The Advanced Light Source: A Third-Generation Synchrotron Radiation Source

The Advanced Light Source (ALS) at the E.O. Lawrence Berkeley National Laboratory (Berkeley Lab) of the University of California is a “third-generation” synchrotron radiation source optimized for highest brightness at ultraviolet and soft x-ray photon energies. It also provides world-class performance at hard x-ray photon energies. Berkeley Lab operates the ALS for the United States Department of Energy as a national user facility that is available 24 hours/day around the year for research by scientists from industrial, academic, and government laboratories primarily from the United States but also from abroad.

X Rays, Synchrotron Radiation, and the Advanced Light Source

Since their discovery in 1898, x rays have tantalized scientists with their ability to see into solid objects. By the time synchrotron radiation was definitively observed almost a half-century later in 1947, the scientific use of x rays was well established. For example, they were, and continue to be, the principal probe of the positions of atoms in crystallized solids, from the comparatively simple structures in metals and semiconductors to the highly complex arrangements in biological molecules, such as proteins and DNA.

By the early 1960s, the potential benefits of synchrotron radiation with its bright, wavelength-selectable beams of x rays were sufficiently apparent that significant attempts to harness it arose around the world. The subsequent growth of synchrotron radiation research has markedly expanded the scope of x-ray investigations. The result is a collection of spectroscopic, scattering, diffraction, and imaging tools that can probe in minute detail both the atomic and electronic structures of all manner of samples, large and extremely small, including gases, liquids, and non-crystalline and inhomogeneous solids.

At first, scientists exploited the ultraviolet and x rays emitted by electrons in synchrotrons built and operated for high-energy physics research. These were the “first-generation” synchrotron sources. By the early 1980s, new facilities based on electron storage rings were springing up in the major industrialized nations. Users of synchrotron radiation soon recognized that brightness is often more important than flux alone for many experiments. So, not only were these “second-generation” sources dedicated to synchrotron radiation, but many were also designed to achieve much higher brightness than previously obtainable.

The importance of brightness traces to statistical-mechanical phase space, which applies to the source of the synchrotron radiation (the electron beam) and to the radiation itself. For electrons, the occupied area in phase-space (the emittance) is the product of the beam size and divergence. The emittance sets a lower limit for the phase-space area of the light beam, defined as the product of the effective source size and radiation cone angle. Brightness is the density of photons in this phase space. Similarly, there is a sample acceptance defined by the spot size and beam divergence required at the sample. Since the highest useful flux delivered to the sample occurs when the phase-space area of the photon beam matches the sample acceptance, brightness is almost always more important than flux alone.

As the flux density in phase space, brightness is an invariant quantity, so that no optical technique can improve it. The cure, therefore, is proper design of the source, the electron beam in the storage ring. For these reasons, within a decade after the first second-generation synchrotron sources began operation, work began on the third generation of facilities, with great expectations for benefits from still higher brightness.

The ALS is one of the first third-generation facilities, with construction completed in March 1993, but there are now several such sources around the world, divided roughly into two types, according to the spectral range they serve. The first comprises large storage rings optimized for the production of hard x rays. Owing to the large size and cost, there are just three of these sources at present, the European Synchrotron Radiation Facility in Grenoble (6 GeV), the Advanced Photon Source at Argonne National Laboratory near Chicago (7 GeV), and Spring-8 in Hyogo Prefecture west of Osaka (8 GeV). The second type is based on smaller storage rings of 1–3 GeV and specializes in the generation of soft x rays. There are now many of these smaller facilities, including the ALS, on several continents.

In the first synchrotron sources, the radiation came from the bend magnets in the curved sectors of an electron accelerator. At any point on the trajectory, the synchrotron radiation emerges in a narrow cone tangential to the path of the relativistic electrons with a flux and a broad spectral range that depends on the electron energy and the magnetic field. As the electron sweeps around the curve, it generates a horizontal fan of light. For the ALS, the beam energy ranges from 1 to 1.9 GeV and the bend-magnet field is about 1.3 Tesla, so that useful fluxes from bend magnets are available at photon energies to above 10 keV. The synchrotron radiation spectrum extends to very long wavelengths, as well, so that the ALS is also an excellent source of diffraction-limited infrared light.

In 2001, superconducting dipole (bend) magnets were retrofitted into three sectors of the 12-fold symmetric ALS storage ring, the first time such a feat has been attempted in an already operating facility (See Figure 4.). The higher magnetic field (5 Tesla) of the superbends has extended the ALS spectral range to above 40 keV, well into the hard x-ray spectral region, thereby enlarging the opportunities for the user community without compromising capabilities in the core soft x-ray region.

