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 and spectroscopy as major tools for materials research primarily at BES-supported user facilities. Development of next-generation instrumentation concepts, software tools for data analysis and modeling, and novel applications of polarized neutrons are important elements of this activity.

Scientific Challenges

Quantum Materials – Quantitative understanding of the new states of matter such as spin liquids, topological insulators, topological magnon insulators, magnetic monopoles and skyrmions, and the collective mesoscale phenomena emerging from the interplay between charge, spin, orbital and lattice degrees of freedom in materials, including high temperature superconductors, multiferroics, thermoelectrics, ferroelectrics, spintronics and quantum magnets, remains a major challenge. Inelastic neutron scattering, diffraction and reflectometry will play major roles in the studies of these materials.

Matter Under Extreme Conditions – Extreme temperature (both ultrahigh and ultralow), high pressure, magnetic and electric fields, shear and combinations thereof are important parameters for material design and synthesis as well as for tuning material properties. Highly optimized neutron scattering spectrometers with novel sample environments will enable *in situ* studies at conditions relevant to understanding the mesoscopic behavior of materials. 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 multi-component systems and thin films of hybrid materials. The role of the structure and dynamics of individual constituents on the emergent behavior in the materials can be readily probed by exploiting the unique contrast variation with isotopes and polarized neutrons using neutron scattering and reflectometry. Highly optimized instruments at the Spallation Neutron Source (SNS) will enable science requiring smaller samples with unprecedented resolution, accuracy, and sensitivity under relevant parametric conditions.

Projected Evolution

The Neutron Scattering activity will continue its stewardship role in fostering growth of 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. Topics that will be emphasized are new states of matter and phenomena in hard and soft condensed matter, spintronics, self-assembly, design principles and collective behavior of multicomponent systems, interfacial science, and mesoscale science where macroscopic properties are manifested. A continuing theme is fostering strong interaction between synthesis, neutron scattering experiments, theory, and high performance computation to accelerate the fundamental understanding needed for predictive design of advanced materials for future energy needs. Areas that are not a high priority are those with a major focus on conventional and high temperature superconductivity and organic photovoltaics.

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 among the most important techniques for elucidating the structure and dynamics of solids, superconductors, fluids, soft matter 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:

- First realization of a novel material that can conduct magnetic waves on its edge, but not within its bulk;
- Demonstration of the tunability of defects in the bulk to control the surface electronic properties of a canonical topological insulator;
- Established the wave-like properties of metallic magnetism and the itinerant character of magnetism in iron-based superconductors;
- Showed that the unconventional superconductivity can be continuously tuned towards a Mott insulator in an iron-based superconductor, indicating the similarity with cuprates that exhibit unconventional superconductivity driven by strong electronic correlations;
- Established evidence for the propagation of magnetic monopoles in a well-known quantum spin ice material and measured their mass;
- First direct observation of the Skyrmion Hall Effect;
- Discovered that the interactions of electrons and atom vibrations responsible for the thermal conductivity and electrical conductivity in materials can be altered with high temperature, a behavior well known to be controlled with high pressures;
- Established a key correlation between the properties of the high-temperature liquid dynamics and the arrested glassy state properties in three prominent classes of glass-formers: metallic, molecular, and network; and
- Developed a novel process known as dopant induced solubility control (DISC) that allows patterning of organic features with unprecedented small sizes.

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 research and instrumentation development at DOE's 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 SNS, the BES facility with the highest pulsed neutron flux in the world and a range of optimized neutron scattering instruments.

Mission Relevance

The increasing complexity of DOE mission-relevant materials including superconductors, magnets, magnetoelectric materials, energy storage devices, photovoltaics, thermoelectrics, materials for gas separation, metallic alloys, organic/inorganic hybrid materials 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 essential tools for characterizing the atomic, electronic, and magnetic structures of materials. The activity is relevant to the behavior of matter in extreme environments including high and ultralow temperature, high pressure, shear, magnetic fields and combinations thereof.

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 supports focused research in the areas of superconductivity, magnetism, thermoelectrics, materials under extreme conditions, interfacial structure and dynamics for energy storage, hydrogen storage, gas separation, carbon sequestration, and catalysis. 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. 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.
- 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 National Science Foundation on research instrumentation infrastructure for such activities as crystal growth and characterization.
- Within the larger federal research enterprise, program coordination is through meetings of the Federal Interagency Materials Representatives (FIMaR).