction dynamics, photochemistry	5–30 eV	None	Now
9.0.2.2	U10 undulator	High-resolution photoelectron and photoionization spectroscopy	5–30 eV	Off-plane Eagle	Now
9.3.1	Bend magnet	Atomic, molecular, and materials science	2.2–6 keV	Double crystal	Now
9.3.2	Bend magnet	Chemical and materials science, circular dichroism, spin resolution	30–1500 eV	SGM	Now
10.0.1**	U10 undulator	High-resolution atomic, molecular, and optical physics; photoemission of highly correlated materials	20–320 eV	SGM	1998
10.3.1	Bend magnet	X-ray fluorescence microprobe	3–20 keV	White light, multilayer	Now
10.3.2	Bend magnet	X-ray optics development, materials science	3–12 keV	White light, four crystal	Now
11.3.2	Bend magnet	EUV lithography	50–1300 eV	VLS-PGM	1998
12.0.1.1	U8 undulator	Surface and materials science, spectromicroscopy	60–320 eV	VLS-PGM	Now
12.0.1.2	U8 undulator	EUV lithography optics testing, interferometry	60–320 eV	VLS-PGM	Now

*The most current information on ALS beamlines is available on the World Wide Web (http://www-als.lbl.gov/als/als_users_bl/bl_table.html).
**The atomic and molecular science beamline will move to 10.0.1 in early 1998.

ALS Storage Ring Parameters

Parameter	Value
Beam particle	Electron
Beam energy	1.0–1.9 GeV
Injection energy	1.0–1.5 GeV
Beam current multibunch mode two-bunch mode	 400 mA 2 × 20 mA
Filling pattern (multibunch mode)	287 bunches
Bunch spacing multibunch mode two-bunch mode	 2 ns 328 ns
Circumference	196.8 m
Number of straight sections	12
Radio frequency	500 MHz
Beam size in straight sections, rms	200 μm horiz. × 20 μm vert.
Natural emittance	3.5 nm-rad
Energy spread ($\Delta E/E$, rms)	8×10^{-4}

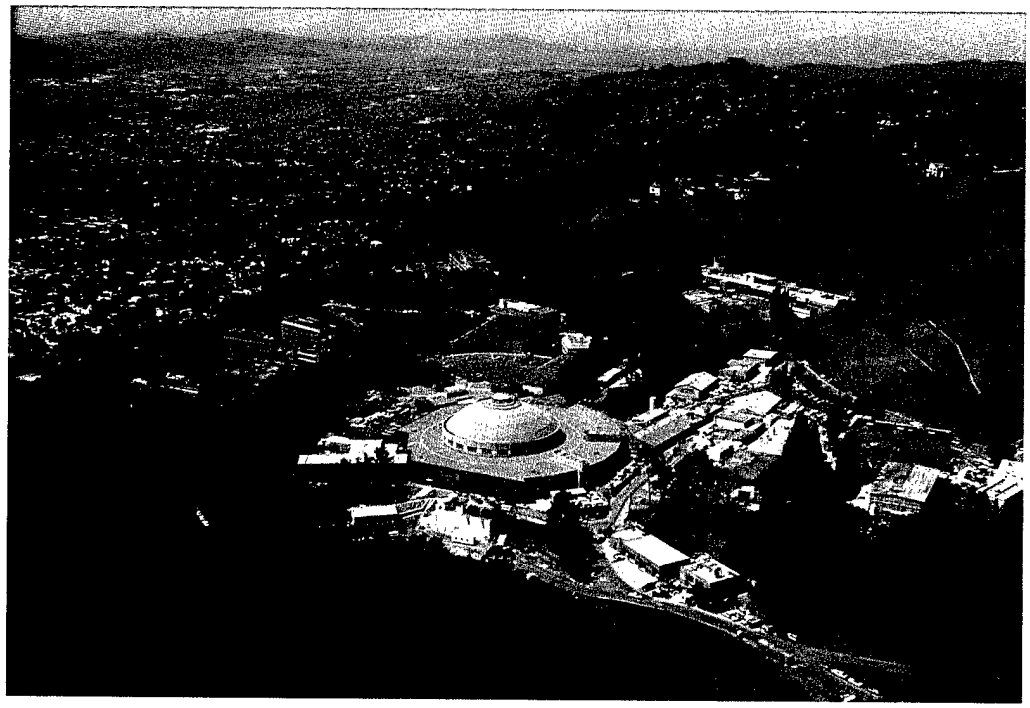
Parameter	Value at 1.5 GeV	Value at 1.9 GeV
Beam lifetime multibunch mode* two-bunch mode	 ~5 hours at 400 mA ~2.5 hours at 40 mA	 ~4.5 hours at 400 mA ~2.5 hours at 40 mA
Horizontal emittance	4 nm-rad	6 nm-rad
Vertical emittance (nominal)**	< 0.1 nm-rad	< 0.1 nm-rad

*Fills in multibunch mode typically occur every four hours for the convenience of our users.
**Vertical emittance can be deliberately increased to improve beam lifetime.

INSERTION DEVICES FOR 1997–1998

Device	Beamline	Status	Energy Range (at 1.5 GeV)	Energy Range (at 1.9 GeV)	Period Length	Number of Periods	Operating Gap Range	Peak Effective Field Range
U5 Undulator	8.0	Operational	50–1900 eV	80–3000 eV	5.0 cm	89	1.4–4.5 cm	0.85–0.10 T
U5 Undulator	7.0	Operational	50–1900 eV	80–3000 eV	5.0 cm	89	1.4–4.5 cm	0.85–0.10 T
U8 Undulator	12.0	Operational	18–1200 eV	30–1900 eV	8.0 cm	55	2.5–8.3 cm	0.80–0.07 T
U10 Undulator	9.0	Operational	5–950 eV	8–1500 eV	10.0 cm	43	2.4–11.6 cm	0.98–0.05 T
U10 Undulator	10.0	Construction in Progress	8–950 eV	12–1500 eV	10.0 cm	43	2.4–11.6 cm	0.80–0.05 T
EPU5 Elliptical Polarization Undulator	4.0	Design and Construction in Progress	60–1000 eV*	100–1500 eV*	5.0 cm	37	1.45–5.5 cm	0.79–0.10 T (vertical field) 0.54–0.10 T (horizontal field)
W16 Wiggler	5.0	Operational	5–13 keV	5–21 keV	16.0 cm	19	1.4–18.0 cm	2.1–0.03 T

*Elliptical polarization mode.



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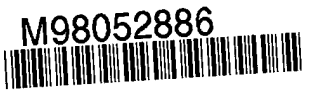

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