

Research Activity: **Neutron and X-ray Scattering Facilities**
Division: Scientific User Facilities
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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 (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 Intensity Flux Reactor (HFIR) at Oak Ridge National Laboratory (ORNL); the Intense Pulsed Neutron Source (IPNS) at ANL; 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 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. Under construction is the Linac Coherent Light Source (LCLS) at SLAC, 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. R&D is underway on the NSLS-II which will be built as a replacement for NSLS-I 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 7,000 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 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 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 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 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, in the thousands.

Scientific Challenges:

The synchrotron radiation light sources. First, completion of SPEAR3 at SSRL requires upgrading the beamlines to make full use of the new more powerful radiation source. 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, 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 SNS must successfully perform its commissioning and early operational phases.

Funding Summary:

Dollars in Thousands

	FY 2005	FY 2006	FY 2007 Request
Advanced Light Source	44,800	42,783	49,802
Advanced Photon Source	100,500	95,890	108,604
National Synchrotron Light Source	36,750	36,196	40,763
Stanford Synchrotron Radiation Laboratory	32,388	25,475	35,836
High Flux Isotope Reactor	46,900	43,330	51,598
Intense Pulsed Neutron Source	16,800	15,500	18,531
Manuel Lujan, Jr. Neutron Scattering Center	9,588	10,000	10,582
Spallation Neutron Source	37,600	101,001	171,409
REDC	4,500	---	---
Neutron and X-ray Scattering Facilities, Total	329,826	370,175	487,125

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 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 mode in order to maintain and increase the tremendous scientific achievements they have facilitated.

The instrumentation and scientific needs required by the future operation of the SNS at ORNL will be identified and addressed. 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 use and judicious increases in the capabilities of SNS as recommended by all advisory committees to DOE.

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 (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.