ADVANCED LIGHT SOURCE

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University of California at Berkeley, California 94720
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 laboratories. Its building incorporates the dome that once housed the 184-inch Cyclotron built by the Laboratory’s founder E.O. Lawrence.

The ALS Activity Report is designed to share the breadth, variety, and interest of the scientific program and ongoing R&D efforts in a form that is accessible to a broad audience. Recent research results are presented in six sections, each representing an important theme in ALS science. These results are designed to demonstrate the capabilities of the ALS, rather than to give a comprehensive review of 1995 experiments. Although the scientific program and facilities report are separate sections, in practice the achievements and accomplishments of users and ALS staff are interdependent. This user-staff collaboration is essential to help us direct our efforts toward meeting the needs of the user community, and to ensure the continued success of the ALS as a premier facility.
Scientists from around the world find tools for their research at the ALS; many also bring their own experiment chambers designed to make optimum use of ALS light. Nearly 100 times brighter than existing second-generation synchrotron light sources and 100 million times brighter than conventional x-ray sources, the ALS has illuminated investigations from the inner structures of atoms and crystals to the best means of fabricating high-quality semiconductor devices. The advantages of a high-brightness source for certain key areas of research draw scientists with similar interests, thus facilitating an exchange of knowledge that moves these areas forward. The pages ahead describe scientists' work in several such areas and give a sampling of what is possible with this exceptional tool.
Activity at the Advanced Light Source is driven by the cooperation of large numbers of people—a process that is evident at any beamline. From first plans to first light and reliable operation, beamlines require the knowledge and skills of engineers, scientists, and technicians. Beamlines, like the machine itself, continue to grow and add capabilities as a research environment grows around them and new needs arise.
Research at the Advanced Light Source (ALS) spans the full spectrum from basic to applied work in a wide range of scientific fields, providing a rich ground for cross-fertilization and collaboration. A broad base of knowledge and a wide variety of skills come into play as expert ALS staff join researchers from academia, industry, and government in bringing their scientific ideas to life.

The ALS provides an ever-growing set of tools for the research community. At its heart are the brightest ultraviolet and soft-x-ray beams available in the world, from one of the world’s first third-generation synchrotron light sources. In 1995, many beamlines and endstations finished their commissioning phases and became available for research, leading to a significant increase in the number of users and scientific results. New construction also continued, with one insertion device and several beamlines coming into service.

The Scientific Facilities Initiative, funded by Congress in October 1995, spurred acceleration in the construction of beamline instrumentation for users. Furthermore, it allowed the ALS to move to a full operations schedule and to increase its technical support to users. These developments have produced rising demand for beamtime, as well as increasing interest from industry in partnerships for research and development.
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Developing the Right Material for the Job

Researchers studying materials make up a generous portion of the ALS user community, bringing ALS beams to bear on a broad range of problems. Some materials scientists use ALS light to analyze the structure of materials, probing such characteristics as the arrangement of atoms in crystals or the properties of interatomic bonds. Others seek new methods of preparing high-quality materials, such as more efficient semiconductors. Still others are developing tools and methods for fabricating the next generation of integrated circuits for the computer industry.

Materials scientists find the ALS a particularly useful tool for several reasons. First, light in the wavelength range produced by the ALS has the right energies for studying the electronic and chemical structure of many important materials. Being able to select the optimum photon energy for an experiment lets researchers zero in on distinct phenomena, such as electronic gaps in semiconductors or bonding at surfaces and interfaces. Second, to examine materials on a local scale, it is necessary to have spatial resolution, and in today’s technologies the relevant scale is often measured in fractions of a micron. The high brightness of the ALS allows the x-ray beams to be focused to sub-micron spot sizes, while retaining sufficient flux to perform traditional spectroscopy. This combination of spectroscopy and microscopy is known as spectromicroscopy, and it is an area of intense activity at the ALS.

Getting the Blues

The semiconductor gallium nitride (GaN) has attracted widespread attention as a material for use in bright blue light-emitting diodes (LEDs), laser diodes, and other electronic devices. It emits a pure and intense blue that completes the spectrum of available colors, making full-color LED-based displays possible. Researchers from LBNL’s Materials Sciences Division are developing a preparation method for thick GaN crystals, using a hard-x-ray fluorescence microprobe to test the quality of the crystals they make. Because of the high brightness of the ALS, the microprobe receives enough flux to measure the concentration of a single element with high accuracy in a spot only 2 μm square.

The microprobe images showed that nickel and iron contaminants were highly mobile and had agglomerated along grain boundaries (boundaries between individual crystallites in the sample). Such groupings of contaminant atoms can cause short circuiting across the crystal. Having a clear view of what’s going on inside the material will help the researchers optimize the crystal growth process to make high-quality GaN.
**Iron**

Gallium nitride (GaN) is a new semiconductor that fills the need for a material that emits a bright and stable blue light. The fluorescence microprobe images above show the spatial distribution of typical contaminants in a thick GaN sample. The contaminants in the crystal had agglomerated along grain boundaries (boundaries between individual crystallites). Such information is helping researchers test new methods of preparing high-quality GaN.

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**Unraveling the Fire-Proof Fiber**

Successful manufacturing processes are often developed without a detailed knowledge of the chemical processes involved. To better understand how heat treatment made a material flame resistant, a maker of fire-proof polymer fibers sought insight into the chemistry involved through spectromicroscopy at the ALS. The analysis revealed the chemical changes in the fiber that occurred with heat treatment. Understanding how the heating process renders the polymer impervious to flame will aid the development of other flame-resistant materials.

A scanning transmission x-ray microscope produced images of cross-sectional samples from a polyacrylonitrile fiber, showing chemical states in the “fresh” polymer and at early and late stages of heat treatment. Spectromicroscopy revealed not only the chemical changes that took place but also the locations of those changes. By analyzing changes in the absorption of x-ray light in the energy range corresponding to carbon–nitrogen triple bonding (C≡N), the researchers observed that C≡N bonds were broken in the center of the fiber as the heat treatment progressed.

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**Polyacrylonitrile fiber research conducted by scientists from Asahi Chemical Company and the ALS using the scanning transmission x-ray microscope at Beamline 7.0.**
Cross sections of a polymer (polyacrylonitrile) fiber in the early (left) and late (right) stages of heat treatment to impart fire resistance. These images were obtained by transmission photoabsorption spectromicroscopy, which specifies chemical states by x-ray absorption. The lighter areas are the portions of the fiber that absorbed less x-ray light in the energy range corresponding to carbon–nitrogen triple bonds (C\(\equiv\)N) and hence contained less C\(\equiv\)N bonding. Comparison of the two images thus reveals that the amount of C\(\equiv\)N bonding has decreased in the center of the fiber with heat treatment. The vertical striations in the early-stage sample are wrinkles (i.e., variations in thickness that occurred in slicing the sample rather than variations in chemical state).

**X Rays Enhance Annealing**

Just as the goal of many an inventor has been to build a better mousetrap, a major goal of materials scientists developing new semiconductors is to build a better crystal. Semiconductors are the basic materials for diodes, transistors, and most other elements of integrated circuits. Production of these circuit elements requires that a substrate such as silicon be implanted with dopants—atoms of another element that alter the conductivity of the semiconductor. Ideally, a dopant should be distributed through the substrate as single atoms, substituting for substrate atoms in a near-perfect lattice structure. Unfortunately, the process of implanting dopants causes damage to the crystal lattice, which must be repaired by a heating process called thermal annealing. A group of researchers has used the high flux of the ALS to make annealing more effective, yielding doped crystals with a more perfect lattice.

The researchers implanted silicon wafers with zinc dopant ions, producing surface damage in the process. They irradiated some of the samples with x rays for several hours and left others untreated. Next they thermally annealed all the samples at 535°C to repair the damage caused by implantation. They found that the irradiated wafers reorganized into single-crystal forms with far fewer defects than the non-irradiated control samples. This improvement in crystal quality could make previously impractical semiconductors usable and improve the stability of existing semiconductors.

*X-ray pre-annealing research conducted by scientists from LBNL's Materials Sciences Division using the fluorescence microprobe at Beamline 10.3.1.*
Spectra showing the increase in crystal quality resulting from the use of x-ray pre-annealing. Two wafers were implanted with zinc atoms, a process that damages the crystal lattice. One wafer was simply annealed to repair the damage; the other was irradiated with x rays before annealing. The $\chi$ value is a measure of imperfection in the crystal's lattice; hence, a low $\chi$ profile indicates a higher-quality crystal.

**Exploring the Limits of Solubility**

Today's materials scientists often know what combination of elements they need to make a material with certain properties, but getting these puzzle pieces to fit together can be problematic. For example, a semiconductor with a desired lattice structure and specific conductive and magnetic properties can be produced by adding the right amount of an additional element (a dopant) to the initial substrate, but the solubility of dopant atoms limits how much of a particular dopant can be added. Thus, potentially useful materials with higher dopant concentrations cannot be produced. To find out if the limit of solubility in one class of semiconductors (the dilute magnetic semiconductors) is related to the arrangement of electrons, researchers at the ALS studied the semiconductors' electronic structure.

Through x-ray absorption spectroscopy, the investigators examined the electronic structure of transition metal dopants in zinc selenide (ZnSe) and zinc sulfide (ZnS). Like gallium nitride, these semiconductors emit blue light. The
researchers wanted to know why dopant solubility decreases as transition metals with higher atomic numbers, from manganese to iron to cobalt to nickel, are implanted. Along this progression, the dopant atoms contain progressively more electrons in the 3d energy band. The study provided a detailed view of the energy band structure in these compounds, showing that electrons in the 3d band actually occupy multiple sub-bands, but that they occupy progressively fewer bands across the series of transition metals. As atomic number increases, the elements' electrons behave more like core (inner-shell) electrons, decreasing their tendency to form bonds with other atoms; this causes the observed decrease in solubility. Understanding the importance of electronic structure in dopant solubility can guide future attempts to increase dopant concentrations in these compounds.

Studies of the electronic structure of zinc sulfide (ZnS) semiconductors, materials that emit blue light, may open the door for new semiconductor variants with specific properties. These soft x-ray absorption spectra for ZnS with varying amounts of iron (left) and cobalt (right) dopants show the decrease in the number of sub-bands with increasing occupancy of the 3d energy band.
Collaborations in Semiconductor Research

In the last 30 years, the semiconductor industry has successfully miniaturized integrated-circuit (IC) chip technology enough to squeeze thousands more transistors onto a chip. To help maintain the miniaturization momentum, the ALS is pursuing ways to address some of the technological challenges faced by the industry as circuit sizes shrink. For example, in collaboration with semiconductor manufacturers, the ALS is developing the analytical techniques needed for research towards the next generation of microcircuit devices. The ALS's strength in materials research and its proximity to Silicon Valley make it well suited to such cooperative efforts.

Integrating Efforts

A new collaborative research agreement involving Intel, the ALS, and LBNL's Center for X-Ray Optics (CXRO) will address some of the technological challenges faced by the semiconductor industry in advancing the state of the art in integrated-circuit performance. The research will focus on two areas identified as major "industry-wide" concerns by the Semiconductor Industry Association: new fabrication techniques that will allow the minimum feature size on integrated circuits to be reduced from the present level (approximately 0.35 μm) to 0.10 μm, and improved methods for silicon wafer surface materials analysis.

One contender in the pursuit to shrink the size of circuit features and the spaces between them is fabrication by extreme ultraviolet (EUV) lithography. The development of EUV lithography depends on fabricating optical surfaces with contour and roughness considerably better than what is available today and on coatings with high reflectivity at shorter (EUV) wavelengths. This requires new test procedures (interferometry) with improved accuracy (smaller wavefront error), operating at the wavelength at which the coated optics are intended to be used. An EUV interferometry endstation on Beamline 12.0 will be used to test the surface figure (i.e., shape and roughness) of multilayer coated optics and optical systems, crucial elements in the EUV lithography process. Information gleaned from this research will enhance CXRO's optics program as well as the semiconductor industry's future lithography plans.

