Research Activity: X-ray and Neutron Scattering

Division: Materials Sciences and Engineering
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Portfolio Description:

This activity supports basic research in condensed matter and materials physics using neutron and x-ray scattering capabilities primarily at major BES-supported user facilities. Research is aimed at achieving a fundamental understanding of the atomic, electronic, and magnetic properties of materials and their relationship to the physical properties of materials. Both ordered and disordered materials are of interest as are strongly correlated electron systems, surface and interface phenomena, and behavior under environmental variables such as temperature, pressure, and magnetic field. Development of neutron and x-ray instrumentation for next generation sources is a major component of the portfolio.

Unique Aspects:

The Department's history and mission has played an important role in BES's current position as the Nation's steward of major neutron and x-ray facilities. Historically, neutron sources descended from the neutron reactors that were constructed in the early 1940s as part of the U.S. Atomic Energy Program. Similarly, synchrotron facilities stemmed from particle accelerators that were developed for high-energy physics research. As part of its stewardship responsibilities, BES maintains strong fundamental research programs in materials and related disciplines that are carried out at these facilities by the laboratory, university, and industrial communities. This activity has evolved from the pioneering, Nobel prize-winning efforts in materials science to the current program that encompasses multiple techniques and disciplines. The activity also supports the research that has motivated the largest BES construction projects in recent years - the ALS, APS, and SNS. BES is a major supporter of both the research and the instrumentation at these and other facilities.

The type of information derived from neutron and x-ray scattering is very diverse with inelastic scattering allowing measurements of elastic, magnetic, and charge excitations (phonons, magnons, crystal field energies) and elastic scattering affording structural information. X-ray scattering allows researchers to "see" where the atoms are as x-ray wavelengths are commensurate with interatomic distances. The dramatic increase in brilliance of synchrotron radiation has directly improved the available photon flux to probe a limited sample volume over a small time domain making in-situ experiments a reality. Neutron scattering can afford information concerning 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 and biological sciences, and high penetrating ability, which allows property measurements deep within a specimen. Neutrons have magnetic moments and are thus uniquely sensitive probes of magnetic interactions. Taken together, neutron and x-ray scattering cover an enormous range of energies and allow multiple length scales and associated phenomena to be probed.

Relationship to Others:

This activity interacts closely with neutron and x-ray scattering research programs supported at other federal agencies, especially in the funding of beamlines whose cost and complexity require multi-agency support. The activity works in concert with the Instrumentation for Materials Research Program (IMR) at the National Science Foundation and the NIST Center for Neutron Research (NCNR) in the Department of Commerce to develop instruments and capabilities that best serve the national user facility needs of the nation. A coordinated effort between the Department of Energy (DOE) and the National Science Foundation (NSF) is being initiated to facilitate the full utilization of the SNS under the auspices of the Office of Science and Technology Policy's Interagency Working Group on Neutron Science.

Significant Accomplishments:

This activity supported the research of Clifford G. Shull at Oak Ridge National Laboratory that resulted in the 1994 Nobel Prize in Physics for the development of the neutron diffraction technique. Shull's work launched the field of neutron scattering, which has proven to be one of the most important techniques for elucidating the structure and dynamics of solids and fluids. Shull and others produced an impressive list of "firsts": first measurement of neutron scattering amplitudes of over 60 elements and isotopes; first direct evidence of antiferromagnetism; first use of neutrons to determine the structure of hydrides; and the first measurements of 3d and 4f electronic form factors. This activity has provided major support for the construction and operation at APS for 10 of the 19 Collaborative Access Teams (CATs). The majority of the CATs are now operational, and the resultant myriad tools provide an invaluable resource to the nation's science community.

The neutron scattering program has been a key player in the effort to understand superconductivity. Jorgenson (ANL) was the first to determine the structure of several high-temperature superconductors using neutron diffraction. In attempting to understand the role of stripes, Tranquada (BNL) provided the first direct evidence that holes segregate into stripes separated by insulating regions of antiferromagnetic order. Mook (ORNL) found evidence of fluctuating stripes suggesting stripes and superconductivity are linked.

Recent accomplishments include the first measurement of protein structure via high resolution x-ray powder diffraction by von Dreele (LANL), the discovery via high resolution x-ray powder diffraction of the universal presence of a previously undetected lower symmetry phase in ferroelectrics with unusually large dielectric responses by Noheda and Shirane (BNL), and the development and demonstration of a new class of instrumentation called the 3-D x-ray crystal microscope that provides precise local information about crystal morphology, orientation, elastic strain and plastic deformation with subgrain 3-D spatial resolution by Ice and Larson (ORNL).

Mission Relevance:

To understand the physical properties of any material, one needs to begin with its structure. The fundamental understanding of the structure and behavior of matter contributes to the Nation's science base and underpins DOE's broad energy and environmental mission and responsibilities. X-ray and neutron scattering are the primary tools for characterizing the atomic, electronic and magnetic structures and excitations of materials. The increasing complexity of such energy-relevant materials as superconductors, semiconductors, and magnets requires ever more sophisticated, specific, and sensitive X-ray and neutron scattering techniques to extract new and useful knowledge and develop new theories for the behavior of new materials. The scientific importance of x-ray and neutron science has been broadly recognized as some 15 Nobel Prizes (14 in x-rays; 1 in neutrons) have been based on research utilizing these tools.

