Research Activity: X-ray and Neutron Scattering Facilities

Division: Materials Sciences
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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; the **Advanced Photon Source** (APS) at Argonne National Laboratory; the **National Synchrotron Light Source** (NSLS) at Brookhaven National Laboratory; the **Stanford Synchrotron Radiation Laboratory** (SSRL) at Stanford Linear Accelerator Center; the **High Intensity Flux Reactor** (HFIR) at Oak Ridge National Laboratory; the **Intense Pulsed Neutron Source** (IPNS) at Argonne National Laboratory; and the **Manuel Lujan Jr. Neutron Scattering Center** (Lujan Center) at Los Alamos National Laboratory.

Under construction is the **Spallation Neutron Source** (SNS) at Oak Ridge National Laboratory, which is a next-generation short-pulse spallation neutron source that will be significantly more powerful than the best spallation neutron source now in existence -- ISIS at the Rutherford Laboratory in England. On the drawing board is the **Linac Coherent Light Source** (LCLS) at Stanford Linear Accelerator Center, which is a free-electron laser that will provide laser-like radiation in the x-ray region of the spectrum that is 10 orders of magnitude greater in peak power and peak brightness than any existing coherent x-ray light source.

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 7,000 users annually from academia, 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 Others:

This activity has very strong interactions with all BES programmatic research that utilizes 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 BER, and the Department of Energy, notably DP, EE, and EM. There are frequent contacts with other agencies in order to better coordinate efforts in optimizing beamlines and instruments. This activity participates in a number of OSTP and NSTC interagency activities, e.g., OSTP Interagency Working Groups on macromolecular crystallography at the synchrotron light sources and on neutron sources and instrumentation. Finally, this activity is starting to establish more frequent contacts with international user facilities such as ESRF, SPring-8, ILL, ISIS, and others. The objective is 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, inelastic x-ray scattering using nuclear resonances, extended x-ray absorption fine structure (EXAFS), and near-edge absorption fine structure (NEXAFS). The BES light sources are used by over 6,500 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, by other agencies, by industry, and by private sponsors includes: high-resolution imaging of precision-fabricated thin films of copper, pointing the way toward much denser magnetic data storage for computers; imaging of contaminants in a polycrystalline silicon solar cell and their removal by heat treatment -- a step toward more efficient, less costly solar cells; development of a high-pressure "diamond anvil cell" enabling the creation of entirely new classes of materials such as biomaterials, semiconductor phases, and dense polymers; the solution of the structure of HIV (the AIDS virus) laying the groundwork for developing a vaccine; and the determination of the structure of a key (immunoglobulin-E) antibody receptor on immune system cells, opening the way to prevention of allergic reactions.

The neutron scattering sources. Since the late 1940s, BES and its predecessors have been the major supporter of neutron science in the United States -- from the earliest work of Clifford Shull and E. O. Wollan at Oak Ridge National Laboratory'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, the Department 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 Oak Ridge, Brookhaven, and Argonne National Laboratories led these pioneering advances. Most of the important techniques used today have been developed at Argonne, Brookhaven and Oak Ridge National Laboratories. 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 automotive gears and brake discs, and defects in airplane wings, engines, and turbine blades.

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, 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 has 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 utilization 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, in the thousands.

Scientific Challenges:

The synchrotron radiation light sources. First, completion of SPEAR3 at SSRL will require upgrading the beamlines to make full utilization of the new more powerful radiation source. Second, the concepts of Participating Research Teams (PRTs) used at the NSLS and Collaborative Access Teams (CATs) used at the APS will be revisited; PRTs were extremely useful in the first decades of operation of NSLS as were CATs in the first years of operation of the APS. However, the larger, more diverse, and less experienced user base at all of the light sources may require new paradigms of operation to address new needs. Third, 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. Fourth, the promise of a coherent, short-wavelength x-ray source from the LCLS will require completely new instrument and experiment concepts.

The neutron scattering sources. First, the upgrades and new instrumentation at HFIR must be completed in a timely way to facilitate a robust user program. Second, the Lujan Center must show reliable, user-friendly operation with its robust suite of new and upgraded instruments.

Funding Summary:

Dollars in Thousands

Operations Funding	FY 2000	FY 2001	FY 2002
Advanced Light Source	30,652	35,605	37,605
Advanced Photon Source	84,783	90,314	90,314
National Synchrotron Light Source	30,955	34,470	34,720
Stanford Synchrotron Radiation Laboratory	22,493	21,696	21,446
High Flux Beam Reactor	18,878	15,341	0
High Flux Isotope Reactor	37,734	37,197	38,485
Intense Pulsed Neutron Source	12,739	13,833	16,080
Manuel Lujan, Jr. Neutron Scattering Center	6,968	9,190	9,190
Spallation Neutron Source	17,900	19,059	15,100
REDC	6,809	6,512	6,712
Total, Operations Funding	269,911	283,217	269,652
Construction and MIE Funding			
Spallation Neutron Source			
Beamline (ALS)	750	1,800	1,950
Instruments (Lujan Center)	3,500		
SPEAR3 Upgrade (SSRL)		10000	9000
HB-2 Beam Tube Extension (HFIR)	1,600	1,150	
Neutron Scattering Instruments (HFIR)		0	2,000
Total, MIE's	5,850	12,950	12,950
Total	275,761	296,167	282,602

Projected Program 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 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. One needs to keep these facilities in an optimal operational mode in order to maintain and increase the tremendous scientific achievements they have facilitated.

One needs to foresee the instrumentation and scientific needs required by the future operation of the SNS at ORNL. The SNS will be for years to come the most important neutron spallation source in the world. It is important to be prepared for full utilization and judicious increases in the capabilities of SNS as recommended by all advisory committees to the Department.

Finally, the proposed 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 (230 femtoseconds 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 create plasmas.

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