A key technique for surface materials analysis is soft x-ray spectromicroscopy, the combination of the traditional macro-techniques of x-ray absorption near-edge structure (XANES) and x-ray photoelectron spectroscopy (XPS) with microscopy. As the minimum feature size of integrated circuits shrinks, obtaining local chemical information becomes more critical but also more difficult. Analytical efforts will focus on two situations common to semiconductor manufacture with shrinking feature sizes: one where a defect (such as a contaminant particle, organic residue,
etc.) is present and chemical information is required in order to localize the defect's origin in the fabrication process, and another where a material used in fabrication alters its behavior when localized in ever smaller areas. In each of these cases, the limitations of traditional laboratory instrumentation are becoming increasingly problematic, but the new capabilities and techniques of spectromicroscopy may provide a way forward. The ALS is collaborating with the semiconductor industry to develop several new spectromicroscopes to meet their needs, including a special scanning photoelectron microscope (see "Experimental Systems," p. 52).

**Improving Analytical Techniques**

The semiconductor industry requires nondestructive, quantitative analysis of surface impurities on the silicon wafers used to manufacture integrated circuits (ICs). The most advanced analytical technique to date is total-reflection x-ray fluorescence (TXRF). This approach involves irradiating a sample with x rays from a conventional source and measuring the wavelength and intensity of the resulting fluorescence x rays to identify surface contaminants and their concentrations. However, advanced ICs now on the drawing boards will require about two orders of magnitude greater sensitivity than conventional x-ray sources can provide. The ALS is cooperating with the Stanford Synchrotron Radiation Laboratory (SSRL) to investigate how much better synchrotron radiation can do.

The group at SSRL has pioneered the use of synchrotron-radiation-based TXRF and is building dedicated instrumentation for this work at an SSRL wiggler beamline. The work at the ALS has a different direction: first, to test a system with conventional geometry on a bend magnet beamline (Beamline 10.3.2), and second, to produce a theoretical framework for understanding the ultimate sensitivity of the technique. Initial experiments have been performed in the horizontal scattering geometry with highly contaminated, calibrated test wafers, confirming the validity of our model. The model shows that, although the ultimate sensitivity can be obtained using the horizontal scattering geometry, practical considerations of the photon flux required to do an experiment in a reasonable time indicate that an optimized vertical scattering geometry is far superior for a bend magnet source. This work will be of great importance if we go on to the next stage, construction of a TXRF endstation, which will depend on customer demand.

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*Total-reflection x-ray fluorescence research conducted by scientists from the Pohang University of Science and Technology, Korea; Stanford Synchrotron Radiation Laboratory; LBNL's Center for X-Ray Optics; and the ALS at Beamline 10.3.2.*

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*Taking advantage of total-reflection x-ray fluorescence (TXRF) analysis of impurities on silicon wafers requires optimizing the relative orientation of sample and light source. Models developed at the ALS indicate that the vertical scattering geometry shown, with an almost in-plane detector, will be much more effective than a traditional horizontal geometry.*
Atoms are the simplest physical systems for which we can test our fundamental understanding of the electronic structure of matter. Thus, careful investigations on the atomic scale can provide a basis for greater understanding of the properties of matter on larger scales.

The prevailing theory of physics on the atomic scale is quantum mechanics, which describes particles' behavior using differential equations known as wave equations. These equations rapidly become complex when more than one particle is involved; in fact, equations describing mutual interactions among three or more particles (as in helium or ionized lithium) cannot be solved exactly. To overcome this problem, atomic theorists have put forth a variety of approximations for use in solving wave equations for "many-body" systems. Validating and refining these approximations requires sensitive experiments that compare the actual behavior of systems with their behavior as predicted by theory. Researchers at the ALS have made excellent use of its high flux, brightness, and energy resolution to gain increases in data quality while avoiding prohibitive decreases in data collection speed or information yield.

Helium at Record Resolution

Researchers testing theories in atomic physics often require extremely high spectral resolution, since the ability to distinguish closely spaced features in a spectrum can make the difference between successful and inconclusive tests of quantum-mechanical approximations. One group using photoabsorption spectroscopy to study helium (the simplest atom for which approximations are required) achieved a new record in spectral resolution using careful experimental methods, high-precision experiment chamber design and fabrication, and fine beamline tuning.

This spectrum shows three helium Rydberg series and demonstrates a resolving power of ~64,000. This is six times higher than was predicted for the beamline and four times higher than the best previous resolving power in the 60–79 eV energy range. All three series represented here stem from double-excitation events in which one electron is excited to the N = 2 and the other to a higher (n = 4, 5, etc.) quantum state.
Using 60–79 eV photons, the group excited helium atoms by double excitation, a process whereby electron-electron interaction (also known as electron correlation) allows one photon to excite both electrons to higher-energy states. The same photon energies can also cause single ionization, in which one electron absorbs all of the photon's energy and leaves the atom. Quantum-mechanical interference between double excitation and single ionization influences the peak energies, line shapes, and other characteristics of the double-excitation resonance spectrum. This detailed spectrum can hence be studied to test key quantum-mechanical approximations for correlated-electron systems.

**Hollow Lithium**

**Results an Excellent Fit**

"Hollow" lithium atoms provide an example of the extremely complex behavior that can occur in an atom with only three electrons. In a recent experiment making use of the ALS's high-brightness beams, theoretical calculations predicting this complex behavior received their first definitive test.

Hollow lithium is produced by exciting all three of lithium's electrons to higher-energy orbitals, leaving its inner (K) shell empty. An inherently unstable state, hollow lithium decays rapidly into a lithium ion (Li⁺ or Li⁺⁺), ridding itself of extra energy by ejecting one or two electrons. The resulting ion can have a variety of different internal energies, depending upon the electrons' final states. Since the electrons can also be excited to a variety of high-energy orbitals, the possible transitions within this system are numerous, and excellent spectral resolution is required to resolve the final states. Previous experimental work on hollow lithium has provided information on lithium's hollow states but not about its final states. Now, using high-resolution photoelectron spectroscopy, researchers have explored the final states in detail: agreement between experiment and theory is excellent.

The excellent agreement between this autoionization spectrum and theoretical R-matrix calculation—both giving the probability that hollow lithium will decay to the Li⁺(1s3s 3S) ionic state—strongly supports the validity of the theoretical calculations. The measured spectrum's resolution exceeds those of previous efforts because the undulator beam's high brightness allowed researchers to narrow the monochromator and spectrometer slits, thereby increasing resolution without a damaging loss of flux.

**Experiment conducted by scientists from Université de Paris-Sud and the ALS, using the Wuilleumier group cylindrical mirror analyzer and lithium oven at Beamline 9.0.1. R-matrix calculations by L. VoKy, published in Diehl et al. Phys. Rev. Lett. 76, 3915 (1996).**
Some of the work going on in many-electron systems focuses not on verifying experimental calculations, but on observing never-before-considered phenomena. This was the case in an experiment involving electron recapture and subsequent autoionization in argon atoms.

The researchers created an electron recapture situation by using ALS photons to eject electrons from the 2p orbitals of argon, such that they emerged with low kinetic energies (and thus slow speeds). The result of this is Auger decay, with one valence electron dropping to fill the 2p hole and another leaving the atom with the resulting excess energy. The Auger electron, with its higher kinetic energy, overtakes the slower photoelectron, suddenly subjecting it to the pull of a larger net positive charge from the argon nucleus. This additional pull can recapture the photoelectron, pulling it back into a high-energy orbital.

By measuring the Ar⁺ and Ar⁺⁺ ions generated as they varied the incoming photon energy, the researchers determined that when the photon energy was barely sufficient to eject electrons from argon’s 2p orbitals, the probability of recapture was 100%. This much had been examined in previous experiments, but the researchers broke new ground when they examined the possibilities for what might happen following electron recapture. According to their measurements, 67% of the recaptured electrons were re-emitted from their atoms (autoionization), carrying excess energy as kinetic energy, while the other 33% dropped to a lower-energy orbital and emitted their excess energy as a photon (fluorescence). This new look at argon’s detailed ionic spectrum was possible because of the high intensity and high spectral resolution of the undulator x rays used.

Research conducted by scientists from the University of Nebraska and the ALS, using the Nebraska mass analyzer endstation at Beamlines 6.3.2 and 9.0.1.

This spectrum of Ar⁺⁺ yield from photoionized argon marks the first time that the re-emission of electrons captured in a Auger process has been addressed by experiment or theory. The purple area represents the expected Ar⁺⁺ yield assuming 100% electron recapture at the L₂ and L₃ thresholds (where photon energy is exactly that required to eject electrons from 2p orbitals). The gold area, representing the disagreement between this assumption and the experimental data, indicates that 100% recapture does occur at threshold, but that 67% of the recaptured electrons are then re-emitted in an autoionization process rather than decaying by fluorescence.
The x-ray microscope provides an excellent complement to other microscopy techniques, offering biologists a precise method for examining samples in near-natural environments. X-ray microscopes provide better resolution than visible-light microscopes without the extensive sample preparation required by electron microscopy. Their ability to image more than the surface of a sample adds depth to information gained from sources such as atomic force microscopes.

X-ray microscopy works in much the same way as visible-light microscopy, except that it uses shorter-wavelength light. While shorter wavelengths make higher resolutions possible, soft x rays in a specific wavelength range, known as the “water window,” are particularly useful for studying cell structure because they are absorbed by carbon but not by water. Thus, many carbon-containing structures within a cell, such as plastids, are more x-ray dense (absorb more x rays) in this range than the surrounding cytoplasm. This difference, along with the ability to resolve depth in thick samples, makes x-ray microscopes ideal for investigating the secrets of the cell.

Focus on Malaria

Among infectious diseases, malaria is one of the leading causes of death worldwide. To halt its spread, scientists around the globe are studying the life cycle and the possible weaknesses of the parasite that causes malaria. Biological microscopy at the ALS has given scientists views of malaria-infected blood cells that were not possible with other types of microscopy.

Transmitted from human to human by the female *Anopheles* mosquito, the malaria parasite matures inside human red blood cells for several stages of its life cycle. Light microscopy has provided limited views of the different stages, but understanding the details of parasite development calls for higher resolution than even the best visible-light microscopes can provide. At the ALS, researchers have collected a series of x-ray images that give new insight into the effects of blood cell abnormalities on the shape of developing malaria parasites. The images should provide clues to the parasites' weaknesses—clues that could one day be exploited in developing new treatments for malarial infection.

Malaria research conducted by investigators from the Center for X-Ray Optics and the Life Sciences Division of LBNL using the XM-1 transmission x-ray microscope at Beamline 6.1.
Visible-light (phase contrast, left) and x-ray microscope (right) images of the malaria parasite (Plasmodium falciparum) in red blood cells. The x-ray images give a clearer view of the parasite's development than visible-light images provide. Upper row: red blood cells with early-stage parasites; lower row: doubly infected red blood cells with mature parasites.
**Exploring the Properties of Magnetic Thin Films**

In recent years there has been a general trend toward miniaturization in all computer components. Miniaturization of the read heads for computer hard disks involves not only changes in scale, but changes in the type of technology used. Read heads hover just over the surface of a disk while the magnetized bits spin beneath them, and the heads must convert the information encoded in the bits into electrical signals. In older read heads, the bits' magnetic fields induce a current in a small conducting coil. The newer heads instead use magnetoresistive materials, whose electrical resistance changes with the magnetic field to which they are exposed.

Although magnetoresistive read heads are already much smaller than inductive devices, even more sensitive materials are required to continue increasing the density of stored data. Promising materials include multilayer films that exhibit giant magnetoresistance (GMR) many times stronger than the iron/nickel alloy now commonly used.