Undulators provide a way to take maximum advantage of the intrinsic brightness of the synchrotron radiation source. Together, undulators and related devices called wigglers are called insertion devices because they are placed in the otherwise empty straight sections that connect the curved arcs of large storage rings. Although designs differ, the most common insertion device comprises two rows of magnets that form a linear array of vertical dipoles with alternating polarity (i.e., N-S-N-S and so on). The array generates a sinusoidal vertical field that drives an electron into an oscillating trajectory in the horizontal plane with the same period as the field.

Constructive interference of the radiation from the poles in an undulator results in one or a few spectrally narrow peaks (a fundamental and harmonics) in a beam that is highly collimated along the axis of the undulator in both the horizontal and the vertical directions and linearly polarized in the horizontal direction. For the values of the periods (5 to 10 cm) and maximum fields (less than 1 Tesla) of the ALS undulators, the spectral range is currently from about 5 eV to 3000 eV. Wigglers are similar to undulators but have higher magnetic fields, so that each dipole acts as an independent bend-magnet source, thereby resulting in a continuous spectrum with a higher flux and a spectrum that extends to shorter wavelengths than bend magnets. The ALS has one wiggler with a spectral range from 5 to 21 keV.

More complicated insertion-device designs can produce variably polarized radiation. At the ALS, there is an increasing number of so-called elliptically polarizing undulators (EPUs). With four rows of magnets, two of which are movable longitudinally, the EPUs are capable of generating linearly polarized radiation with any transverse orientation of the polarization vector and left- or right-handed circularly polarized light. The long-term plan at the ALS is to place two short EPUs in the straight sections to enhance the number of beamlines receiving this high-quality radiation.

Spectrum of Science at the Advanced Light Source

Almost all of the commonly observed properties of matter depend directly on the atomic structure (i.e., where the atoms are) and on electronic structure (e.g., chemical bonding). There are two basic types of x-ray interactions, scattering and absorption, that give this type of information. For example, the pattern of elastically scattered radiation contains information about the spatial structure of the scattering object. Since scattering is most informative when the wavelength is somewhat less than the size of the scattering object, x-rays with short wavelengths near 1 angstrom are ideal for investigating the positions of atoms.

X-ray absorption provides a way to study electronic structure because the energy range of x-ray photons nicely matches that needed to excite electrons from core to valence quantum states or from one band to another. Dissipating the energy of the photoexcited electrons can have many consequences, such as the emission of electrons (photoemission), photons (fluorescence), or ions from the surface, all of which give rise to spectroscopic techniques to monitor the electronic structure. Inelastic scattering also provides spectroscopic information.

Optimized for high brightness in the VUV/soft x-ray photon-energy range, the ALS traditionally has had a strong program in spectroscopy based primarily (but not exclusively) on excitation of atomic core levels. Since the presence or absence of long-range order does not strongly affect core levels, they are particularly suited for probing short-range order and local properties (e.g., atomic coordination and oxidation states). Because of their localized nature, they inherently provide elemental identification in spectroscopy experiments. Complicated materials can be dissected element by element by tuning to the absorption edges of the constituent elements.

Increasingly explored are the capabilities of the ALS at higher photon energies. The potent performance of the ALS in this range was for a long time not widely recognized. More recently, with the availability of hard x rays from the wiggler and the superbends, protein crystallography, spatially resolved (micro) diffraction, high-pressure diffraction, and microtomography have become increasingly important at the ALS. The high brightness of the ALS together with the growing power of x-ray focusing elements makes spatially resolved spectroscopy and imaging practical with resolution down to 20 nm for soft x rays and less than 1 μm for hard x rays.

The ALS scientific program is divided into the following categories, some of which overlap:

<u>Complex materials.</u> The term “complex materials” is used to describe materials characterized by strong coupling between the electronic, spin, and structural degrees of freedom. The strong coupling is at the heart of the novel behavior of these materials, such as high-temperature superconductivity and colossal magnetoresistance. The ultrahigh resolution made possible by modern instrumentation and the high brightness of the ALS is making it one of the most productive synchrotron radiation facilities for studying the electronic structure of complex materials with high energy and angle resolution by means of angle-resolved photoemission.

<u>Magnetism and magnetic materials.</u> Current research is driven both by the interesting physics and the technological relevance of magnetic nanostructures comprising ferromagnetic, antiferromagnetic, and nonmagnetic layers with nanometer thicknesses. Interfacial structure and behavior are important to understanding the origin of giant magnetoresistance, exchange bias, perpendicular magnetic aniostropy, and other phenomena of commercial as well as basic scientific interest. The photoemission electron microscope allows spatially resolved absorption spectroscopy with a resolution of around 20 nm (2 nm is on the drawing boards). (See Figure 54.)

<u>Polymers, soft matter, and biomaterials.</u> The applications of polymers and soft condensed matter range from the nanoscopic (e.g., biomolecular material and copolymeric mesophases) to the microscopic (microelectronics) to the macroscopic (high performance structural composites). An area of interest at the ALS is the spatially resolved structure, composition, and interfacial properties of multiphase polymer systems, such as polymer blends with microscopic precipitates, polymer beads surrounded by shells, and multilayer systems. Polymer research at the ALS is based on the use of scanning transmission x-ray microscopy and photoemission electron microscopy. (See Figure 6.)

