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 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 nuclear 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. Neutron and x-ray scattering are well-established techniques for investigating the microscopic properties of materials. With the advent of both high brightness x-ray beams produced by third generation synchrotron radiation facilities and intense pulsed neutron beams provided by accelerator-based neutron sources, a number of totally new capabilities will become possible.

Neutron Scattering. Neutron scattering provides information on the positions, motions, and magnetic properties of solids. With unique characteristics such as sensitivity to light elements, neutron scattering has proven to be invaluable to polymer and biological sciences. The high penetrating ability of neutrons allows property measurements and nondestructive evaluation deep within a specimen. Neutrons have magnetic moments and are thus uniquely sensitive probes of magnetic species within a sample. The wavelength of neutrons used in scattering experiments is commensurate with interatomic distances, and their energy (meV) is comparable to both lattice and magnetic excitations (phonons and magnons) making them an ideal probe for both structure and dynamics.

X-ray Scattering. The unique properties of synchrotron radiation – high flux and brightness, tunability, polarizability, high spatial and temporal coherence, along with the pulsed nature of the beam – afford a wide variety of experimental techniques in diffraction and scattering, spectroscopy and spectrochemical analysis, imaging, and dynamics.

Relationship to Others:

This activity interacts closely with research instrumentation 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 -- Major Instrumentation Projects (IMR-MIP) 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. A coordinated effort between the Department of Energy (DOE) and the National Science Foundation (NSF) is ongoing to facilitate the full utilization of the nation's neutron scattering facilities under the auspices of the Office of Science and Technology Policy's Interagency Working Group on Neutron Science. Interaction with ISIS and ILL in the training of post-doctoral fellows and neutron detector development is also underway. In FY2003, the program coordinated with the DOE's SBIR Program which resulted in 6 Phase I and 2 Phase II awards in the area of neutron detectors, monochromators and other scattering instrumentation.

Significant Accomplishments:

Neutron Scattering. 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. The program supports major efforts in neutron scattering centered primarily at the DOE laboratories- Ames, ANL, BNL, ORNL, LANL- and these groups have pioneered virtually all the instruments and techniques in neutron scattering, spectroscopy, and imaging.

X-ray Scattering. As in the neutron scattering effort, the program supports large research groups that utilize synchrotron radiation to understand the intrinsic properties of materials. These groups have contributed to the development of such powerful techniques as magnetic x-ray scattering, inelastic x-ray scattering, extended x-ray absorption fine structure (EXAFS), x-ray microscopy, microbeam diffraction, time-resolved spectroscopy and others.

Recent accomplishments include the development of ^{3}He spin filters for the production of polarized neutrons, the first evidence of icosahedral ordering in liquid metals by in-situ x-ray diffraction, the first measurements of local deformation in bulk materials on the mesoscale using combined x-ray microscopy and nanoindentation, the demonstration of the existence of electron-lattice polarons in colossal magnetoresistive manganites via single crystal x-ray and neutron scattering, the confirmation of stripe domains in ferroelectric thin films as shown by in-situ x-ray diffraction, and the formation of "nanowater wires" in zeolites by applying simultaneous pressure and temperature using a hydrothermal diamond anvil cell.

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. Additionally, neutrons will play a key role in the President's Hydrogen Fuel Initiative as they provide atomic- and molecular-level information on structure, hydrogen diffusion, and interatomic interactions, as well as the nanoscale and macroscopic morphologies that govern useful properties in catalysts, membranes, proton conductors, hydrogen storage materials, and other materials and processes related to hydrogen production, storage, and use.

Scientific Challenges:

Programmatic Challenges:

Neutron Scattering. The ongoing enhancements at the HFIR 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 research effort in neutron scattering to take full advantage of the improved sources and to prepare for the SNS. Another includes maintaining the strength of the DOE lab-based neutron scattering groups 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.

X-ray scattering. Major instruments at the synchrotron light sources have a lifetime of 7-10 years. Thus a challenge to the program is to provide support for the 10-15% of the instruments which must be upgraded or replaced each year to keep the facility at the forefront of science.

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. 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. 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. With the development of the SNS, innovative focusing optics, more sensitive detectors and emerging next-generation pressure cells, high pressure research at neutron sources can approach the routine pressure ranges available with diamond anvil cells at synchrotron x-ray sources. With the dramatic advances in techniques for preparing and investigating single crystals, studies of more complex materials become tractable. Similarly, scattering experiment performed in the presence of magnetic fields 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 facilitating rapid experiments and in-situ configurations. Smaller samples can be probed with unprecedented resolution, accuracy, and sensitivity under various parametric conditions. 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 2003	**FY 2004**	**FY 2005 Request**
37,821	41,877	42,058

Performer	**Funding Percentage**
DOE Laboratories	76%
Universities	24%

Major DOE laboratory performers include Ames, ANL, BNL, ORNL, LANL, SSRL.
This activity also provides support for the construction of seven instruments at the SNS including; High-Resolution Chopper Spectrometer (ARCS), Cold Neutron Chopper Spectrometer (CNCS), Ultra High Pressure Diffractometer (SNAP), High Resolution Thermal Chopper Spectrometer (SEQUOIA), Single Crystal Diffractometer (SCD), Disorder Materials Diffractometer (NOMAD) and the Hybrid Spectrometer (HYSPEC). Also under construction at DOE synchrotron radiation facilities are: APS; Inelastic Scattering Beamline, High Pressure Beamline, Powder Diffraction Beamline; NSLS; Microdiffraction beamline; ALS; Inelastic Scattering Beamline, AMO physics beamline upgrade; SSRL; Soft-X-ray Facility for Nanoscale Materials and Phenomena.

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 and neutron scattering activity will continue in fully developing the capabilities at the DOE facilities 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 is vital to US interests.