The interest in GMR materials is part of a larger field of study which includes a host of magnetic films, multilayers, and alloys. The ALS produces bright photon beams that span the key energy ranges for many of these materials. High brightness is an advantage for researchers who need large signals from low-yield techniques, high spectral resolution without sacrificing too much signal, or high flux for experiments with tight physical tolerances.

**Strange Behavior for a Semiconductor**

Giant magnetoresistance (GMR) is normally observed only in structures with alternating layers of a magnetic material, such as cobalt, and a non-magnetic metal, such as copper, each layer a few tens of angstroms thick. Thus, researchers at Argonne National Laboratory were surprised when, in 1993, they observed GMR in an iron/silicon multilayer even though silicon is a semiconductor rather than a metal. Electron microscopy experiments suggested that the non-magnetic layer was actually an iron-silicon compound (iron silicide) formed by intermixing of iron and silicon atoms during the preparation process, but it was not possible to determine whether the iron silicide was a metal or a semiconductor.

A group working at the ALS resolved the conflict by using two forms of soft-x-ray fluorescence spectroscopy to measure the energies of electron orbitals in the iron silicide. These measurements were useful because the key difference between metals and semiconductors is that semiconductors have an energy gap (called a band gap) between their occupied and unoccupied orbitals, whereas metals have no such gap. The spectroscopy experiments demonstrated the absence of a band gap and, hence, the metallic nature of the iron silicide.

Fluorescence (a photon-in, photon-out technique) was the right tool for this experiment because fluorescent photons...
These soft-x-ray fluorescence spectra (blue) and absorption spectra (red, measured using fluorescence yield) map the occupied and unoccupied orbitals, respectively, of an iron silicide layer in a giant-magnetoresistance multilayer. Comparison spectra for crystalline silicon, a semiconductor, show a clear band gap between the two sets of orbitals; the absence of such a gap in the iron silicide layer demonstrates that it is a metal.

What Changes in Thinner Layers?

The thickness of layers in a giant-magnetoresistance (GMR) material is a variable of keen interest to researchers who want to miniaturize GMR-based devices. It is possible to grow thin films of magnetic materials only a few atoms thick, but these films can behave differently from bulk materials. This is partly because as atoms are deposited slowly on a substrate, the first several atomic layers tend to arrange themselves according to the crystal-line structure of the substrate (pseudomorphic growth). This arrangement has higher energy than their ordinary bulk structure, a situation known as pseudomorphic strain.

A group of researchers working at the ALS investigated whether pseudomorphic strain alters a phenomenon known as invar quenching, whereby iron/nickel (FeNi) alloys suddenly lose their magnetic properties when the...
concentration of iron in the alloy exceeds a certain percentage (about 75% in bulk samples). They used magnetic x-ray linear dichroism, taking photoelectron spectra from thin layers of FeNi with various iron concentrations. By comparing spectra taken from each sample with two opposite magnetizations, they could gauge the magnetic properties of the different samples. They concluded that invar quenching does occur in pseudomorphic layers, but that it appears at a lower iron concentration than in bulk samples.

Magnetic x-ray linear dichroism experiments conducted by scientists from Lawrence Livermore National Laboratory, Pennsylvania State University, and the ALS, using the x-ray photoelectron diffractometer endstation at Beamline 7.0.

These photoelectron spectra from iron/nickel alloys with 50% (top) and 70% (bottom) iron concentrations demonstrate invar quenching in films about 5 atomic layers (10 Å) thick. In the 50% iron alloy, the large peaks in the difference spectrum show a high degree of magnetic asymmetry, which is almost entirely missing from the 70% iron spectrum (note the magnified difference scale). These results are similar to those for bulk samples except that the loss of magnetic asymmetry occurs at a lower concentration of iron.
Isolating Elemental Magnetic Behavior

A key property for materials to be used in magnetic storage devices is their ability to sustain a given magnetization. This ability is often gauged by measuring the material's hysteresis loop, the closed path traced by its magnetization as a function of an applied magnetic field. One phenomenon sometimes used to measure magnetization is called magneto-optical rotation (MOR): the degree to which the polarization plane of a beam of light rotates when the beam passes through or reflects from a magnetized medium.

Researchers working at the ALS have taken the first measurements of MOR hysteresis loops using soft x rays. Soft x rays can penetrate deep into a material to obtain information from buried layers and interfaces. The soft x-ray spectrum also includes many absorption edges for important magnetic materials; tuning the incoming photon energy to these edges can produce much larger MOR effects than are observed in other spectral regions. In the ALS experiment, measurements at absorption edges allowed researchers to measure separate hysteresis loops for iron and chromium in an iron/chromium multilayer. Two characteristics of the ALS bending magnet beam were also important to the experiment's success: a very high degree of linear polarization to allow sensitive measurements of the degree of MOR, and high brightness to deliver sufficient flux to a polarizer with limited angular acceptance.

Magneto-optical rotation experiments conducted by researchers from LBNL's Center for X-Ray Optics, using their tunable soft x-ray polarimeter at Beamline 6.3.2.

These element-specific hysteresis loops for iron (top) and chromium (bottom) in an iron/chromium multilayer reveal that chromium has a significant magnetic moment in the multilayer—it usually has none—with the opposite orientation of the iron moment. The hysteresis loops were recorded by measuring the magneto-optical rotation of linearly polarized x rays reflecting from the multilayer sample.
New Tools Make New Investigations Possible

The scientific method is based on forming hypotheses and then devising experiments to test these hypotheses—yet what can researchers do when they lack the tools to perform the necessary experiments? Before the advent of third-generation synchrotron light sources such as the ALS, certain experiments were difficult or impossible to perform, leaving some hypotheses without a suitable means of testing. Now, however, the high brightness, tunability, and other characteristics of ALS light are making it possible to evaluate both old and new hypotheses which could not otherwise be tested.

What makes the ALS such an improvement over existing tools? Researchers using spectroscopy techniques would cite its high brightness, which makes high spectral resolution available without a prohibitive loss of photon flux. Those using low-yield techniques such as fluorescence spectroscopy appreciate both high flux and brightness, which increase the amount of data they can acquire within a given time. Researchers who need tunability over a broad range of photon energies can widen or narrow the undulator gap for their beamline without disrupting experiments at other beamlines. For some experiments, even the high degree of linear polarization of ALS photon beams (related to the electron beam’s small vertical size and low vertical emittance) can make a critical difference.

New Paths to Ozone Formation

The photochemistry of ozone has been a matter of concern in recent years, as scientists have explored the processes by which ozone is formed and destroyed in the earth’s protective ozone layer. Each new process that is well-understood allows a better grasp of the dynamics of the ozone layer as a whole; this grasp, in turn, provides a tool for shaping effective environmental policy. Recently, the reaction product dynamics for one ozone-formation process were significantly clarified by a group working at the ALS.

In the stratosphere, solar ultraviolet light is constantly dissociating ozone (O₃) into oxygen molecules (O₂) and atoms (O). Theorists had recently proposed that if the O₂ were sufficiently vibrationally excited during dissociation, it could recombine with ground-state O₂ to form O₃ + O, thus providing a mechanism for the formation of stratospheric ozone. To test this idea, experimenters at the ALS used an ultraviolet laser to mimic the action of sunlight in dissociating O₃ molecules. An undulator beam then ionized the products, and an ion detector measured their time-of-flight spectrum.

Using a tunable undulator beam to ionize the dissociation products combines the strengths of two techniques used in previous experiments: ionization by electron bombardment, which gives access to any molecule over a wide
energy range but is not selective, and laser-induced ionization, which can select particular vibrational states but requires detailed prior knowledge of the target molecules' spectra. Ionization by undulator beam allowed the researchers to correlate peaks in the time-of-flight spectrum to the vibrational states they represented, and thus to confirm that the vibrational state of O$_2$ required for the proposed ozone-formation mechanism is present.

Ozone research performed by researchers from LBNL, Taiwan's Academia Sinica, the University of California at Berkeley and the University of California at Santa Barbara, using the crossed molecular beam endstation at Beamline 9.0.2.1.

This time-of-flight spectrum shows several vibrational states of O$_2$ created from the laser-induced dissociation of ozone (O$_3$), including one vibrationally excited state of O$_2$ that could combine with ground-state O$_2$ to form new ozone molecules. Selective ionization of the dissociation products using a tunable undulator beam allows a direct correlation between peaks and the particular products they represent. The spectrum's high resolution is due in part to the ionizing undulator beam's tight focus, which creates O$^+$ and O$_2$+ ions at a well-defined point in space. This precisely defines the path length traveled by the dissociation products and thus gives accurate flight times.
One of the fundamental ideas of quantum mechanics is that a physical system (such as a molecule, or in Erwin Schrödinger’s famous thought experiment, a cat) can exist in a combination of two or more distinct states. Largely taken on mathematical faith in the past, this idea has now received direct, experimental support in resonant soft x-ray emission spectroscopy (SXES) studies involving the symmetric molecules oxygen ($O_2$) and nitrogen ($N_2$).

The researchers in this study used precisely tuned photon beams to excite specific resonant transitions in their target molecules ($O_2$, $N_2$). As an x-ray struck a molecule, it excited...
an electron from the core shell of one of the molecule's two atoms to a higher-energy state. One of various electrons could then drop to fill the core hole, emitting an x ray in the process. The foregoing description is classical, not quantum-mechanical, in that it describes a core hole which is localized at one atom or the other. This would break the symmetry of the molecule, whereas quantum mechanics allows for core-electron excitation to occur without breaking molecular symmetry.

The research group tested for symmetry-breaking by looking for violations of the parity-selection rules that govern which orbitals may be involved in electronic transitions within a symmetric molecule. (It is the ability of resonant SXES to detect parity violations that prompted the researchers to choose it over non-resonant techniques such as photoelectron spectroscopy.) If they had found evidence of transitions not allowed by parity-selection rules, this would indicate that molecular symmetry had been broken. However, the spectra showed only parity-allowed transitions, indicating that molecular symmetry was preserved.

Furthermore, the broad peaks in the N₂ spectrum indicate that the core-hole state is relaxed and well-defined, with a bond length distinct from those of the ground state and the final state. This supports the localized-core-hole view. In order to reconcile a localized core hole with the preservation of molecular symmetry, one must consider the excited molecule as existing in a combination of two states, one for each of the possible locations of the core hole.

Molecular symmetry research conducted by scientists from Sweden's Uppsala University and Linköping University, the ALS, and the University of Oregon, using the soft x-ray fluorescence endstation at Beamline 7.0.

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**Experiment Challenges Adsorption Assumptions**

The bonding of molecules to surfaces interests a wide variety of researchers in surface and interface science. A group working at the ALS has been able to test various concepts and models used to describe surface bonding. One of the group's surprising findings is that all molecular orbitals contribute to the surface chemical bond, not only the highest occupied and lowest unoccupied molecular orbitals as has often been assumed.

The group performed x-ray emission spectroscopy (XES) experiments on a sample of nitrogen (N₂) molecules adsorbed on a nickel (100) surface. Diatomic nitrogen bonds to nickel in a "standing-up" position, so the energies of the two nitrogen atoms' orbitals are slightly shifted by the greater proximity of one of the atoms to the nickel surface. Thus, the researchers could tune the incoming x rays to excite transitions selectively in either the outer or
the inner nitrogen atoms, separating their spectral contributions from each other and from those of the nickel substrate. The clear differences between the outer and inner nitrogen atoms' spectra—differences absent in non-adsorbed $N_2$—show that all molecular orbitals in $N_2$ are involved in the surface bond to the nickel. It was the possibility of making this atomic-level separation that brought the group to the ALS; its high-intensity, highly monochromatic undulator light enabled them to perform an experiment that was impossible using conventional techniques.

Surface bonding research conducted by scientists from Uppsala University, Sweden; and IBM Almaden Research Center, using the Uppsala x-ray emission spectrometer at Beamline 8.0.