<u>Semiconductors and nanostructures.</u> Nanostructures are low-dimensionality material systems with at least one dimension measured in nanometers. These novel materials have electronic, optical, structural, chemical, or even biological properties that are different from those of the bulk parent compounds and also of the constituent atoms and molecules. In addition to enabling research on artificial and natural nanostructures in any of several forms, such as the magnetic nanolayers and polymers already described, the ALS is slated to play a key role in the Molecular Foundry, a U.S. Department of Energy

Nanoscale Science Research Center scheduled to open for business at Berkeley Lab in early 2006.

Surface and interface science. Surface and interface science has crucial implications for most technologies and for the environmental and life sciences. The controlling role of interfacial phenomena already described in magnetic nanostructures is a prime example. The frontiers are in working at higher pressures, shorter time scales, and higher spatial resolutions, as well as studying more complex systems (e.g., with lateral and vertical heterogeneity and lacking long-range atomic order) than in the past. A growing area of research at the ALS for which new experiment chambers are becoming available consists of wet surfaces.

Environmental and earth science. Recently, a new discipline has arisen, molecular environmental science, which focuses on studying at the molecular level the structure, composition, chemical speciation, and interactions of the many constituents that are found in complex, often wet, real-world environments, such as soils and water systems that have been contaminated by industrial and military waste. Spatially resolved fluorescence, absorption, and diffraction at existing beamlines are already contributing to the identification of chemical species in contaminated soils. A dedicated MES soft x-ray facility will soon be available.

Protein crystallography. The high brightness of the ALS combined with wiggler and superbend sources makes the facility competitive with any in the world for protein structure determination. Researchers at the ALS are pursuing state-of-the-art studies involving very high resolution, microcrystals of proteins that are difficult to crystallize, large macromolecular complexes, and rapid structural determination of large numbers of samples in coordinated project, such as needed for structural genomics and in iterative structure-based pharmceutical design. Provision of automated sample handling and data gathering is a major thrust. (See Figure 7.)

Soft x-ray microscopy. Soft x-ray imaging of cellular structures within biological cells offers higher spatial resolution than optical microscopy but does not require the potentially structure-altering preparation techniques used in transmission electron microscopy. The use of fluorescently labeled antibodies to localize proteins in the light microscope has led to major advances in the understanding of cell structure and function; similar techniques are now under way that take advantage of the higher spatial resolution of an x-ray microscope. The use of tomography to obtain high-resolution, three-dimensional information about protein localization in whole, hydrated cells is also being explored.

Atomic and molecular science. The scientific motivations in atomic and molecular physics include the fundamental quest to understand the interactions of photons with atomic, molecular, and cluster systems and phenomena that impinge on other areas, such as biology, atmospheric physics, astrochemistry, radiation physics, materials science, and environmental science. An area of specific interest at the ALS is electron-electron correlations, where even the three-body helium atom presents challenges. Time-of-flight photoelectron spectroscopy, a unique ion beamline, and a “momentum microscope” that tracks all the products of a photoexcitation event are some of the experimental tools available.

Chemical dynamics. Lasers and molecular beams have had a dramatic impact in chemical dynamics, but the unique features of the ALS offer solutions to a number of previously insoluble problems. The chemical dynamics beamline at the ALS is the first in the world to combine dedicated, intense undulator radiation with state-of-the-art molecular-beam machines. Breakthroughs have been achieved in photoionization studies, photochemistry, and crossed-beam reactive scattering. A particularly effective approach for ultrahigh-resolution spectroscopy has been the combination of pulsed-field ionization (well known to laser chemists) with photoemission spectroscopy and photoelectron–photoion coincidence.

Technology. Built and operated at the ALS under the auspices of Berkeley Lab”s Center for X-Ray Optics, metrology beamlines for at-wavelength interferometry, reflectometry, and mask inspection have been instrumental in a 5-year, $250-million industry–national laboratory effort to bring extreme ultraviolet (EUV) lithography to fruition. EUV lithography is the future chip-printing technology that the Semiconductor Industry Association is backing as the likely successor to the current optical lithography. The EUV promise is that with wavelengths 50 times smaller than those of visible light, it will be able to draw circuit patterns just tens of nanometers wide. (See Figure 8.)

For additional information about the ALS, including how to become a user, visit our Web site at www-als.lbl.gov.