Scientific Challenges:

Programmatic Challenges:

The ongoing enhancements at the HFIR and the LANSCE will not only increase the nation's neutron scattering capacity, but, in many cases, will provide instruments with resolution and flux on sample that is equal to or greater than existing benchmark instruments. The SNS will push instrument capacity and performance even further. One challenge for this activity will be to support an increased effort in neutron scattering to take full advantage of the improved sources and to prepare for the SNS. Another includes maintaining the strength at the DOE laboratories that have traditionally been strong in neutron scattering and rebuilding strength in neutron sciences in the academic community. Education and training of the next generation of neutron scientists especially those familiar with instrumentation and performance of TOF methods remains a high priority. Strategies to replace or ameliorate the capabilities lost from the closing of HFBR, especially triple axis instrumentation, continue to be discussed including support from other agencies.

Scientific Challenges*:*

Correlated Electron Systems: The effects of strong electron-electron interactions give rise to a remarkable range of anomalous behavior in condensed matter systems, producing phenomena as varied as metal-insulator transitions, colossal magnetoresistance, and high temperature superconductivity in heavy fermion metals, insulators and magnets. In particular, high-temperature superconductivity is a singularly spectacular example of the cooperative macroscopic phenomena such as the interplay of charge, spin, and lattice degrees of freedom that can arise from correlated electron behavior. Techniques such as inelastic x-ray scattering and neutron diffraction, among others, have enabled scientists to unravel the crystallographic and microscopic electronic structure of these materials, including stripes. This information will ultimately be used to answer questions such as what is the mechanism for superconductivity, how high can the temperature be for materials to remain superconducting, and will that temperature ever be room temperature.

Matter Under Extreme Conditions: Opportunities in high pressure research address a broad range of new scientific problems involving matter compressed to multimegabar pressures. Highly collimated and intense synchrotron beams provide the ideal source for ultrafine and sensitive x-ray diffraction microprobes necessary to measure concentrated high stresses in a very small area. Extreme pressures provide a fertile ground for the formation of new materials and novel physical phenomena as compression changes the chemical bonds and affinities of otherwise familiar elements and compounds. Likewise, the coupling of magnetic fields during a scattering experiment can be used to study materials during phase transitions (magnetic, structural, superconducting) thus allowing researchers to segregate magnetic field effects or to simulate effects normally observed via doping (for example).

In-situ Studies of Complex Materials: Recent advances in both sources and instrumentation have yielded gains in intensity on sample not just facilitating rapid experiments but also in-situ configurations. Also smaller samples at higher concentrations can be probed. In-situ synchrotron radiation techniques provide real-time observations of atomic arrangements with high spatial sensitivity and precision, which are important features in the development of novel processing techniques and in the search for new exotic materials. In-situ studies of complex materials including those undergoing time-dependent structural or magnetic phase transformations, disordered systems such as alloys and amorphous materials, organic thin films and self-assembled systems, and other condensed matter systems can be probed with a variety of scattering, reflectivity and spectroscopic techniques.

Funding Summary:

Dollars in Thousands

FY 2000	FY 2001	FY 2002
$22,076	$31,682	$36,293

Performer	Funding Percentage
DOE Laboratories	70.0%
Universities	29.0%
Other	1.0%

Major DOE laboratory performers include Ames, ANL, BNL, ORNL, LANL, SSRL.

This activity also supports diverse Collaborative Access Teams at the APS including; MRCAT (Materials Research CAT; Notre Dame, U. Florida, ANL), MUCAT (Midwestern Universities CAT; Ames, Missouri, Washington U., etc.), PNCCAT (Pacific Northwest CAT; U. Washington, PNNL, U. Florida), UNICAT (University-National Lab-Industry CAT; Illinois, NIST, UOP, ORNL), HP-CAT (High Pressure CAT; Carnegie Institute, UNLV, LLNL), BESSRC (Basic Energy Sciences Synchrotron Radiation Center; ANL), MHATTCAT (University of Michigan, Howard U., Lucent), CMCCAT (Complex Materials Consortium; Exxon, Princeton, U Penn, BNL, LANL, ORNL, etc.), IMMCAT (IBM, McGill, MIT), and DNDCAT (DuPont, MWU, DOW).

This activity also provides support for the construction of two instruments at the SNS including the High-Resolution Chopper Spectrometer (ARCS) instrument led by Brent Fultz at CalTech and the 10-100□eV Multi-Chopper Spectrometer instrument led by Paul Sokol.

Projected Evolution:

Advances in neutron and x-ray scattering will continue to be driven by the scientific opportunities presented by improved source performance and instrumentation optimized to take advantage of that performance. The x-ray scattering activity will continue in fully developing the capabilities of the third generation sources by providing instrumentation and research support. A continuing theme in the scattering program will be the integration and support of materials preparation (especially single crystals) as this is a core competency that has all but vanished in the US. An example of this integrated program is the high magnetic field/low temperature synchrotron facility at SSRL funded in conjunction with single crystal growth and characterization capabilities at Stanford.