These spectra from nitrogen molecules ($N_2$) adsorbed on a nickel (100) substrate show the involvement of all of nitrogen's molecular orbitals in the surface bond to nickel, contradicting previous assumptions about surface bonding. The surface bond causes differences between the spectral contributions of each atom's molecular orbitals that would not be observed in free (non-adsorbed) $N_2$. Peaks in the spectra are labeled with the corresponding molecular orbitals; orbitals created by the surface bond are indicated by the $\tilde{\pi}$ symbol.
Beyond the Dipole Approximation

The precise tools available at the ALS have encouraged several researchers to challenge the validity of common assumptions in their fields. One group using the ALS has now brought into question the dipole approximation used in atomic and molecular physics. In experiments using photons, especially at energies of a few keV or less, the dipole approximation states that only the electric dipole field ($E_1$) of the incoming photon beam, and not its electric quadrupole ($E_2$) or magnetic dipole (M1) fields, affects photoemission measurements.

The group's results indicate that this approximation is valid as long as measurements are taken in the plane perpendicular to the direction the incoming photons travel (which can be called the dipole plane). However, the research group showed that for measurements taken outside this plane, $E_2$ and M1 effects can be more significant than has previously been assumed. This is important because a wide variety of angle-resolved photoemission results have long been characterized using the dipole approximation, and the well-known dipole parameter $\beta$, for energies below a few keV. The group's neon photoemission experiment indicates that this may be inappropriate even for energies well below 1 keV.

The angular dependence and the comparatively small size of the $E_2$ and M1 effects observed in this experiment made it necessary to use a high-intensity, highly linearly polarized source such as the ALS to reveal their significance. However, these non-dipole effects may carry implications for all angle-resolved photoemission measurements made with x rays outside the dipole plane, even those performed at second-generation synchrotron sources.

Non-electric-dipole photoemission research conducted by researchers from the University of Nevada at Las Vegas, the University of Tennessee at Knoxville, the ALS, the Indian Institute of Technology at Madras, and Georgia State University, using the ALS x-ray atomic and molecular spectroscopy program's electron time-of-flight spectrometer at Beamline 8.0.

These spectra from neon demonstrate the effects of non-electric-dipole fields on photoemission spectra, effects assumed in most previous experiments to be negligible below 2 keV photon energy. The blue spectrum was taken in the dipole plane, where non-dipole effects vanish. The red spectrum was taken outside the dipole plane and normalized so that both spectra have equal area under the Auger peak. The differences between the two spectra at the 2s and 2p peaks show the effects of the electric quadrupole and magnetic dipole fields on measurements outside the dipole plane.
Studying Crystals with Photoelectron Diffraction

When scientists want to study a material's atomic structure, element specificity assumes a critical role. Researchers often need a technique that is specific enough to let them zero in on atoms of a single element and examine the structure around those atoms. X-ray photoelectron diffraction (XPD) offers this capability. Furthermore, it allows researchers to differentiate between oxidation states of the same element, or between bulk atoms and surface or interface atoms in the same sample. Through such detailed information, XPD reveals the relative positions of neighboring atoms in a crystal lattice (both distances and angles). These types of structural parameters are what define the chemical behavior of a material and, ultimately, the material's uses. Diffraction studies can take advantage of the ALS's high brightness to collect data quickly at high spectral and angular resolution, and researchers can explore a wide range of effects by using both linearly and circularly polarized light.

How Photoelectrons Reveal a Structure

In XPD studies, x-ray photons excite electrons in a sample with enough energy to eject the electrons from the atoms to which they are bound. As they pass through the crystal lattice, the ejected electrons scatter from near-neighbor atoms and emerge at various angles. A detector then collects emitted electrons over nearly a hemisphere above the sample. The intensities of emitted electrons vary from one angle to the next because of the way the electrons scatter. Mapping these intensities gives an angle-dependent diffraction pattern, which is usually presented as a planar projection of the intensity variations. Such a diffraction pattern can be interpreted to give information about the structure of the crystal lattice.

The relationship between the photon energy of incoming light and the kinetic energy of outgoing electrons is the key to XPD's specificity. The kinetic energy of a photoelectron depends on the energy of the light that excited the electron and the type of atom from which it came (the element and its chemical environment). By varying the incoming photon energy and the kinetic energy at which they collect electrons while keeping the difference between the two constant, scientists can detect electrons coming from a single type of atom in a sample and thus study the crystal structure around it. This tracking of the two energies allows for generation of multiple diffraction patterns, each at a different kinetic energy, revealing information from the different types of scattering that occur at various incoming photon energies.
**A Gold Mine of Copper Data**

Holography holds the promise of turning x-ray photo-electron diffraction (XPD) data directly into a three-dimensional representation of a crystal's structure through a simple mathematical transformation, giving scientists a straightforward view of how the crystal's atoms are arranged. Such transformations require diffraction data sets that cover many angles and many electron kinetic energies, sampled closely enough to provide smooth variations. The slowness of data collection is often a limiting factor in the completeness of such data. With the high flux that the ALS can provide at high photon-energy resolutions, however, XPD studies can be performed quickly enough that finely detailed data sets can be generated in just a few working shifts.

One group of investigators has assembled an extremely rich data set for copper. The researchers built the data set by collecting angle-dependent diffraction patterns at enough discrete kinetic energies to show, for the first time, the continuous variation in angle-dependent diffraction patterns with changes in kinetic energy. Since this crystal's structure is well understood, the data can be used to test how well holographic transformations reproduce crystal structure.

Copper research conducted by scientists from the University of Wisconsin at Milwaukee and the University of Oregon using the ultraESCA endstation at Beamline 7.0.1.

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The photoelectron diffraction data set (right) for copper [Cu (100), bulk 3p emission] represents diffraction data for about 480 angles at 75 distinct kinetic energies. Each horizontal slice through the solid represents one angle-dependent diffraction pattern like the one at left. Stacked up by kinetic energy (center), they reveal the continuity of intensity variation across three distinct regimes, each dominated by a different type of scattering.
Diffraction with a Twist

The first experiments with circularly polarized light at the ALS gave a distinctive twist to x-ray photoelectron diffraction (XPD). Since the light source naturally generates circularly polarized synchrotron radiation above and below the plane of the electron orbit, a group of researchers gained access to circularly polarized light by adding a new vertically scanning slit assembly to their beamline. Photoelectron diffraction with circular polarization is particularly useful for studying magnetic materials, such as those used in the computer and data storage industry.

An intriguing effect known as peak rotation occurs with this variation of XPD: the photoelectron diffraction pattern is rotated relative to the pattern obtained from the same sample with linearly polarized light. In experiments on an oxidized tungsten surface, patterns for both tungsten and tungsten oxide (4f peaks) were rotated about 6° counterclockwise for left circularly polarized light and about 6° clockwise for right circularly polarized light. Understanding and quantifying this phenomenon in nonmagnetic materials is crucial in new methods that use similar effects to study magnetic order in magnetic materials.

Tungsten oxide research conducted by scientists from the University of California at Davis, Pennsylvania State University, Osaka University, LBNL's Materials Sciences Division, and the ALS, using the photoelectron spectrometer/diffractometer at Beamline 9.3.2.

Photoelectron diffraction patterns for tungsten oxide made with left circularly polarized light and right circularly polarized light show peak rotation relative to the pattern for linearly polarized light. (These "annular" patterns correspond to the outer portions of full angle-dependent patterns.) Because circularly polarized light imparts an angular momentum to the photoelectrons, the intensities in the diffraction patterns shift from the locations they would have when measured with linearly polarized light. This peak rotation and similar effects are important for measuring magnetic order in materials for use in computers and data storage.
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 optimized to run at an energy of 1.5 GeV, although it can run from 1.0 to 1.9 GeV, allowing flexibility for user operations. At 1.5 GeV, the normal maximum operating current is 400 mA in multibunch operation. The spectral range of undulator and wiggler beamlines extends from photon energies of roughly 5 eV to 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 13 operating beamlines with several more under construction by the end of 1995.
### Beamlines 1995-1997

<table>
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<td>7.3.1.2</td>
<td>Bend magnet</td>
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<td>260–1200 eV</td>
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<td>9.0.2.1</td>
<td>U10 undulator</td>
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<td>3–12 keV</td>
<td>White Light, Four Crystal</td>
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<td>60–320 eV</td>
<td>VLS-PGM</td>
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*LIGA will move to 7.3.3 in the late summer of 1996.*

*See key at right.*
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Generating the high brightness beams of the ALS is an intricate and demanding process, requiring teamwork and first-class engineering—two areas in which the ALS excels. Along with our R&D expertise, these are key contributors to the wealth of scientific results being produced by our users and to the realization of the ALS’s full potential as a premier research facility.

Our high performance and technical achievements have led to continued strong support from the scientific community, allowing us to significantly increase the number of beamlines to meet the ever-increasing user demand. By the end of 1995, the ALS had 13 beamlines in operation with 7 more set for completion in 1996.
The success and growth of the ALS scientific program depends directly on the quality of operations the facility provides. In 1995 the ALS again demonstrated its ability to deliver a high-quality beam to user experiments on a reliable schedule and maintain an efficient and safe work environment for users. The success of these efforts depends on the cooperation among ALS groups and between the ALS and users.

In November 1995 we substantially increased our operations for users and our level of customer support because of increased funding from the Scientific Facilities Initiative. User beamtime now occupies 16 eight-hour shifts per week, an increase of 78% as compared to the previous funding-limited schedule. This increased level of funding is key if the ALS is to continue to be able to meet the ever-growing needs of the user community and if it is to be fully utilized as a national user facility.

**Enhanced Performance**

The ALS successfully maintained its tradition of reliably providing beam with the advertised quality or better to a rapidly growing community of users. The brightness of the ALS, its prime performance metric, exceeded the advertised value at the normal operating values of current and beam energy owing to below-design-value vertical beam emittances. Achieving this performance was aided by the new coupled-bunch feedback systems implemented in 1995 (see “Accelerator Physics,” p. 44). No matter how bright the beam is, however, its usefulness is diminished if it is not delivered on the promised schedule. Despite an unscheduled 17-day outage in May caused by failure of a
storage-ring bellows liner called a flex band, our overall availability of beam to user shifts (actual/scheduled) was 89.1%. Without this problem, the availability would have been 93.7%—an exemplary record. For more information on the outage, see “Diagnostic Flex Band on Duty,” p. 43.

April 1995 marked the first shift of user operation at a storage-ring energy of 1.9 GeV (nominal storage-ring energy is 1.5 GeV), and the long-term scheduling process gradually emphasized operation at the higher energy. The availability of 1.9-GeV beams increases the variety of experiments that can be performed efficiently on ALS beamlines by providing more usable photon flux at high photon energies.

**A Growing Facility**

We scheduled two major shutdowns during 1995, each of which helped the ALS toward its goal of serving users over its entire spectral range and enhancing the facility’s productivity. During the first shutdown in January and February, workers replaced the wide-gap vacuum chamber in the 5-cm-period (U5) undulator in sector 7 with a smaller vacuum chamber (minimum magnetic gap 14 mm, down from 23 mm). The smaller gap extended the spectral range of the undulator at the operating energy of 1.5 GeV down to its design value of 50 eV, giving access to a key silicon absorption edge at 99 eV and allowing important studies on the oxidation of silicon and its interaction with adsorbed metal layers. Installation of a second narrow-gap chamber for the U5 undulator in sector 8 is planned for 1997.

The second shutdown began in mid-September and continued through October. Major tasks included moving the 8-cm-period (U8) undulator in sector 9 to sector 12 and installing a new 10-cm-period (U10) undulator in its place. The longer-period U10 will permit chemical dynamics experiments using photon energies in the ultraviolet range at a storage-ring energy of 1.5 GeV rather than 1.0 GeV. The relocated U8 serves Beamline 12.0, which began operation in December 1995 with LBNL’s Center for X-Ray Optics as its primary user.