Figure 1 (XBD9904-00696.jpg). Aerial view of the ALS at the Ernest Orlando Lawrence Berkeley National Laboratory. The ALS building consists of an older central portion (under the dome) and the newer annular structure around it. The dome was retained from the historic 84-Inch Cyclotron, whose large size prompted Lawrence to establish a new laboratory on the hillside above the University of California, Berkeley, campus during the World War II years. (Lawrence Berkeley National Laboratory Photographic and Digital Imaging Services)

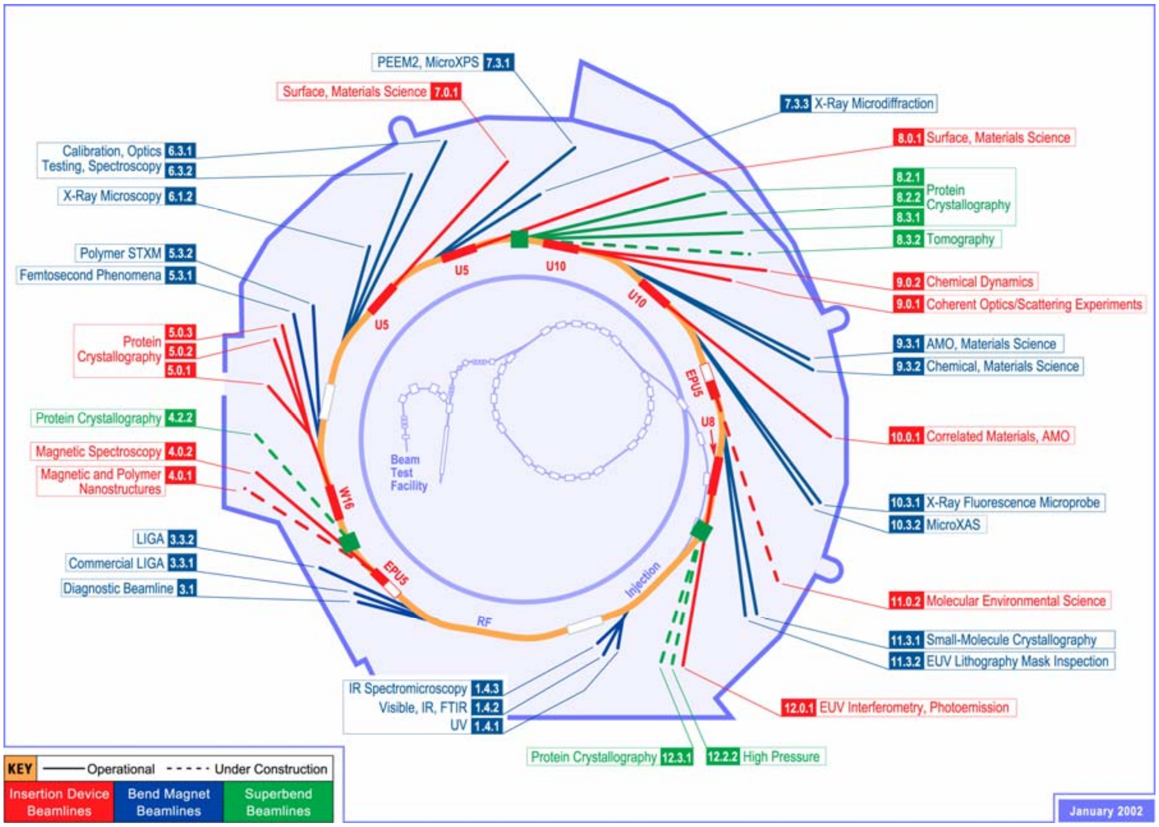

Figure 2. Floor plan of the ALS showing the accelerator complex (50-MeV linear accelerator, 1.5-GeV booster synchrotron, and the electron storage ring), and the beamlines that are operational or under construction. The storage ring has 12 sectors comprising a straight section and a downstream curved arc. Each sector has five possible ports for synchrotron radiation, where port 0 is an insertion-device port; ports 1, 2, and 3 are bend-magnet ports; and port 4 is a bend-magnet port suitable only for an infrared beamline because of space restrictions. The maximum practical number of beamlines is around 50.

