Electron and Scanning Probe Microscopies

Portfolio Description

This activity supports basic research in materials sciences that utilizes and advances electron and scanning probe microscopy and spectroscopy techniques to address forefront challenges related to atomic, electronic, and magnetic structures and properties of materials. This activity also supports the development of new instrumentation concepts and quantitative techniques, including ultrafast electron diffraction and imaging techniques, for basic science and materials characterizations for energy applications. The goal is to develop a fundamental understanding of materials through advanced microscopy and spectroscopy.

Unique Aspects

Materials properties at macroscopic scale originate from microscopic details, via a hierarchy of length scales. This activity is driven by the need for quantitative characterization and understanding of the structure, chemistry and physical properties of materials at near-atomic length scales. High spatial resolution in electron and scanning probe microscopy and spectroscopy provides unique opportunities to characterize atomic and mesoscale structures in technologically-important materials. This activity supports comprehensive microscopy research groups which undertake the development, implementation, and exploitation of a variety of electron beam and scanning probe techniques for fundamental understanding, characterization, and analysis of materials. Research results are increasingly coupled with first-principles theory, which offers quantitative insights into the atomic origins of materials properties.

Relationship to Other Programs

This activity interfaces with other programs in BES, including the activities under X-Ray and Neutron Scattering, Condensed Matter Physics, Synthesis and Processing, Physical Behavior, Materials Chemistry, Biomolecular Materials, Mechanical Behavior and Radiation Effects, Catalysis, Energy Frontier Research Centers, and the DOE Experimental Program to Stimulate Competitive Research. In addition, interactions outside of BES include:

- With the DOE Office of Energy Efficiency and Renewable Energy through activities in solar energy, hydrogen and energy storage technologies.
- 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. BES further coordinates nanoscience activities with other federal agencies through the National Science and Technology Council (NSTC) Nanoscale Science, Engineering, and Technology Subcommittee that leads the National Nanotechnology Initiative.
- Predictive materials sciences activities and the associated theory, modeling, characterization and synthesis research are coordinated with other federal agencies through the NSTC Subcommittee on the Materials Genome Initiative.
- Active interactions occur with the National Science Foundation through workshops, joint support of National Academy studies in relevant areas, and communication about research activities.

Significant Accomplishments

This program has been a major U.S. supporter of microscopy research for developing a fundamental understanding of materials. Scientific achievements in this program include the development of leading U.S. capabilities for materials characterization at subangstrom length scales that are coupled with advances in detectability limits and precision quantitative analytical measurement. Historical accomplishments include: the development of the Embedded Atom Method to study defects in materials, which revolutionized computational materials science by permitting large scale simulations of materials structure and evolution; the successful correction of electron microscope lens aberrations that allowed the first spectroscopic imaging of single atoms within a solid; the development of dynamic transmission electron microscopy, which couples high time resolution (~nanoseconds) with high spatial resolution (~nanometers), providing a unique tool for probing and understanding materials dynamics; and the visualization of electronic structure at the nanometer and atomic scale by spectroscopic imaging scanning tunneling microscopy which contributed to the understanding of the electronic transport mechanisms for superconductivity.

Recent accomplishments include:

- The discovery of the first solid-state triple point in vanadium dioxide.
- A new mechanism of thermal transport using electron thermal microscopy.
- The direct observation of nanoscale ferroelectric switching in real-time.
- New insights on the superconductivity of heavy fermions and magnetic superconductors through the developments of state-of-the-art scanning tunneling microscopy techniques.

Mission Relevance

This activity is relevant to materials research and energy technologies through the structural and functionality determination of mesostructured materials for a wide range of energy generation and use technologies. The nation's long-term energy needs present many fundamental challenges that require new materials and characterization tools such as electron beam and scanning probes. Performance improvements for environmentally acceptable energy generation, transmission, storage, and conversion technologies depend on a detailed understanding of the atomic, electronic, and magnetic structures found in advanced materials; electron and scanning probe microscopies and associated spectroscopy are among the primary tools for characterization of these structures. Analysis of the surface and interior of nano- or meso-scale structures related to the functionality of materials often require *in situ* and *in operando* microscopy techniques under various environments.

Scientific Challenges

Researchers addressing major scientific challenges supported by this activity require utilization of advanced, innovative imaging and spectroscopy to solve forefront scientific problems in understanding materials properties and functionality. Relevant research challenges are: imaging functionality at the near-atomic or mesoscale; development of a fundamental understanding of electron scattering and nanoscale ordering phenomena in matter; utilization of high-resolution, quantitative analysis of nano- and mesoscale materials to understand the origin of macroscopic properties and enable the design of high-performance materials; understanding the correlation between electrons and spins at nanoscale, and their dynamics and transport properties; determination of interface structures and understanding the link between surface/interface/defect structures and materials properties; combining electron and scanning probes to study complex properties; probing the local properties of materials at the atomic or molecular scale with *in situ* and *in operando* microscopy in the end-use application environment; development of time-resolved microscopy with high spatial, temporal and energy resolutions to study the atomic level mechanisms during structural or phase transformations; and the application of first principles theory to understand the data obtained from microscopy instrumentation and how to use this information to predict the structures of real materials.

Projected Evolution

The emphasis of the program will be basic research for the fundamental understanding of materials using advanced microscopy and spectroscopy techniques. This program will use currently available electron and scanning probe microscopy capabilities; develop new, innovative instrumentation and techniques; and use advanced scattering, imaging and spectroscopy methods to understand functionality, fundamental processes and dynamics of materials at the near-atomic to mesoscopic length scales.

To address forefront scientific challenges, new state-of-the-art experimental and theoretical techniques will need to be developed. This activity will continue to support the development and use of advanced microscopy instrumentation/techniques, and the associated theoretical tools to understand the experiments, for research on imaging materials functionality and understanding the properties of materials. New advances are needed in time-resolved microscopy and related spectroscopy, in high-resolution analyses of energy-relevant soft matter and for quantitative *in situ* analysis capabilities under perturbing parameters such as temperature, stress, chemical environment, and magnetic and electric fields. The combination of multiple probes in a single experiment is expected to address complex and challenging materials science problems. Significant improvements in resolution and sensitivity in microscopy and related spectroscopy techniques will provide an array of opportunities for groundbreaking science.