"Moving Day" took on special meaning September 19 as the U8 undulator in sector 9 was moved to its new location in sector 12 and the U10 undulator was installed in its place. Shown is the U10 passing above the U8 on the way to its new berth. (The booster to storage ring transfer line is visible in the lower right.)
Critical Survey and Alignment Work

Gradual settling of the ALS floor means that every year or two the girders holding the storage ring magnets need to be surveyed and aligned, and this was one of the primary tasks of the fall shutdown. Plans called for surveying all the magnets in the ring and then aligning as many girders as possible, with five girders programmed as a reasonable estimate. However, improvements designed to streamline the alignment procedure helped save enough time so that all twelve girders could be aligned within the shutdown schedule. The dedicated work of the ALS Survey and Alignment Section, aided by these time-saving advances, yielded a ring alignment well within 150-μm tolerances.

A well-aligned storage ring benefits users in several significant ways. Having the stored electron beam in its ideal position around the ring means that the photon source points are where they should be, the beamlines can be erected on their ideal coordinates, mirrors are illuminated centrally (conserving the original photon beam brightness), and image distances are what they were planned to be. Moreover, the state of alignment of the

![Alignment of the storage ring sector 1 girder magnets before and after realignment work during the fall 1995 shutdown. One can see the girder had a pronounced pitch (open circles) which was removed during alignment. At the conclusion of the shutdown, the average alignment error for all 12 storage ring girders was only 60 μm.](alignment_graph.png)
storage ring magnets affects the dynamic behavior of the electron beam. Misalignment can lead to tune changes, thus disrupting the functioning of the feed-forward tables that are used to keep the beam positions stable while insertion device gaps are being changed. Finally, the fast transverse and longitudinal feedback systems can lose control if tunes change too much, leading to beam flickering and source-size increase, both highly undesirable.

**User Services Improvements**

A ground-breaking ceremony marking the beginning of construction for the new Structural Biology Support Facilities (SBSF) in the ALS building and in the contiguous Building 80 took place on May 15. The SBSF, funded at $7.9M, will include laboratory facilities, computers for data reduction and visualization, and office space. Slated to open in October 1996, it will support all structural biology work at the ALS, including research at the protein crystallography beamline scheduled for first experiments shortly thereafter. Rapid construction progress suggests these goals will be met. Within a year after the main construction contract for the SBSF project was awarded in the fall of 1994, steel supports and all rough utility installation were completed, the elevator shaft was finished, and more than half of the standard equipment purchased.

The ALS is working closely with current users and members of the Users' Executive Committee (UEC) to improve our level of service, such as a new procedure to ensure a timely response to all comments and suggestions noted by users on the User Services Questionnaire (our customer satisfaction survey). Recent additions and improvements include more user office space and a new chemistry laboratory in Building 10 (adjacent to the ALS experiment floor area). The new laboratory, near the existing user machine shop
and the clean assembly room, is equipped with a fume hood with cabinets for flammables and acids, a refrigerator for flammable materials, a de-ionizing high-purity water system, and an ultrasonic cleaner. The ALS also set up a new shipping and receiving area to help expedite the delivery of user equipment.

The Structural Biology Support Facilities project will provide offices for researchers, laboratories for sample preparation and characterization, and computer workstations on portions of the second floors of Building 80 (below) and the ALS building (right) for protein crystallography and other life sciences research. (Inset) Interior view of the second floor of the ALS building shows metal studs defining SBSF user offices and laboratories.
Diagnostic Flex Band On Duty

In addition to the year's advances, 1995 will be remembered for "the outage." In April, toward the end of a shift that was being used to test coupled-bunch feedback at high currents, the beam was lost. Thereafter, no beam could be stored under normal magnet settings. A search to find a magnet-based problem proved fruitless. An ALS operator found the fault when he hit on a set of steering corrector settings that permitted some beam to be injected and stored. With this stored beam, it was quickly established that the storage ring aperture was being partially blocked by one of the fingers of a bellows liner, known as a flex band. Quickly thereafter, the beam was restored for normal operation.

This exercise took 17 days to complete, however, and the cause of the failure of the flex band is still not fully understood. Our investigations, which have included the addition of a specially instrumented "diagnostic flex band," have led to new insights into the heating of these thermally isolated devices and to investigation of other parts of the storage ring vacuum vessel where thermal loading might be a problem (e.g., in the coated ceramic pipes in the injection straight section). The diagnostic flex band/bellows assembly was designed and produced by ALS physicists and engineers in collaboration with LBNL's Center for Beam Physics.

The flex band in this position in the storage ring is now monitored by a special diagnostic assembly shown at right. The top of the device is fitted with a zinc selenide infrared window and an infrared pyrometer, which measures temperatures inside the flex band. Two rf ports, one on the side of the bellows and one on the bottom, monitor the electric and magnetic components of the rf fields within. The remaining side port allows a naked-eye view of the interior of the bellows assembly.

A beam's-eye view of the flex band that failed during tests of the coupled-bunch feedback system. One "finger" bends down into the center of the vacuum chamber, blocking the normal path of the electron beam. As part of the succeeding shutdown, other flex bands were examined for signs of related trouble; all those examined were given a clean bill of health.
The accelerator physics group will remember 1995 as the year in which the ALS accelerators came of age. We made significant progress in our continuing mission to ensure reliable performance for users by improving beam stability, standardizing operating conditions, and increasing our efficiency in changing from one operating condition to another.

To give users more stable photon beams, we improved electron beam stability and installed the diagnostics necessary to observe real-time electron beam motions as small as half a micron so that operators can instantly recognize errant conditions. We made important strides toward implementing feedback systems to combat coupled-bunch instabilities (which produce a significant degradation in the quality of both undulator and bend-magnet radiation). As requested by the user community, we established standard operating conditions for different operating energies. We also improved the ramping algorithm for raising the electron beam energy from 1.5 GeV to 1.9 GeV to make the change more quickly and without losing beam current. In addition, users can now take advantage of another operating condition—two-bunch operation with a maximum current of 20 mA per bunch—which is made practical by running close to a coupling resonance to enhance beam lifetime.

Beam Stability—Diagnostics and Improvements

As always, beam stability is a major concern for the user community. Since any movement of the electron beam results in movement of photon beams, monitoring the electron beam’s position is essential to control photon beam stability. During 1995, we installed three highly sensitive electron-beam monitors, one in straight 4 and the others at each end of straight 7. They can detect beam movements of less than 0.5 μm rms. With three of these monitors, we are able to distinguish true electron beam motion (where all monitors indicate the same motion) from apparent beam motion, which is caused by the motion of individual monitors or by different electronic drift in each monitor. We will eventually bring the number of these advanced beam-position monitors (BPMs) in the ring to 20.

The new monitors have already made an important contribution toward improving beam stability. Data from the BPMs confirmed that there was vertical beam motion caused by temperature variations of around 1°C in the ALS’s low-conductivity water (LCW) supply. With the help of LBNL’s Facilities Department, we traced this to variations in the cooling-tower reservoir temperature and thence to variations in the speeds of cooling fans that control the evaporation from the reservoir—a large excursion indeed from the area in which accelerator physicists usually ply their trade. The temperature problem was brought under control by adjusting the output temperature of the LCW and running the fans at constant speed.
Fast and Efficient Energy Ramping

To accommodate users of both 1.9-GeV and 1.5-GeV operating conditions without losing beamtime, we have streamlined the process of switching from one energy to another. Since the booster synchrotron cannot inject electrons into the storage ring with energies higher than 1.5 GeV, the storage ring energy has to be ramped up to operate at 1.9 GeV. Ramping the energy of stored electrons requires nearly synchronous control of many of the accelerator systems, particularly the main storage ring magnets: bend magnets (controlled by one power supply), quadrupole magnets (49 power supplies), and sextupole magnets (two power supplies). Complicating matters, the six families of magnets have different properties. This makes control of the energy ramp extremely difficult, and if the ramping is not done correctly, some beam current may be lost.

To aid navigation through this sea of potential beam-loss phenomena, we undertook a thorough evaluation of the properties of the different magnetic fields by using the exhaustive measurements generated when the magnets were first installed. The results of this painstaking work are outstanding. Initially, ramping from 1.5 GeV to 1.9 GeV took 20 minutes, and 20% or more of the beam was lost. Now the ramping is accomplished in a little more than one minute with no loss of beam.

Further work has been aimed at establishing a ramping loop whereby the beam can also be decelerated from 1.9 GeV to 1.5 GeV and current can be “topped off” (filled again to maximum rather than dumping and refilling from zero) before ramping back to 1.9 GeV. Such a scenario could substantially reduce the 1.9-GeV refill time.
**Coupled-Bunch Feedback System**

To prevent the instabilities that arise when electron bunches interact with each other, a full coupled-bunch feedback system was commissioned this year. The result of a collaboration between scientists and engineers from Stanford Linear Accelerator Center, the LBNL Beam Dynamics Group, and the ALS, the system monitors the longitudinal, horizontal, and vertical motion of each bunch in the storage ring (up to 324 bunches) and feeds back a correction signal through broad-band kicker electrodes to minimize the motion. With the systems on, the stored beam conforms to all its design parameters at the full current of 400 mA. The longitudinal part of the system is fully digital (including signal filtering and delay generation) and features some of the fastest digital processing chips (250 MHz) available.

Earlier in the year, when the digital processing system was only partially complete, attempts were made to control the coupled-bunch instabilities with only 56 bunches in the machine. It is likely that the high peak current (more than 6 mA per bunch) with feedback on and the high average current (350 mA) were responsible for melting one of the strips in a flex band, leading to a 17-day outage. We have therefore designed and built a diagnostic flex band, equipped with an infrared pyrometer and ports for monitoring electric and magnetic fields. This assembly was installed during the fall shutdown (see “Diagnostic Flex Band on Duty,” p. 43).

**Accelerator Characterization**

To understand problems related to the storage ring’s optics (such as variations in the width of the beam around the ring), we are characterizing the storage ring in detail through beam-based measurements. This involves measuring the response of the accelerator (the change in the closed orbit, the dispersion function, the betatron tunes, the chromaticity, etc.) to a change in a single element, such as a corrector magnet. By making such measurements for different elements, we have built up response matrices, also called sensitivity matrices, for the machine. Our analysis of these matrices has substantially improved our understanding of the signals from the beam position monitoring system in both the first turn mode (measurements for one turn around the ring) and the more sensitive averaging (over many turns) mode.

As a direct result of this characterization work, we have discovered an abnormally high modulation of the ring’s beta function (which is a determinant of the size of the beam from point to point around the ring). This beta beat could be responsible for the diminishing injection efficiencies we have observed (because it limits the range of working parameters over which we can inject) as well as the anomalously low tune shifts caused by the undulators. (Undulators have a focusing effect on the beam that shifts the betatron tune—the number of oscillations an electron makes in a full circuit around the ring. The shifts caused by the ALS undulators are lower than predicted.)
Determining the source of the beta beat (irregular variations in the storage ring beta function), which causes variation in beam size around the ring, required elimination of the sextupole magnets as a possible source. These plots show the changes in the beta function ($\beta_y$) in the various positions where the beam's vertical path is corrected. The finding of a strong similarity between the beta beat with sextupole magnets turned on (top) and with the sextupole magnets off (bottom) ruled out the sextupoles as a source of the problem.
The sources of the beta beat are under investigation, but we have already made notable progress in identifying them. Since the sextupole magnets were a possible source, the analysis required full accelerator characterization with the sextupoles turned off. This was a challenge because of the short beam lifetimes available under such conditions. To gather the necessary data, we began upgrading the data-taking capabilities of the BPM system. These improvements are already helping to speed up other accelerator physics tasks as well. For example, determining the relative alignment of quadrupole magnets and adjacent BPMs now takes only two hours rather than two shifts. In addition, the undulator feed-forward correction tables (used to maintain beam position as undulator gaps are varied) can be generated in less than two hours for all four undulators. The time savings has allowed us to keep more accurate tables by acquiring them routinely on startup.

