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. Emphasis will be on the application of neutron scattering, spectroscopy, and imaging as major tools for materials research primarily at BES-supported user facilities. Development of next-generation instrumentation concepts, innovative neutron optics, advanced high resolution detectors, rigorous modeling software tools, training next generation neutron scattering scientific community, and application of polarized neutrons for materials research are distinct aspects of this activity.

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 principal supporter of both the research and the instrumentation at the major U.S. neutron scattering facilities. It maintains strong fundamental research programs in materials and related disciplines at these facilities that serve to drive advancements in both the techniques and 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 in the world and a range of optimized neutron scattering instruments.

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

Relationship to Other Programs

This activity interacts closely with the BES Scientific User Facilities Division in the development of new instrumentation concepts and sophisticated software tools for data analysis and coordination on complementary scientific portfolios. It serves several BES-supported Energy Frontier Research Centers with focused research in the areas of superconductivity, magnetism, thermoelectrics, organic photovoltaics, materials under high pressure, structural materials under extreme conditions, and interfacial structure and dynamics for energy storage, hydrogen storage, carbon sequestration and catalysis. In addition, there are coordination activities with other federal agencies:

- Coordination with the National Institute of Standards and Technology's Center for Neutron Research helps to ensure development of instrumentation and capabilities that best serve the broad neutron scattering user community.
- Nanoscience-related projects in this activity are coordinated with the Nanoscale Science Research Center user facilities and reviews in the BES Scientific User Facilities Division.
- Predictive materials sciences activities and the associated theory, modeling, characterization and synthesis research are coordinated with other federal agencies through the National Science and Technology Council Subcommittee on the Materials Genome Initiative.
- Active interactions with the National Science Foundation through workshops, joint support of National Academy studies in relevant areas, and communication about research activities.
- Coordination with other federal agencies on research instrumentation programs, especially in the funding of beam lines whose cost and complexity require multi-agency support.

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, fluids and magnetic materials.

Neutron scattering groups supported by this activity at the DOE national laboratories 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. Recent scientific accomplishments include:

- Phase diagrams for the recently discovered high temperature iron pnictide superconductors and heavy fermions;
- The first experimental determination of spin liquids, a new state of magnetism;
- Mechanisms responsible for the giant negative thermal coefficient materials and high performance thermoelectrics;
- Emergent magnetism at the interfaces of complex oxide heterostructures offering a new pathway for oxide spintronics;
- Rich phase behavior of protein-polymer block copolymers offering a new platform to assemble functional biomaterials at high concentrations; and
- Neutron focusing optics to increase neutron flux in the instruments.

Mission Relevance
The increasing complexity of DOE mission-relevant materials including superconductors, magnets, batteries, photovoltaics, thermoelectrics, metallic alloys and polymer nanocomposites requires ever more sophisticated scattering techniques to investigate the structure and dynamics at relevant length and time scales and to develop theories which can predict the behavior of these materials. Neutron scattering probes are among the primary tools for characterizing the atomic, electronic, and magnetic structures of materials. The activity is relevant to the behavior of matter in extreme environments, high pressure, shear and magnetic fields.

Scientific Challenges

Strongly Correlated Electron Materials – 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, thermoelectrics, spintronics, and magnets, remains a great challenge; inelastic neutron scattering, diffraction and imaging will play major roles in the studies of these materials.

Matter Under Extreme Conditions – Extreme temperature (both ultrahigh and ultralow), pressure, magnetic and electric fields, shear and combinations thereof are important parameters for material synthesis as well as to tune the material properties. Highly optimized neutron scattering spectrometers with novel sample environments will enable *in situ* studies at high pressures. Similarly, scattering experiments at high magnetic fields can be used to study materials during phase transitions, allowing separation of magnetic field effects as well as to simulate effects normally observed via doping.

Multi-component Complex Materials – Interfaces play strong roles in the behavior of these materials. The role of individual constituents on the emergent behavior in these materials can be readily probed using unique contrast variation techniques. Highly optimized instruments at the SNS will enable the science with smaller samples with unprecedented resolution, accuracy, and sensitivity under various parametric conditions.

Projected Evolution

The Neutron Scattering activity will continue its stewardship role in fostering growth in the U.S. neutron scattering community in the development of innovative time-of-flight neutron scattering and imaging instrumentation concepts and their effective utilization for transformational research. A continuing theme will be the integration and support of materials preparation as this is vital for relating neutron structural measurements to materials properties.