	Beamlines 2002	Branchlines	Source	Operational since	Techniques	Energy Range
1	1.4	1.4.1	Bend		Ultraviolet photoluminescence	1.6–6.2 eV
		1.4.2	Bend	Jul-98	Visible and FTIR spectroscopy	0.002–3 eV
		1.4.3	Bend	Jul-98	FTIR spectromicroscopy	0.05–1 eV
2	3.3.1	3.3.1	Bend	Apr-01	Deep-etch x-ray lithography (LIGA)	3–12 keV
3	3.3.2	3.3.2	Bend	Apr-98	Deep-etch x-ray lithography (LIGA)	1–20 keV
4	4.0.2	4.0.2	EPU5	Sep-99	Spectromicroscopy, circular dichroism	60–1800 eV
5	5.0.1	5.0.1	W16	Sep-00	Monochromatic protein crystallography	12.4 keV
6	5.0.2	5.0.2	W16	Sep-97	Protein crystallography: monochromatic and multiple-wavelength anomalous diffraction (MAD)	3.5–14 keV
7	5.0.3	5.0.3	W16	Sep-00	Monochromatic protein crystallography	12.4 keV
8	5.3.1	5.3.1	Bend	Jul-00	Femtosecond Laser slicing	0.1–12 keV
9	5.3.2	5.3.2	Bend	Nov-01	Scanning transmission x-ray microscopy	150–650 eV
10	6.1.2	6.1.2	Bend	Jul-94	High-resolution zone-plate microscopy	300–900 eV
11	6.3.1	6.3.1	Bend	Mar-99	Calibration and standards, optics testing	500–2000 eV
12	6.3.2	6.3.2	Bend	Sep-94	Calibration and standards, optics testing	50–1300 eV
13	7.0.1	7.0.1	U5	Feb-94	Spectromicroscopy, photoemission, absorption	50–1200 eV
14	7.3.1	7.3.1.1	Bend	Oct-98	Photoemission electon microscope (PEEM)	175–1500 eV
		7.3.1.2	Bend	Jan-97	Micro x-ray photoelectron spectroscopy	175–1500 eV
15	7.3.3	7.3.3	Bend	Mar-98	X-ray microdiffraction, technique development	6–12 keV
16	8.0.1	8.0.1	U5	Dec-93	Soft x-ray fluorescence, photoemission	65–1400 eV
17	8.2.1	8.2.1	Sbend	Dec-01	Protein crystallography: monochromatic and MAD	6–18 keV
18	8.2.2	8.2.1	Sbend	Feb-02	Protein crystallography: monochromatic and MAD	6–18 keV
19	8.3.1	8.3.1	Sbend	Oct-01	Protein crystallography: monochromatic and MAD	2.4–15 keV
20	9.0.1	9.0.1	U10	Aug-94	Speckle, coherent optics	200–800 eV
		9.0.2	U10	Mar-95	Photochemistry	5–30 eV
21	9.3.1	9.3.1	Bend	Nov-94	NEXAFS, TOF spectroscopy	2.2–6 keV
22	9.3.2	9.3.2	Bend	Apr-94	Spectroscopy, Circular dichroism	30–1400 eV
23	10.0.1	10.0.1.1	U10	Jun-98	Angle-resolved photoemission spectroscopy	17–340 eV
		10.0.1.2	U10	Jun-98	Ion spectrometer	17–340 eV
		10.0.1.3	U10	Jun-98	Gas-phase photoelectron spectroscopy	17–340 eV
24	10.3.1	10.3.1	Bend	Oct-93	X-ray fluorescence microprobe	3–20 keV
25	10.3.2	10.3.2	Bend	Oct-94	Micro x-ray absorption spectroscopy	3–17 keV
26	11.3.1	11.3.1	Bend	Dec-01	Small-molecule crystallography	6–17 keV
27	11.3.2	11.3.2	Bend	Oct-99	Inspection of EUV lithography masks	50–1000 eV
28	12.0.1	12.0.1.1	U8	Dec-95	EUV optics testing, interferometry, coherent optics	60–320 eV
		12.0.1.2	U8	Dec-01	Angle-resolved photoemission spectroscopy	20–320 eV

Figure 3. Table of operational beamlines. Beamlines at the ALS are numbered x.y.z., where x is the sector number, y is the port number within the sector, and z is the branchline number. Branchlines generally have their own monochromators and may service multiple end stations. In the table, “beamlines” are defined as branchlines that can operate simultaneously. By this criterion, the ALS has 28 beamlines.