**Studies of Symmetry Breaking**

Breaking the storage ring's symmetry by adding a new insertion device to the lattice can have a profound effect on the quality of photon beams generated all around the ALS. To model the dynamics of the storage ring when symmetry is broken, we have adopted a technique called Frequency Map Analysis, developed by French astronomer Jacques Laskar to study the dynamics of the solar system. With the help of Dr. Laskar, we have examined the onset of chaos and increased instability when symmetry is broken.

We have also explored symmetry breaking, and compensation thereof, experimentally. This work involved investigating the tails of the transverse beam distribution by moving a thin scraper into the aperture and measuring the bremsstrahlung radiation produced as the electrons in the tails of the beam hit the scraper. By such measurements, we have found that the effects of symmetry breaking caused by an undulator are clearly recognizable before effects on beam lifetime or beam size become apparent. We also discovered that we could suppress the effects of symmetry breaking by adjusting individual quadrupole strengths.

**Short X-Ray Pulse Production with the ALS Accelerators**

Because of mounting user interest in experiments that use sub-picosecond x-ray pulses, LBNL accelerator physicists have been exploring new ways of operating the accelerators. To meet this need, we are collaborating with LBNL's Center for Beam Physics to construct a Compton scattering facility using the ALS 50-MeV linac. Such a facility could generate x-ray pulses on the order of 100 femtoseconds. A possible extension of this idea is to use the booster synchrotron to produce very-low-emittance electron beams at 150 MeV that could interact many times with femtosecond laser pulses. The multiple interactions of the electron beam with the laser pulses could greatly enhance the flux of short-pulse x rays. Tests so far have confirmed that the electron beam can be maintained in the booster during a cycle in which the electrons are accelerated to 700 MeV, there allowed to damp, and then decelerated to 150 MeV.

Another way of producing short pulses of x rays is to operate the storage ring with a momentum compaction factor (the path length difference between high-energy and low-energy particles) close to zero to get shorter bunches. Initial tests of such a configuration indicate that we can inject into this modified machine, but higher-order effects limit how closely we can approach a momentum compaction factor of zero. Even so, we were able to reduce the bunch length by nearly a factor of three, from 15 ps to 6 ps.
With the aid of Frequency Map Analysis, we are modeling the dynamics of the storage ring when its symmetry is broken. The frequency maps represent a ring with perfect symmetry (top) and one with broken symmetry (bottom). Each colored point plotted in "tune space" corresponds to an electron orbiting the ring. An electron's horizontal and vertical tunes are the respective numbers of horizontal and vertical oscillations it makes in one turn around the ring. Electrons whose oscillations have small amplitudes orbit with horizontal tunes near 14.27 and vertical tunes near 8.18 (upper right corner of the plots). Electrons that oscillate with large amplitudes have tunes that are shifted downward and to the left.

The color of each point represents the diffusion rate, or rate of movement in tune space, of the electron. Blue indicates that the electron is stationary in tune space (no diffusion). Red indicates that the electron is moving rapidly in tune space (large diffusion). Large diffusion rates indicate that the motion of the electron is chaotic and the electron may become lost. Diffusion rates increase in regions of tune space near strongly excited resonances (seen here as lines of color). As can be seen from the plots, breaking the ring's 12-fold symmetry excites more resonances and reduces the stable region of the frequency map.
**Plans for 1996**

Bringing the coupled-bunch feedback system into routine operation is the highest priority for 1996. This improvement will bring about new challenges, including shorter beam lifetimes and a greater sensitivity of the beam to operating conditions. These dynamics must be understood before they can be improved. We will enhance our diagnostics, in part by augmenting the diagnostic beamline with equipment to measure bunch length and bunch purity routinely. Accelerator characterization will continue, and through it we hope to determine the sources of error that currently limit the performance of the light source. The installation of a new insertion device, the powerful 2-tesla wiggler, brings with it new constraints for operation and beam dynamics. Meanwhile, the elliptical polarization undulator, a still more exotic device, is progressing toward its installation date early in 1997.

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**ALS Storage Ring Parameters**

<table>
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<tr>
<th>Parameter</th>
<th>Value</th>
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<td>Beam lifetime* (multibunch mode)</td>
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*Beam lifetime defined as the time for the beam to decay from 400 mA to 147 mA. ($= \frac{1}{e} \times 400$)
ALS Storage Ring Lattice Structure

(Upper) The ALS storage ring has 12 arc-shaped and 12 straight sections. (Middle) One superperiod of the ALS triple-bend achromat lattice. A compact structure is achieved by including vertically focusing gradients in the bend magnets (B) and by using a single quadrupole family (QFA) to control the dispersion function, a quadrupole doublet family (QF and QD) to match the betatron tunes, and two families of sextupoles (SF and SD) to correct the chromaticity. (Lower) Horizontal and vertical beta functions and dispersion for one superperiod of the storage ring lattice.
Development of state-of-the-art experimental systems for the ALS is fully as challenging as work on the accelerator, and is vital if users are to take full advantage of the machine's capabilities. Through R&D, commissioning, and scientific support for users, the Experimental Systems Group is primarily responsible for ensuring that our array of research tools continues to expand to serve user needs now and in the future. We gratefully acknowledge the superb support of the Mechanical and Electrical Engineering Groups of the ALS which is essential to the success of our efforts.

**Beamline Commissioning**

The inauguration of the chemical dynamics beamline (Beamline 9.0.2) in 1995 represented a major increase in capability for atomic and molecular science, and the Experimental Systems Group took a lead role in its commissioning. The beamline is equipped with special molecular-beam endstations and a selection of advanced infrared, visible, and ultraviolet lasers to complement the vacuum-ultraviolet beams of the ALS. It is designed to help scientists probe the fundamentals of chemical processes including the reactions and photochemistry of transient radicals, and to investigate the possibility of selectively driving reactions to produce particular product molecules (bond-selective photochemistry).

*Schematic of the chemical dynamics beamline, excluding lasers and showing the geometry of the Eagle monochromator in Branchline 2. A time-sharing arrangement allows undulator light to reach Beamline 9.0.1 or either branch of Beamline 9.0.2, depending on the positions of M2 and M3.*
The shapes of the resonance peaks in this photoionization spectrum of neon demonstrate a spectral resolving power ($\Delta \lambda / \lambda$) of 54,000 for the Beamline 9.0.2 monochromator.

To avoid contamination of high-resolution spectra in Beamline 9.0.2 due to undulator harmonics other than the fundamental, we designed a gas-filled filter that suppresses the harmonics by more than a factor of 10,000 with no attenuation of the fundamental. The photo shows the passage of the hair-thin undulator beam through the cell.
The first commissioning activity was to take transmission grating spectrometer (TGS) measurements characterizing the performance of the beamline’s novel harmonic filter. The windowless, differentially pumped rare-gas filter lets the low-energy (8–25 eV) undulator fundamental pass through unattenuated, while suppressing higher undulator harmonics to typically $10^4$ of their original flux, for spectral purity unprecedented in a raw undulator beam. In the absence of gas, a number of undulator harmonics were observed using the TGS. With neon in the filter, the harmonic peaks in the spectrum were suppressed by more than four orders of magnitude with little or no attenuation of the fundamental. (The 8-cm-period undulator (U8) in use when the beamline came on-line was replaced by a U10 in September 1995, lowering the beamline’s minimum photon energy to 5 eV at an operating energy of 1.5 GeV.

Flux

We measured the flux in both branches of the beamline. In the branch leading to the crossed molecular beam endstation (where there is no monochromator), we found the measured flux in the undulator fundamental to be within a factor of two of the calculated value. In the photoelectron photoion coincidence (PEPICO) endstation on the other branchline we found the measured photon flux, with the monochromator set for a resolving power ($\lambda/\Delta\lambda$) of 25,000, to be significantly lower than the calculated values. This is due to a combination of factors. The replica grating has a lower diffraction efficiency than expected, which is being addressed by its replacement with a holographic master grating. In addition, the reflectivity of a number of mirrors appears lower than expected, in one case due to a substrate problem and in others to surface contamination. Steps are being taken to resolve these problems and fully realize the high flux of the beamline.

Resolution

The Eagle monochromator is equipped with two gratings: 4800 lines/mm and 1200 lines/mm. We investigated the resolution with the two gratings by performing photoionization efficiency measurements on neon and on nitrogen oxide, respectively, using the PEPICO endstation. The photoionization of neon is dominated by two series of resonances with very narrow natural linewidths. By measuring the effect of the monochromator on the resonance lineshapes, we observed the monochromator to have a resolving power of 54,000 at the resonances near 21.6 eV using the 4800 lines/mm grating. The main limit on the resolution appears to be the figure error of the grating, and this should be substantially improved when the new holographic grating is installed.

Research and Development

On the instrumentation front, our primary focus is exploiting the high brightness of the ALS by emphasizing techniques with spatial resolution, such as x-ray microscopy and spectromicroscopy in all its diverse forms.

New Microscopes

With the dramatically enhanced brightness of the ALS, x-ray absorption near edge spectroscopy (XANES) and x-ray photoelectron spectroscopy (XPS) of atomic core levels can be carried out to obtain elemental composition, chemical state, and local structural information from complex materials, all on a microscopic scale. To make such measurements, we currently have two instruments in use: a scanning transmission x-ray microscope (STXM) and a full-field imaging x-ray photoelectron emission microscope (X-PEEM). To increase this arsenal, we are now developing two scanning photoelectron microscopes that have electron energy analysis: one aimed at 0.1-μm resolution on Beamline 7.0 and the other for 1.0-μm resolution on Beamline 7.3.1.2. We are also developing a new X-PEEM capable of better than 0.1-μm resolution for Beamline 7.3.1.1 (see below for a description of Beamlines 7.3.1.1 and 7.3.1.2).

The scanning transmission x-ray microscope (STXM) is installed on undulator Beamline 7.0 and uses a Fresnel zone plate lens to produce a microfocus. Currently we are achieving a resolution around 100 nm. The new high-resolution scanning instrument we are developing, the scanning photoelectron microscope (SPEM), combines the
features of the STXM with an electron-energy analyzer in an ultra-high vacuum environment.

The second SPEM, the lower resolution version, will be used on Beamline 7.3.1.2 and was designed specifically to meet the needs of the semiconductor industry. The microscope uses a pair of spherical mirrors, rather than a zone plate, to generate a spot size of about 1 μm and also has an electron-energy analyzer for XPS. The bend-magnet source is sufficient for the system to produce XPS images at 1-μm resolution because of the high brightness of the ALS. This version of SPEM has large sample capability (50 mm x 50 mm), submicron sample-position encoding, high-resolution optical microscopy for sample registration, and a sophisticated sample preparation and transfer system. Another important feature is that the low cost of this beamline should allow duplication of the system at other ALS beamlines for a relatively modest cost, when demand becomes too high for 7.3.1.2.

In the X-PEEM, the entire area of interest (typically 50 μm in diameter) is illuminated, and an image is formed by electron optics that focus the photoemitted electrons at high magnification onto a detector. Our current X-PEEM achieves a spatial resolution of around 0.3 μm, limited by chromatic aberrations (focusing depends on electron energy). We are constructing a higher-voltage version of this microscope that should give resolutions better than 0.1 μm and which offers a much more sophisticated microscopy environment.
**Magnetic Microscopy and MicroXPS**

Brightness and the large number of bend-magnet ports at the ALS combine to provide an opportunity for so-called "application-specific" beamlines optimized for a well-defined class of experiments. Beamline 7.3.1, designed for full-field photoelectron microscopy of magnetic surfaces, is a prime example.

