Neutron Scattering

Portfolio Description

This activity supports basic research on the fundamental interactions of neutrons with matter to achieve an understanding of the atomic, electronic, and magnetic structures and excitations of materials and their relationship to materials properties. Major emphasis is on the application of neutron scattering, spectroscopy, and imaging for materials research, primarily at BES-supported user facilities. Development of next-generation instrumentation concepts, innovative optics, novel detectors, advanced sample environments, data analysis tools and polarized neutrons are distinct aspects of this activity. Capital equipment funding is provided for items such as detectors, monochromators, focusing mirrors, and beamline instrumentation at the facilities.

Unique Aspects

The DOE history and mission have played important roles in shaping BES' current position as the nation's steward of major neutron 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. This activity has evolved from the pioneering, Nobel prize-winning efforts of Clifford G. Shull in materials science to the current program that encompasses multiple techniques and disciplines. BES is a major supporter of both the research and the instrumentation at the major US neutron scattering facilities. It maintains strong fundamental research programs in materials and related disciplines at these facilities that serve to drive advancements in the instrumentation. High impact science from this activity provided the scientific case to motivate the construction of the Spallation Neutron Source (SNS), the BES facility with the highest pulsed neutron flux and a range of optimized neutron scattering instruments.

Neutron scattering provides information on the positions, motions, and magnetic properties of materials. The neutrons used in scattering experiments with wavelengths commensurate with the inter-atomic distances have energies in the meV range that is comparable to both the lattice and magnetic excitations (phonons and magnons). This fundamental property makes neutrons an ideal probe for both the structure and dynamics in condensed matter. The high sensitivity to light elements and large difference in scattering cross-section of certain isotopes offer unique contrasts and a range of versatile tools for the investigation of ordered and disordered as well as hybrid nanostructured materials. Their high penetrating ability and low energy allow nondestructive evaluation of the structure and dynamics of materials deep within the specimens, and their magnetic moment offers as an important probe of magnetic phases in materials.

Relationship to Other Programs

This activity serves several BES supported Energy Frontier Research Centers (EFRC) with focused research in the areas of superconductivity, organic photovoltaics, materials under high pressure, structural materials under extreme conditions and interfacial structure and dynamics for energy storage and catalysis. It supports fundamental research on hydrogen storage materials through coordination with the Office of Energy Efficiency and Renewable Energy and high pressure research with the National Nuclear Security Administration. It interacts closely with the BES Scientific User Facilities Division in the development of new instrument concepts and tools for neutron scattering and coordination on complementary scientific portfolios as well as with research instrumentation programs supported by other federal agencies, especially in the funding of beam lines whose cost and complexity require multi-agency support. It coordinates with the program for Instrumentation for Materials Research – Major Instrumentation Projects at the National Science Foundation and the National Institute of Standards and Technology's Center for Neutron Research to develop instruments and capabilities that best serve the national user facility needs. Nanoscience related projects in this activity are coordinated with the BES Nanoscale Science Research Center activities. BES further coordinates the nanoscience activities with other federal agencies by participating in the National Science and Technology Council's Nanoscale Science, Engineering, and Technology subcommittee, which leads the National Nanotechnology Initiative.

Significant Accomplishments

BES supported the pioneering research of Clifford G. Shull in the development of the neutron diffraction technique at Oak Ridge National Laboratory that led to the 1994 Nobel Prize in Physics. 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. Recent scientific accomplishments include the rich magnetic and electronic structures of correlated electron materials, such as conventional and high temperature superconductors, ferroelectrics, mutiferroics, cobaltites, colossal magnetoresistance materials and layered heterostructures. Also in the areas of high temperature thermodynamics of metallic systems; pressure-temperature stability and thermodynamics of clathrates, hydrides, boranes, crown ethers and Xe-H_2; superfluidity and phase boundaries in quantum solids and fluids; dynamic phase transitions in deeply super-cooled water; polymer and polymer brush behavior under nano-confinement; and metal-organic frameworks for hydrogen storage.

