X-ray and Neutron Scattering Facilities

Portfolio Description

This activity supports the operation of four synchrotron radiation light sources and three neutron scattering facilities. These are: the Advanced Light Source (ALS) at Lawrence Berkeley National Laboratory (LBNL); the Advanced Photon Source (APS) at Argonne National Laboratory (ANL); the National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory (BNL); the Stanford Synchrotron Radiation Laboratory (SSRL) at the Stanford Linear Accelerator Center (SLAC); the High Flux Isotope Reactor (HFIR) at Oak Ridge National Laboratory (ORNL); the Manuel Lujan Jr. Neutron Scattering Center (Lujan Center) at Los Alamos National Laboratory (LANL); and the Spallation Neutron Source (SNS) at ORNL, which is the most powerful short-pulse spallation neutron source in existence. The construction of the free-electron laser facility, Linac Coherent Light Source (LCLS) at SLAC will be completed in June 2010, providing laser-like radiation in the short x-ray region of the spectrum with 10 orders of magnitude greater peak power and brightness than that available from any existing synchrotron radiation x-ray light source. Under construction is the NSLS-II which will replace NSLS to enable the study of material properties and functions at the nanoscale level and to provide the world's finest x-ray imaging capabilities.

Unique Aspects

The synchrotron radiation light sources and the neutron scattering facilities are the most advanced facilities of their kind in the world. Together, they serve more than 10,000 users annually from academia, Department of Energy (DOE) national laboratories, and industry, a number that has more than tripled in the past decade and that can more than double again in the next decade as current facilities and those under construction are fully instrumented. These light sources and neutron scattering sources represent the largest collection of such facilities operated by a single organization in the world. Conception, design, construction, and operation of these facilities, which in current costs are in the hundreds of millions to in excess of a billion dollars, are among the core competencies of the BES program.

Relationship to Other Programs

This activity has very strong interactions with all BES programmatic research that use synchrotron and neutron sources. This includes research in atomic physics, condensed matter and materials physics, chemical dynamics, catalysis, geosciences, high-pressure science, environmental sciences, engineering, biosciences, and much more. Interaction also exists with other parts of the Office of Science, notably the Office of Biological and Environmental Research, and DOE, notably the National Nuclear Security Administration, the Office of Energy Efficiency and Renewable Energy, and the Office of Environmental Management. There are frequent contacts with other federal agencies in order to better coordinate efforts in optimizing beamlines and instruments. This activity participates in a number of Office of Science and Technology Policy (OSTP) and National Science and Technology Council (NSTC) interagency activities, e.g., OSTP Interagency Working Groups on macromolecular crystallography at the synchrotron light sources and on neutron sources and instrumentation. This activity is establishing more frequent contacts with international user facilities such as ESRF, SPring-8, ILL, ISIS, and others. The objectives are to share experiences and to make optimal use of present facilities.

Significant Accomplishments

The synchrotron radiation light sources. During the past two decades, BES has been the nation's major supporter of synchrotron x-ray light sources. BES support pioneered new storage ring lattices for improved beam stability and brightness; developed wiggler and undulator insertion devices that provide 10-12 orders of magnitude greater brightness than the best conventional x-ray sources; and discovered or developed such powerful experimental techniques as magnetic x-ray scattering, microbeam diffraction, x-ray microscopy, photoelectron spectroscopy and holography, x-ray nanoprobe, full-field and diffraction imaging, Rapid Acquisition Pair Distribution Function (RA-PDF), inelastic x-ray scattering using nuclear resonances, extended x-ray absorption fine structure (EXAFS), and near-edge absorption fine structure (NEXAFS). The newly constructed fourth generation light source, LCLS, the world's first "hard" x-ray free-electron laser, has achieved its full performance specification and its first experimental station has successfully been commissioned. The unique capabilities of this facility have attracted 107 proposals involving 672 scientists from 22 countries for the Fall 2010 run.   The BES light sources are used by over 9,000 researchers annually from academia, government laboratories, and industry for state-of-the art studies in materials science, physical and chemical science, geoscience, environmental science, bioscience, medical science, and pharmaceutical science. Recent research at the light source facilities supported by BES, other agencies, industry, and private sponsors includes: infrared transmission measurements of dual-gated bilayer graphene revealed that electric field control of its bandgap may allow it to become a remarkably flexible component of nanoscale electronic devices; structural determinations of one of many human antibodies, H5-F10, which is able to neutralize different types of flu viruses including H5N1 'bird flu' and 1918 H1N1 'Spanish flu', points the way towards developing immunotherapy for curing viral diseases; determination of atomic to nanometer scale structural information to make the essential link between the synthesis and optimization of industrial process gas sensors will increase the combustion efficiency of combustion burners in furnaces and process heaters saving valuable energy; high-energy x-ray scattering data providing information on length scales from atoms to porous networks under various pressures within the oil shale may lead to the development of strategies enabling the economic and environmentally acceptable recovery of this fossil fuel resource; and particularly significant was the award of the 2009 Nobel Prize in Chemistry for studies on ribosome which works as a protein factory for all life organisms. This work was performed at the four BES supported synchrotron radiation facilities.