The first branchline (Beamline 7.3.1.1) is specifically adapted to the characteristics of the ALS and combines simplicity with high performance. It includes a mechanical chopper for alternating between right- and left-handed circularly polarized light, a spherical-grating monochromator, and a single elliptical mirror. The monochromator grating and the mirror will focus the light to a spot size of approximately 50 μm. The small vertical size of the ALS electron beam (and thus the photon beam) eliminates the need for entrance slits. An x-ray photoelectron emission microscope (X-PEEM) endstation will image the photoelectrons emitted from the sample.

The second branchline (Beamline 7.3.1.2) is designed for "micro" x-ray photoemission spectroscopy of the micro-structures in integrated circuits (ICs) and of the silicon wafers from which ICs are made. For investigating device failure mechanisms in next-generation (smaller) devices, as well as identifying microscopic surface contaminants that can render a wafer useless, this branchline will use a small part of the flux from the bend magnet and divert it to an experiment station specifically designed for measurements on ICs and silicon wafers.

**Circular Polarization Facility**

We are developing a circular polarization facility to apply the high brightness available from undulators to fundamental studies of spin dependent phenomena, from aligned metal centers in metallo-proteins to magnetic surfaces and thin films. Scheduled for development in phases, the facility will ultimately include up to four undulators to produce the radiation for two independent

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Image of experimental setup for magnetic microscopy and microXPS.
The circular polarization facility in sector 4 of the ALS storage ring will ultimately consist of two pairs of interchangeable elliptical polarization undulators, a set of translating mirrors to guide the light from the undulators to either of two beamlines, and beamlines for high-resolution magnetic spectroscopy and magnetic imaging using circularly polarized x rays. Both scanning and full-field imaging microscopes will be available.

beamlines, one for high resolution spectroscopy (Beamline 4.0.1) and one for microscopy (Beamline 4.0.2). The first undulator and the spectroscopy beamline are scheduled for completion in fall 1997; the microscopy beamline will be finished thereafter.

To produce circularly polarized radiation, an elliptical polarization undulator is being designed (see "Insertion Devices," p. 60). The undulator will be roughly half the length of the devices constructed up to now, so that two will fit in one straight section at the same time. In addition, a translation mechanism will allow either of two side-by-side devices covering different spectral ranges to be placed in the beam, thereby accommodating a maximum of four devices.

The beamlines are designed for making measurements at important absorption edges of magnetically important elements, such as transition metals and rare earths, but they are also separately tailored to suit the different requirements of high-resolution spectroscopy and microscopy. Two experiment-station positions will be accommodated on the spectroscopy beamline. Mounting these experiment stations on a rotating platform will make rapid changeover from one experiment to the next possible, providing researchers with greater access to beamtime. The microscopy beamline will have two branches, one equipped for full-field photoemission microscopy and the other optimized for scanning microscopy.

**Protein Crystallography**

The macromolecular crystallography facility being constructed at the ALS will offer structural biologists from industry, government, and academia a choice of crystallographic techniques with semi-automated operation and rapid sample turnaround, making it fully competitive with the best synchrotron sources in the United States. The heart of the crystallography facility is Beamline 5.0, which will deliver x rays from a multipole wiggler to up to three automated experiment stations for high-quality data collection. Users will also have access to the Structural Biology Support Facilities located near the beamline; these support facilities will be available in fall 1996.
Innovative New X-Ray Detector

Synchrotron radiation offers several advantages for the study of the structure of biological molecules and other materials by x-ray diffraction, including high flux, high brightness, and tunability over a broad range of wavelengths. However, to make better use of the high intensity of the beam than is now possible, faster x-ray detectors that can also record diffraction information with high resolution over large areas are necessary. Scientists from LBNL's Engineering and Structural Biology Divisions, the ALS, and the University of California at San Diego are addressing this challenge by collaborating on a multiyear project to build a high-speed, two-dimensional (area), x-ray detector for the ALS.

Called a pixel detector, the new device will eventually find a home in the x-ray crystallography beamline at the ALS (Beamline 5.0). In a major advance, the pixel detector will be able to read-out diffraction data as soon as it is detected to a data-storage computer. This means there are no unproductive intervals in which the detector cannot register data as is the case with current state-of-the-art electronic systems such as that initially planned for the crystallography beamline. Hence the pixel detector will ensure even more efficient use of the beamline, which is expected to be heavily subscribed.

The idea behind the pixel detector is conceptually simple. To provide position sensitivity over an area, the designers split the detector into rows and columns of identical elements (pixels), each of which has its own autonomous processing electronics. The basic unit is an array of x-ray sensitive semiconductor (PIN) diodes bonded to custom-designed integrated circuit chips (application-specific integrated circuits or ASICs). Each array comprises 50 by 50 pixels. Four such units are then assembled into a module with additional circuitry for read-out based on columns of pixels. Finally, a full detector of the desired size is constructed using the requisite number of modules arranged in a matrix. The collaborators are aiming for an operational detector with an area of 15 cm by 15 cm containing one million pixels.

The basic unit of the pixel detector is a 50 by 50 pixel array of semiconductor detectors (PIN diodes) bonded to a 50 by 50 channel application-specific integrated circuit (ASIC). Four such units are then assembled into a module from which a large-scale pixel detector can be constructed.
Based on current construction progress, we plan to have the first, central station ready for use shortly thereafter. This multi-purpose station for fixed wavelength, multiple-wavelength, and time-resolved techniques will receive the on-axis, brightest portion of the wiggler light. It will offer cryo-cooled sample environments and beamline optics that are self-aligning onto sample collimators. In a separate project, we are also developing a high-speed x-ray detector that will dramatically enhance the rate of data transfer to computers, a major bottleneck in even the fastest existing electronic detectors (see “Innovative Detector,” p. 56). Funding for the endstations is being sought from individual pharmaceutical companies, so far with a positive response. It is expected that full industrial funding will be secured in 1996.

**Infrared Beamline**

Infrared spectroscopy has been a mainline analytical tool for decades, both in industry and in the laboratory, owing to its ability to identify molecular constituents of complex materials from their vibrational spectra (molecular fingerprints). In the last decade, advanced optics and detectors have made spatially resolved infrared spectroscopy (spectromicroscopy) a popular technique for the analysis of inhomogeneous samples and small particles, but resolution has been limited because of the low brightness of black-body sources.

Synchrotron radiation, on the other hand, is a very bright source of infrared radiation, and the use of synchrotron radiation in infrared spectromicroscopy has already extended the basic technique to new levels of performance and resolution for molecular characterization of materials. The ALS is developing a beamline for infrared spectromicroscopy based on the strong desire expressed by the scientific community for such a facility. Construction is now under way with initial operation scheduled for late 1996.

The primary wavelength range of the ALS beamline for spectromicroscopy will be in the mid-infrared, 2 to 25 μm, where the ALS is at least 1000 times brighter than a blackbody source. Research at the ALS will center on this important wavelength range because many materials have vibrational modes there that provide a unique fingerprint for constituent compounds. The primary experiment station will be a commercially available Fourier-transform infrared (FTIR) microscope.

![Brightness is the key parameter for spectromicroscopy. In the mid-infrared spectral range at which the ALS infrared beamline will operate, the ALS will be more than 1000 times brighter than conventional black-body sources.](image)
Insertion Devices

The ALS has specified the major parameters for seven insertion devices. By the end of 1995, four undulators were in operation and the wiggler for the crystallography beamline was ready for spring 1996 installation. Other devices underway included a novel elliptical polarization undulator and a 10-cm-period U10 undulator, both headed for operation in 1997.

We completed and installed a 10-cm-period U10 undulator in storage-ring sector 9 during the fall 1995 shutdown. With a longer period compared to previous undulators, the U10 can generate high brightness beams with photon energies as low as 5 eV for chemical dynamics experiments. Our usual rigorous magnet testing program showed that rms field errors were 0.22%, about a factor of 1.5 better than required to meet brightness specifications.

The size of the vacuum chamber is one of the chief factors limiting the spectral range of an undulator at low photon energies. During the January-February shutdown, we installed a small-gap vacuum chamber in the 5-cm-period U5 undulator illuminating Beamline 7.0 (minimum magnetic gap 14 mm, down from 23 mm), thereby allowing the undulator to reach photon energies down to 50 eV when the ALS operates at 1.5 GeV. In October 1995 work started on a second small-gap vacuum chamber for the U5 undulator in Beamline 8.0.

Our first wiggler, with a 16-cm-period (W16), is being constructed for the protein crystallography beamline (Beamline 5.0). The long period and high field (about twice as high as that of a bend magnet) of the W16 combine to generate the high flux and continuous spectrum characteristic of a wiggler, making it an ideal source for crystallography. By year’s end, we had assembled and aligned most of the major systems comprising the device (the wiggler was installed during the April-May 1996 shutdown).

In early 1995 we decided to build a newly designed elliptical polarization undulator (EPU) rather than the elliptical wiggler originally planned, because the undulator can produce circularly polarized beams several orders of magnitude brighter. Of a type pioneered by Shigemi Sasaki, the 5-cm-period EPU will produce both elliptically and circularly polarized light, as well as horizontally and vertically polarized light. Completion is slated for summer 1997.


<table>
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<tr>
<th>Device</th>
<th>Beamline</th>
<th>Status</th>
<th>Energy Range (at 1.5 GeV)</th>
<th>Energy Range (at 1.9 GeV)</th>
<th>Period Length</th>
<th>Number of Periods</th>
<th>Operating Gap Range</th>
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<td>U5 Undulator</td>
<td>8.0</td>
<td>Operational</td>
<td>130–1900 eV</td>
<td>210–3000 eV</td>
<td>5.0 cm</td>
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<td>2.3–4.5 cm</td>
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<td>U5 Undulator</td>
<td>7.0</td>
<td>Operational</td>
<td>50–1900 eV</td>
<td>80–3000 eV</td>
<td>5.0 cm</td>
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<td>1.4–4.5 cm</td>
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<td>18–1200 eV</td>
<td>30–1900 eV</td>
<td>8.0 cm</td>
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<td>2.5–8.3 cm</td>
<td>.80–07 T</td>
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<td>U5 Undulator</td>
<td>9.0</td>
<td>Operational</td>
<td>5–950 eV</td>
<td>8–1500 eV</td>
<td>10.0 cm</td>
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<td>Design in progress</td>
<td>8–950 eV</td>
<td>12–1500 eV</td>
<td>10.0 cm</td>
<td>43</td>
<td>2.4–11.6 cm</td>
<td>.80–05 T</td>
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<td>EPU Elliptical Polarization Undulator</td>
<td>4.0</td>
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<td>Operational</td>
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<td>5–21 keV</td>
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<td>19</td>
<td>1.4–18.0 cm</td>
<td>2.1–03 T</td>
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1 A narrow gap vacuum chamber will be installed in spring 1997.
2 Installed in May 1996.
Photon flux as a function of photon energy for the ALS undulators and wiggler. The flux values plotted here are for a 1.5-GeV, 400-mA electron beam with a horizontal aperture of ± 2.5 mrad. The undulator plots show the curves for the first, third, and fifth harmonics.

Brightness as a function of photon energy for the ALS undulators and wiggler. The brightness values plotted here reflect a 1.5-GeV, 400-mA electron beam. The undulator plots show the curves for the first, third, and fifth harmonics.
Circular polarization merit function brightness for the elliptical polarization undulator with a 1.9-GeV, 400-mA electron beam. The solid lines in the plot show the first, third, and fifth harmonics for the elliptical case. The dashed line shows the first harmonic for the helical case. The merit function brightness is defined as $M_B = P_c^2 B$, where $P_c$ is the degree of circular polarization and $B$ is regular brightness.