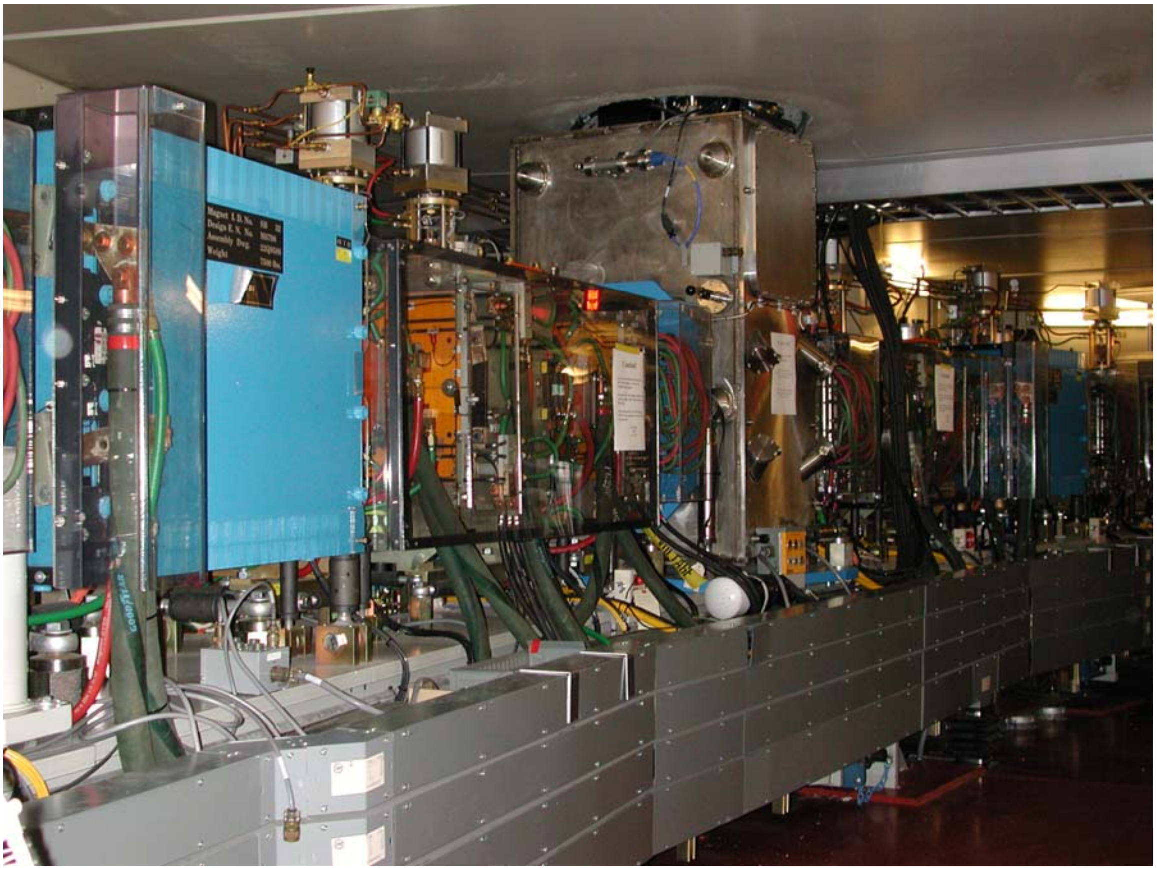

Figure 4. Superconducting dipole magnet (large silver-colored magnet in center) in the Advanced Light Source storage ring. Since the August 2001 installation of the superbends in three of the 12 sectors , which has extended the ALS spectral range well into the hard x-ray spectral region, several new beamlines for protein crystallography have become operational. Additional beamlines are under construction or planned for crystallography, tomography, and high-pressure research (diffraction and spectroscopy).