The neutron scattering sources **.** Since the late 1940s, BES, and its predecessors, has been the major supporter of neutron science in the United States—from the earliest work of Clifford Shull and E. O. Wollan at ORNL's Graphite Reactor in the 1940s to the Nobel Prize in Physics shared by Clifford Shull and Bertram Brockhouse in 1994 for their work on neutron scattering. Based on its experience in nuclear reactors and particle accelerators over the years, DOE developed research reactors and spallation sources as high-flux neutron sources for spectroscopy, scattering, and imaging and helped pioneer virtually all the instruments and techniques used at these facilities. Researchers at ANL, BNL, and ORNL led these pioneering advances. Most of the important techniques used today have been developed at ANL, BNL, and ORNL. Neutron scattering provides important information on the positions, motions, and magnetic properties of solids. Neutrons possess unique properties such as sensitivity to light elements, which has made the technique invaluable to polymer, biological, and pharmaceutical sciences. Neutrons also have magnetic moments and are thus uniquely sensitive probes of magnetic interactions. Neutron scattering studies have led to higher strength magnets for more efficient electric generators and motors and to better magnetic materials for magnetic recording tapes and computer hard drives. Finally, the high penetrating power of neutrons allows nondestructive property measurements deep within a specimen and has been used to study defects in automotive gears and brake discs and in airplane wings, engines, and turbine blades.

Recent research at the neutron scattering sources supported by BES includes: evidence that the same mechanisms responsible for superconductivity could be present for copper-based high temperature superconductors and the recently discovered iron-based superconductors; the study of enzymatic digestion of cell wall cellulose biopolymer whose breakdown into fermentable sugars is critical to producing biofuels for transportation; the study of the mobility of ions in room temperature ionic liquids which are promising ionic charge-carrying media for advanced batteries and supercapacitors; and the study of the atomic structure bond lengths and angles of new geopolymer-based concrete which emits 80 to 90 percent less carbon dioxide than standard concrete during the curing process. Curing reactions in traditional concrete are estimated to account for 5 to 9 percent of anthropogenic carbon dioxide emissions. In addition, at HFIR there was an ongoing program for the production of important medical and industrial isotopes and for studying the effects of neutron irradiation on nuclear materials for fission and fusion reactors.

Mission Relevance

These facilities were born from the most fundamental of needs, i.e., the need to characterize materials at the atomic and molecular level. In order to understand, predict, and ultimately control materials properties, it is necessary to determine the atomic constituents of materials, the positions of the atoms in materials, and how the materials behave under the influence of external perturbations such as temperature, pressure, magnetic or electric field, chemical attack, and excitation by photons, electrons, and other particles. A large number of experimental and theoretical tools are used to achieve these ends. In the last two decades, the experimental demands have motivated the development of centralized facilities, like the ones in existence for synchrotron radiation and neutron scattering. Such highly sophisticated and expensive tools are by nature centralized and staffed with specialists that provide to the user community expertise in order to optimize the scientific use of the facility. The development, construction, and operation of these facilities are one of the most important missions and core competencies of BES. The scientific accomplishments of these facilities, as determined by triennial peer review, are reflected in the large number of publications appearing annually in the most important scientific journals.

Scientific Challenges

The synchrotron radiation light sources. First, the x-ray beam stability has always been a top priority and challenge for synchrotron facilities. The ability to produce nanoscale size x-ray beam has amplified this challenge. Second, the facilities must be operated optimally, which means optimizing instrument-hours of operation, not just accelerator hours of operation, and making the instruments widely available to the general user community. Third, optimal utilization of the LCLS coherent short-wavelength x-ray source will require successful fabrication, installation, and commissioning of advanced instruments.

The neutron scattering sources. New instrumentation at HFIR and SNS must be successfully integrated into robust user programs producing world-class scientific results.

Projected Evolution

X-ray and neutron scattering will continue to play a central role in the growth of BES programmatic science. The facilities will need continuous growth and advanced in terms of beamline upgrades, new neutron scattering instruments, and increase in availability of user time. The set of instruments associated with these facilities provides unique scientific and technical capabilities, rarely available in other parts of the world. These facilities need to be kept in an optimal operational condition in order to maintain and increase the tremendous scientific achievements they have facilitated.

The SNS at ORNL will be for years to come the most important neutron spallation source in the world. It is important to foster full use and judicious increases in the capabilities of SNS in order to optimize its utilization by the scientific community.

Finally, the LCLS will have properties vastly exceeding those of current x-ray sources in three key areas: peak brightness, coherence, and ultrashort pulses. The peak brightness of the LCLS is 10 orders of magnitude greater than current synchrotrons; the light is coherent or "laser like" enabling many new types of experiments; and the pulses are short (70 femtoseconds in standard operation with planned improvements that will further reduce the pulse length), enabling studies of fast chemical and physical processes. These characteristics open new realms of scientific applications in the chemical, material, and biological sciences including fundamental studies of the interaction of intense x-ray pulses with simple atomic systems, structural studies on single nanoscale particles and biomolecules, ultrafast dynamics in chemistry and solid-state physics, studies of nanoscale structure and dynamics in condensed matter, and use of the LCLS to study matter under extreme conditions.