

Research Activity: **Neutron and X-ray Scattering**
Division: Materials Sciences and Engineering
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Portfolio Description:

This activity supports basic research in condensed matter physics and materials physics using neutron and x-ray scattering capabilities, primarily at major BES-supported user facilities. Research seeks to achieve a fundamental understanding of the atomic, electronic, and magnetic structures and excitations of materials as well as the relationship of these structures and excitations to the physical properties of materials. The continuing development and improvement of next-generation instrumentation including a full range of elastic, inelastic, and imaging techniques as well as ancillary technologies such as novel detectors, sample environment, data analysis, and technology for producing polarized neutrons is also supported.

Unique Aspects:

The Department of Energy (DOE) history and mission have played important roles in BES' 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 Advanced Light Source (ALS), Advanced Photon Source (APS), and Spallation Neutron Source (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, and 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 Other Programs:

This activity interacts closely with research instrumentation programs supported at other federal agencies, especially in the funding of beam lines 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 (NSF) and the National Institute of Standards and Technology (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 DOE and NSF is ongoing to facilitate the full use of the nation's neutron scattering facilities under the auspices of the Office of Science and Technology Policy Interagency Working Group on Neutron Science.

Significant Accomplishments:

Neutron Scattering - This activity supported the research of Clifford G. Shull at Oak Ridge National Laboratory (ORNL) 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 national laboratories of Ames, Argonne, Brookhaven, Oak Ridge, and Los Alamos; 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 use synchrotron radiation to understand the intrinsic properties of materials. These groups have contributed to the development of such powerful techniques as inelastic x-ray scattering, extended x-ray absorption fine structure (EXAFS), x-ray microscopy, microbeam diffraction, time-resolved spectroscopy, and resonant techniques providing specific chemical, magnetic, and excitation contrast in the scattering signal.

Recent accomplishments include sensitive measurements of surface segregated atomic and electronic structure in new catalysis alloys, as well as measurements of distortions in the atomic ordering resulting from the interfacial constraints on perovskites oxide films, leading to unique magnetic and electron transport behavior. Progress in understanding the rich magnetic and electronic structure of correlated electron materials continues in terms of mapping out phase boundaries and determining the nature of the competing quantum interactions behind transitions in physical properties. Refinements with in-situ techniques (including x-ray diffraction microscopy and grazing incidence surface x-ray scattering) have become more adept at probing small samples, surfaces, and interfaces under extreme processing environments of temperature, pressure, and reactive gases.

Mission Relevance:

The increasing complexity of energy-relevant materials currently of interest to the Office of Energy Efficiency and Renewable Energy such as superconductors, semiconductors, and magnets requires ever more sophisticated scattering techniques to extract useful knowledge and to develop new theories for the behavior of these materials. X-ray and neutron scattering, together with the electron scattering probes supported under Structure and Composition of Materials, are the primary tools for characterizing the atomic, electronic, and magnetic structures of materials. 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. The program is relevant to National Nuclear Security Administration in its activity on the behavior of matter in extreme environments, especially high pressure. This is the Nation's largest program in neutron and x-ray scattering in condensed matter physics and materials physics supporting the science performed with scattering tools, and the concomitant development of techniques and instrumentation. Consequently it underpins the facility stewardship role of DOE by enabling full exploitation of the BES synchrotron light sources and neutron scattering facilities. The scattering program interfaces with other programs in BES, including: Theoretical Condensed Matter Physics in scattering theory and models; Materials Chemistry and Biomolecular Materials in scattering probes and techniques for soft matter and biophysical materials interrogation such as spin echo spectroscopy, neutron reflectometry, and grazing incidence small angle scattering; Geosciences Research in high pressure neutron and x-ray scattering techniques and tools; and Heavy Element Chemistry in molecular level and surface actinide speciation information.

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 and how high can the temperature be for materials to remain superconducting?

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, and 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

<u>FY 2007*</u>	<u>FY 2008*</u>	<u>FY 2009*</u>
38,943	38,940	52,098
<u>Performer</u>	<u>Funding Percentage</u>	
DOE Laboratories	78%	
Universities	22%	

*Based on FY2007

Major DOE national laboratory performers include Ames, Argonne, Brookhaven, Oak Ridge, Los Alamos, and the Stanford Linear Accelerator Center.

Also supported is the operation of HPCAT (High Pressure Collaborative Access Team).

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 careful structural measurements related to materials properties.

Neutron Scattering - The ongoing enhancements at the High Flux Isotope Reactor (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 Spallation Neutron Source (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 such as the SNS. Another includes maintaining the strength of the DOE national laboratory-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. Coupled with new instrumentation will be support for new technique development that is enabled by advances in sources and detection capability.