Circular polarization merit function flux for the elliptical polarization undulator with a 1.9-GeV, 400-mA electron beam. The solid lines in the plot show the first, third, and fifth harmonics for the elliptical case. The dashed line shows the first harmonic for the helical case. The merit function flux is defined as $M_F = P_c^2 F$ where $P_c$ is the degree of circular polarization and $F$ is regular flux.
The ALS opened its doors to nearly 2000 visitors as part of a Laboratory-wide Open House in October. Activities at the ALS focused on science as fun, stimulating, and accessible to all. On the outside terrace, science enthusiasts of all ages and interests enjoyed a variety of entertaining demonstrations including what happens inside a vacuum, the effects of liquid nitrogen on different materials, and the science of light and bubbles. Inside the ALS, exhibits and hands-on activities exploring everything from the properties of light to how to make an electron move were part of a thematic tour around the experiment floor.
At the Open House, young and old alike had a chance to participate actively in activities ranging from "Puzzling Polarizers" to the "Electronics Petting Zoo" where children were encouraged to take apart meters, computer drives, and more to see how they work. Staff and users were available to answer questions and discuss their research in terms that all could understand.
The ALS developed a poster for the Open House called “Inside the ALS” as a take-home souvenir and a resource for science teachers. Showing how the ALS works using cartoons, key concepts, and diagrams, the poster is the cornerstone of an educational outreach program designed to keep the doors of the ALS open to the scientists of the future. Workshops at the ALS for teachers will provide the framework for incorporating the poster, hands-on activities, and student tours of the ALS into their science programs.

An additional outreach tool to connect classrooms with ALS science is Microworlds, an electronic magazine on the World Wide Web developed by LBNL for teachers and students. The on-line magazine contains a series of articles related to how the ALS works and the scientific research done at the ALS. Each article has learning activities to help students understand basic concepts related to the research described. The URL for Microworlds is http://www.lbl.gov/MicroWorlds/
The opportunity to view the latest scientific results from the growing number of beamlines and to hear some hopeful words about the prospects for federal science funding for FY96 attracted over 200 attendees to the Annual Meeting of the ALS Users’ Association on October 23 and 24. In opening the meeting, Laboratory Director Charles Shank set the tone for the proceedings by putting the emphasis on the high-quality science being done by an enthusiastic user community intent on exploiting the high brightness of the ALS.

Organized by Users’ Executive Committee Chair Tom Callcott (University of Tennessee), the program began with a panel discussion of the funding prospects for science in FY96. Panelist Michael Lubell (City College of New York), who serves as public affairs officer for the American Physical Society, noted that there was strong support for the Scientific Facilities Initiative in Congress. The initiative (now funded) provides a $100 million boost for operation and instrumentation at several DOE “user facilities,” including synchrotron radiation sources. Other panelists included Bill Oosterhuis (DOE Office of Basic Energy Sciences) and Tom Weber (National Science Foundation).

ALS Director Brian Kincaid outlined priorities for use of the additional funding anticipated from the Scientific Facilities Initiative. These include expanding user operations from nine to 16 shifts per week (a change that took place on November 1, 1995), enhancing the level of scientific support for users, increasing outreach to potential industrial and academic users, augmenting support of R&D for instrumentation, and, to the extent possible, stepping up the pace of beamline construction.

Instrumentation Developments

The scientific presentations began with Maya Kiskinova (Sincrotrone Trieste) who reviewed the first few months of experiments with the scanning photoemission electron microscope beamline on the ELETTRA storage ring. Samples investigated included gold-coated carbon films, polycrystalline tin before and after oxidation, metal carbide phases in tool steel, and gold-coated silicon surfaces.

The third annual Halbach Prize for outstanding instrumentation in the field of synchrotron radiation at the ALS was presented at the users’ meeting to Jeffrey Kortright, Marybeth Rice, and Keith Franck for their spectroscopic polarimeter. This continuously tunable instrument uses a laterally graded multilayer to polarize x rays linearly by reflecting them at 45°.
Jeff Bokor (University of California at Berkeley and LBNL) followed with a progress report of his group's work on interferometry for at-wavelength testing of EUV optics at ALS Beamline 9.0.1. The point diffraction interferometer used has revealed irregularities in tests of zone-plate lenses. Jim Underwood (LBNL's Center for X-Ray Optics) reported on the operation of ALS Beamline 6.3.2, designed for calibration and standards in the EUV spectral region from 40 to 400 eV. The beamline is based on a variable-line-spacing plane-grating monochromator and an EUV reflectometer, although other experiment chambers can be attached.

Atomic and Molecular Science

Arthur Suits (LBNL's Chemical Sciences Division) led off the afternoon session with an account of the first results from ALS Beamline 9.0.2, including a study of the photodissociation of ozone. The beamline features two branches, both equipped with molecular-beam endstations with various modes of excitation and detection.

Nora Berrah (Western Michigan University) continued with an overview of the atomic and molecular physics work by several groups at Beamline 9.0.1. Focused on the theme of investigating many-electron effects in photoionization, Berrah's overview included ultra-high-resolution (resolving power of 60,000) absorption spectra for doubly excited helium; partial photoionization cross sections and angular distributions, also in two-electron excitation of helium; photoelectron spectroscopy of hollow lithium atoms; and Auger resonant Raman spectroscopy to eliminate lifetime broadening.

Dennis Lindle (University of Nevada at Las Vegas) reported on experiments based on ion and electron time-of-flight spectroscopy, which can effectively use the roughly 50 ps time structure and high brightness of the ALS to obtain
high-resolution spectra from small sample areas. Lindle demonstrated his argument with results from argon, atomic and molecular oxygen, methyl chloride, and non-dipole effects in neon.

**Materials Science**

The second day began with a review of high-resolution photoelectron diffraction at Beamline 7.0. Jonathan Denlinger (University of Wisconsin-Milwaukee) and Eli Rotenberg (University of Oregon) set a new standard for presentations with computer-generated slides and animations, an approach made necessary by the densely packed data sets in both angular and energy variables. Results were shown for bulk copper, tungsten surfaces, and silicon surfaces.

John Carlisle (Lawrence Livermore National Laboratory) highlighted some of the many experiments by the large group using Beamline 8.0. Carlisle showed results for photoabsorption of oxynitride films on silicon, photoemission of boron nitride on silicon, and soft x-ray fluorescence of iron-silicon multilayers.

Anders Nilsson (Uppsala University, Sweden), representing another group at Beamline 8.0, reported on the use of soft x-ray core-level spectroscopies as a local probe of the surface chemical bond of adsorbates on metals, placing particular emphasis on soft x-ray emission. Systems studied included nitrogen on nickel, benzene on nickel, a copper monolayer on nickel, and the interface between a copper film sandwiched between bulk nickel.

The theme for the concluding presentations of the meeting was microscopy. Tony Warwick (ALS) provided an overview of the spectromicroscopy instruments currently in place and anticipated in the near future. In addition to a small-spot (50 mm) ESCA system on Beamline 7.0, there is an imaging photoelectron microscope and a scanning transmission x-ray microscope. A scanning photoelectron microscope will be added to Beamline 7.0 in fall 1996, as will an imaging photoelectron microscope on Beamline 7.3.

Werner Meyer-Ilse (LBNL’s Center for X-Ray Optics) closed out the session with a presentation of biological microscopy on Beamline 6.1. The microscope uses two zone plates, a condenser to illuminate the sample and a micro zone plate to image the transmitted light. Examples shown included malaria parasites in human blood cells, chromatin packing in mouse sperm cells, the green alga Chlamdomonas, and human chromosomes.

The users’ meeting featured ample opportunity for participants to peruse the vendor exhibits on the ALS experiment floor.
Max Cornacchia (SSRL) described the way he and Klaus designed modified sextupole magnets that achieve chromaticity correction near the axis, but whose fields away from the axis are changed to allow higher dynamic aperture. These ideas can be used even more profitably with octupole magnets. Richard Post (Lawrence Livermore National Laboratory) reported on how he uses Halbach motor/generator magnets in very high energy density flywheel storage systems for motor vehicles. These systems have greater energy output per pound than batteries or internal combustion engines; the Halbach magnet array is used to relax otherwise tight mechanical tolerances.

Kwang-Je Kim (LBNL) then presented his new theory of transition radiation generation from insertion devices. When an electron beam enters such a device, its net drift velocity is reduced. In a phenomenon analogous to conventional transition radiation, the electron beam emits infrared radiation of high brightness; for a typical storage ring insertion device, this infrared photon beam will be squeezed into a few milliradians, as opposed to perhaps 100 mrad for a bending magnet.

After lunch, Shigemi Sasaki (Japan Atomic Energy Research Institute) described how one can design an undulator that does not produce harmonics of the fundamental spectral peak, and so does not contaminate monochromatized radiation. Rodolfo Bonifacio (INFN Milan) reported on how one may generate harmonic radiation from a series of free electron lasers, where each uses the bunched beam from the preceding ones. Simon Yu (LBNL) concluded the meeting with a talk on the use of low-field permanent-magnet quadrupole magnets in a two-beam linear accelerator design. In this scheme, the radio-frequency energy that drives a high-energy beam is derived from a parallel low-energy electron beam that acts as a klystron, feeding energy to the high-energy beam every two meters.
Refereed Journals


Non-Refereed Journals


Refereed Conference Proceedings


Conference Proceedings


S. Caspi, R. Schlueter, and R. Tatchyn, "High-field strong-focusing undulator designs for x-ray linac coherent light source (LCLS) applications," in Proceedings of Particle Conference & International Conference on High-Energy Accelerators (Dallas, TX, 1995).


D. Robin, C. Kim, and A. Sessler, "Compton scattering in the Advanced Light Source booster," in Proceedings of Particle Conference & International Conference on High-Energy Accelerators (Dallas, TX, 1995).


W. Thur and T. Lauritzen, “Surveying the monument system at Lawrence Berkeley Laboratory’s Advanced Light Source accelerator,” in Proceedings of Particle Conference & International Conference on High-Energy Accelerators (Dallas, TX, 1995).


Books


**Theses based on work done at the ALS**


**General ALS Publications**


Science Policy Board, 1995
Advises the Director of LBNL on high-level policy issues affecting the ALS.

E. Morton Bradbury, School of Medicine, University of California at Davis
William F. Brinkman, AT&T Bell Laboratories
John C. Browne, Los Alamos National Laboratory
Bernd Crasemann, University of Oregon
Dean E. Eastman, IBM Thomas J. Watson Research Center (chair)
J. McEwan Paterson, Stanford Linear Accelerator Center

Program Advisory Committee, 1995
Advises the Director of LBNL on the ALS scientific program through the ALS Director.

Franco Cerrina, University of Wisconsin at Madison
Charles S. Fadley, University of California at Davis and Lawrence Berkeley National Laboratory (to July 1995)
Roger Falcone, University of California at Berkeley (from July 1995)
Keith O. Hodgson, Stanford Synchrotron Radiation Laboratory
Christof Kunz, University of Hamburg, Germany (chair)
Gerald J. Lapeyre, Montana State University at Bozeman (to July 1995)
Robert C. McDonald, Intel Corporation
David A. Shirley, Pennsylvania State University
Neville V. Smith, Lawrence Berkeley National Laboratory (ex officio)
Joachim Stöhr, IBM Almaden Research Center (from July 1995)
Robert Stroud, University of California at San Francisco (from July 1995)
François Wuilleumier, University of Paris-South, France

Users' Executive Committee, 1995
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.

Harald W. Ade, North Carolina State University
Nora Berrah, Western Michigan University
Jeffrey Bokor, University of California at Berkeley (vice-chair)
Thomas A. Callcott, University of Tennessee (chair)
Norman M. Edelstein, Lawrence Berkeley National Laboratory
Marjorie A. Olmstead, University of Washington
Linda S. Powers, Utah State University
Eli Rotenberg, University of Oregon
Mahesh G. Samant, IBM Almaden Research Center
Louis J. Terminello, Lawrence Livermore National Laboratory
Michael G. White, Brookhaven National Laboratory (past chair)
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