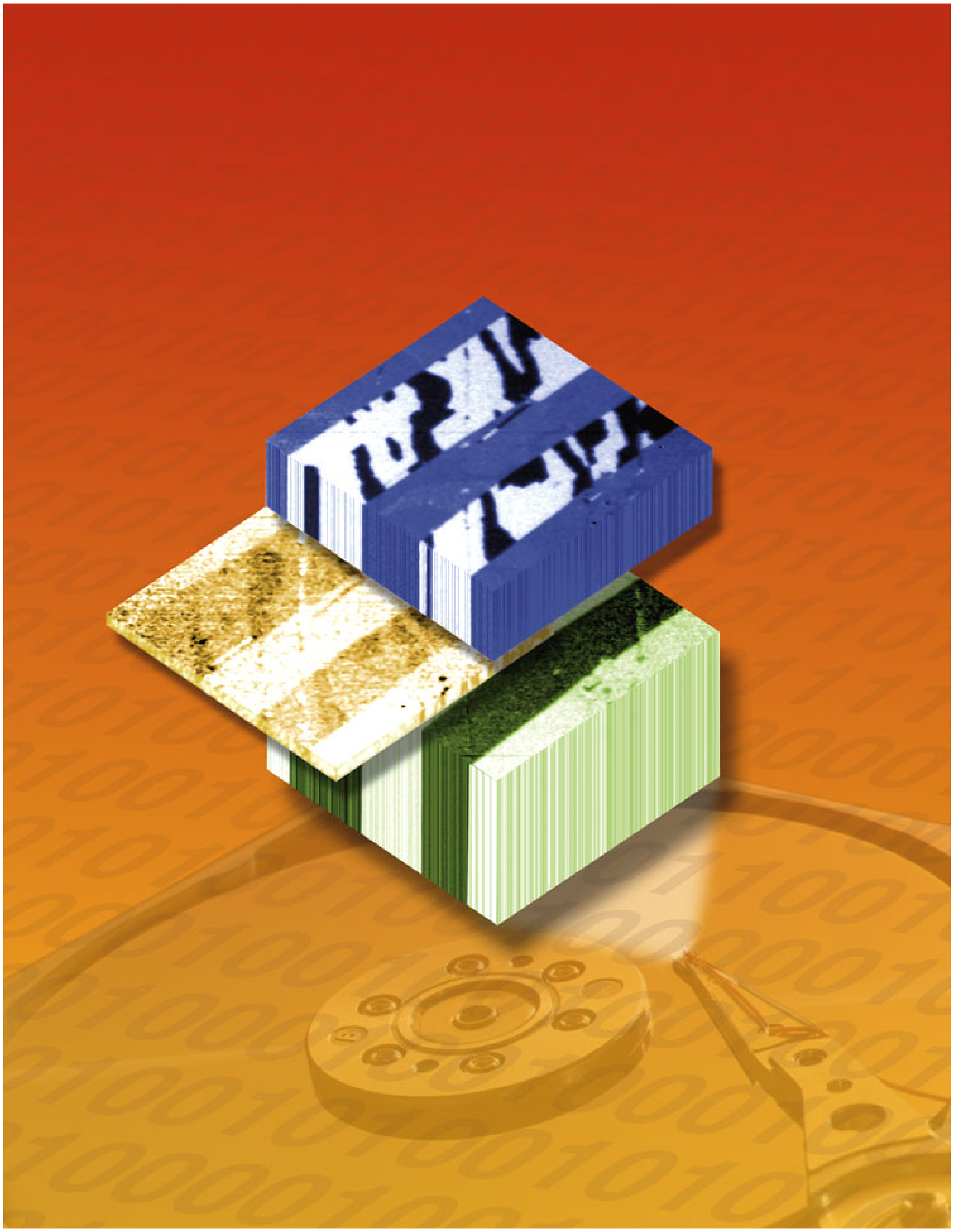

Figure 5. The phenomenon of exchange bias plays a key role in advanced magnetic-device technology based on the giant magnetoresistance (GMR) effect. Photoelectron microscopy of the magnetic domain structure in the multiple nanometer-thick layers comprising GMR devices is providing a large scientific collaboration a look at how exchange bias works. (Image courtesy of Hendrik Ohldag, Universität Düsseldorf, Stanford Synchrotron Radiation Laboratory, and Advanced Light Source)

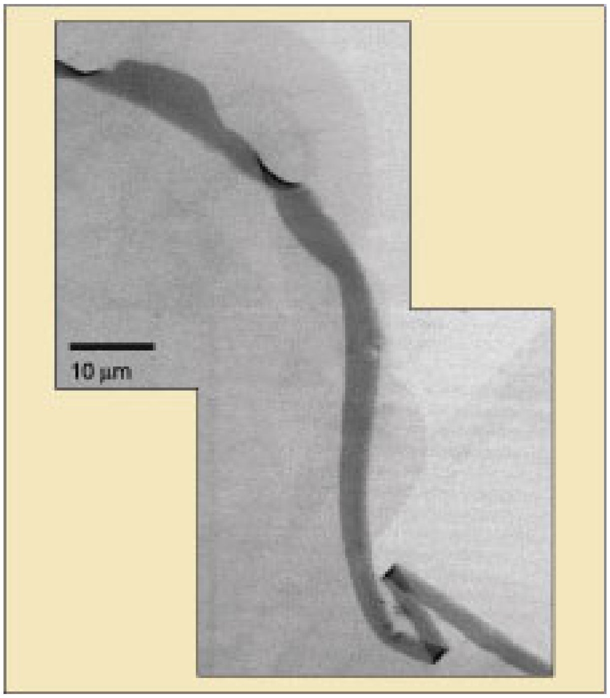

Figure 6. The global market for disposable diapers is $20 billion annually, and superabsorbent polymers are a key ingredient. Researchers from the Dow Chemical Company received the company's highest research award for their work, including an x-ray microscopy study of the shell surrounding beads of polymer, a study that was instrumental to the design of the process technology in a new superabsorbent-polymer manufacturing plant. (Image courtesy of Gary Mitchell, Dow Chemical Company)