Neutron scattering groups supported by this activity at the DOE national laboratories (Ames, Argonne, Brookhaven, Oak Ridge, and Los Alamos) provided the leadership and expertise in the pioneering design and development of virtually all the current highly optimized time-of-flight instruments and techniques in neutron scattering and spectroscopy at the SNS. In addition, this activity supported the development of the spin-echo small-angle scattering measurement technique that extends the measurement length scales to several microns; ^{3}He spin filters for the production of polarized neutrons for the study of magnetism; neutron scattering confinement cell to probe polymer brushes under confinement; and neutron focusing optics for a number of applications.

Mission Relevance

The increasing complexity of DOE mission-relevant materials such as superconductors, semiconductors, magnets, batteries, photovoltaics, thermoelectrics and polymer nanocomposites requires ever more sophisticated scattering techniques to extract useful knowledge and to develop theories which can predict the behavior of these materials. X-ray and neutron scattering probes are some of the primary tools for characterizing the atomic, electronic, and magnetic structures of materials. Additionally, neutrons play a key role in hydrogen research as they provide atomic- and molecular-level information on structure, diffusion, and interatomic interactions for hydrogen. They also allow access to the morphologies that govern useful properties in catalysts, membranes, and protonic conductors. The activity is relevant to the behavior of matter in extreme environments such as high temperature and high pressure.

Scientific Challenges

Correlated Electron Systems – The effects of strong electron-electron and electron-phonon interactions give rise to a remarkable range of anomalous behavior in condensed matter systems. Quantitative understanding of the cooperative macroscopic phenomena emerging from the interplay between charge, spin, and lattice degrees of freedom in materials including high temperature superconductors, multiferroics and magnets remains a great challenge and inelastic neutron scattering and neutron diffraction will play major roles in the studies of these materials.

Matter Under Extreme Conditions – Extreme pressures provide a fertile ground for the formation of new materials and novel physical phenomena as compression perturbs significantly the chemical bonds and affinities of otherwise familiar elements and compounds. Highly optimized spectrometers with novel sample environment will enable *in situ* studies at high pressures at pressure ranges available at the synchrotron x-ray sources. Similarly, scattering experiments at high magnetic fields can be used to study materials during phase transitions, allowing researchers to segregate magnetic field effects as well as to simulate effects normally observed via doping.

In-situ Studies of Complex Materials – Highly optimized instruments at the SNS will enable the science with smaller samples with unprecedented resolution, accuracy, and sensitivity under various parametric conditions. *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 other condensed matter systems can be probed with a range of scattering, reflectivity, and spectroscopic techniques.

Projected Evolution

The 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 as this is a core competency that is vital to careful structural measurements related to materials properties. This program will continue its stewardship role in fostering growth in the US neutron scattering community in the development of innovative time-of-flight neutron scattering instrumentation concepts and its effective utilization for high profile research.

Correlated and Complex Materials – Realization of the enormous potential in functionality of correlated electron systems requires a complete understanding of the underlying mechanisms and phenomena to ultimately control the complexities to achieve desired functionality. In addition to cuprates, the recently discovered iron pnictides family will provide as yet another platform to investigate high Tc superconductivity. Elastic and inelastic neutron scattering techniques will remain as essential tools for the investigation of complex correlated electron systems.

Research at the Intersection of Hard and Soft Condensed Matter Sciences – Polymers, biomaterials and hybrid nanocomposites are ubiquitous in the modern world. Surfaces and interfaces play strong roles in hybrid materials relevant to such applications as organic photovoltaics, thermoelectrics, fuel cells, Li-ion batteries, organic light emitting diodes, and materials for carbon sequestration and hydrogen storage. Neutron scattering will play a major role to understand the effects of interfaces on the collective behavior of these multi-component systems, enabling science in the emerging areas in soft condensed matter science.