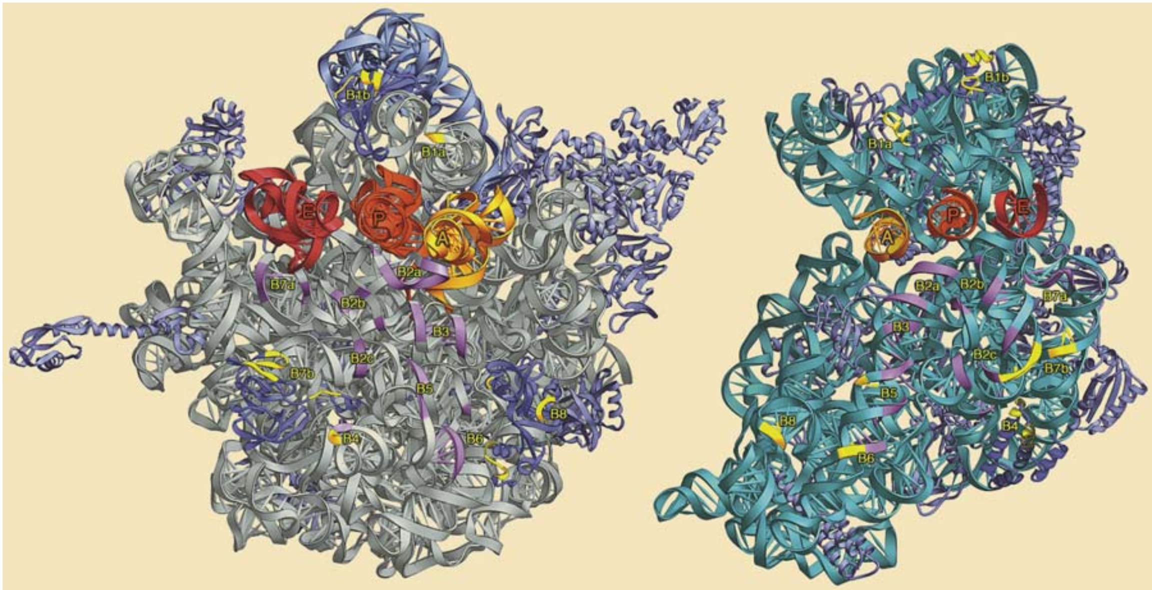

Figure 7. Scientists from the University of California, Santa Cruz, and their co-workers have determined the structure of a complete ribosome to the highest spatial resolution yet. Large multicomponent complexes responsible for manufacture of proteins following the formulas encoded in cellular DNA, ribosomes play an essential role in all living organisms. (Image courtesy of Harry Noller, University of California, Santa Cruz)

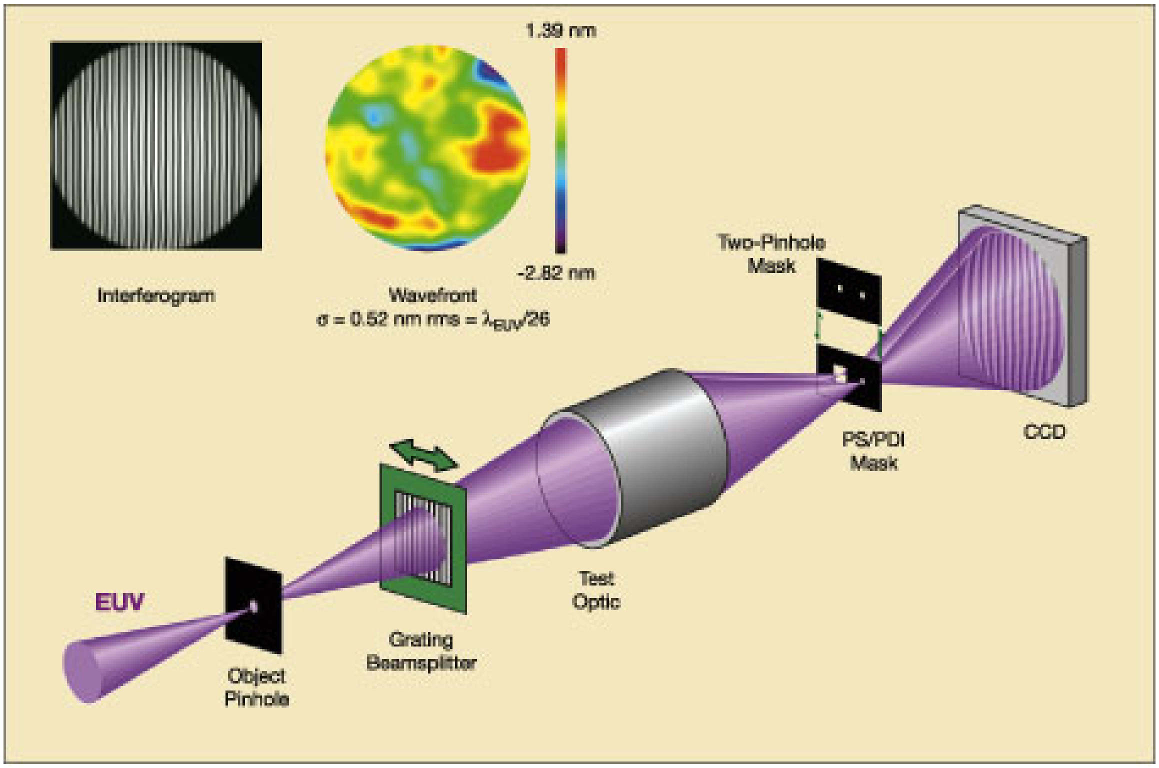

Figure 8. As microchip features grow ever smaller, Intel and other chip manufacturers have joined with DOE national laboratories to develop extreme ultraviolet (EUV) lithography as the next-generation technology for imprinting circuit patterns. As part of this project, EUV interferometry measures any errors in the shape of the reflecting mirrors, essential components of the prototype lithography systems now being tested. (Images courtesy of Kenneth Goldberg, Lawrence Berkeley National Laboratory)