Electron and Scanning Probe Microscopies

Portfolio Description

This activity supports basic research in condensed matter physics and materials science using electron and scanning probe microscopy and spectroscopy techniques. The research includes experiments and theory to understand the atomic, electronic, and magnetic structures and properties of materials. This activity also supports the development and improvement of electron scattering and scanning probe instrumentation and techniques, including ultrafast diffraction and imaging techniques. Capital equipment funding is provided for items such as new scanning probes and electron microscopes as well as ancillary equipment including high resolution detectors.

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 materials over atomic to micron length scales. High spatial resolution provides unique opportunities to characterize nanoscale 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, Physical Behavior, Mechanical Behavior and Radiation Effects, Synthesis and Processing, Materials Chemistry and Biomolecular Materials, Catalysis, Energy Frontier Research Centers (EFRCs), Electron-beam Microcharacterization Centers, Nanoscale Science Research Centers, and DOE Experimental Program to Stimulate Competitive Research. The research is also relevant to the DOE Office of Energy Efficiency and Renewable Energy activities in solar energy, hydrogen and energy storage technologies. This research activity also interfaces with the National Science Foundation in materials research activities, and with other federal agencies through the National Nanotechnology Initiative.

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 the 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 successful correction of electron microscope lens aberrations that allowed, for the first time, the direct imaging of materials at sub-Angstrom resolution and the first spectroscopic imaging of single atoms within a bulk solid; the development of dynamic transmission electron microscopy, which couples high time resolution (~nanoseconds) with high spatial resolution (~nanometers) in both images and diffraction patterns, providing a unique tool for probing and understanding materials dynamics; and the development of the Embedded Atom Method which revolutionized computational materials science by permitting large scale simulations of materials structure and evolution. Recent accomplishments include the development of a method to map complete electron wave functions, including internal quantum phase, from measured probability densities. Quantum measurement (scanning tunneling microscopy) of these “quantum drums” revealed that isospectrality provides an extra topological degree of freedom enabling robust quantum phase extraction. A new world record was set for the smallest writing, with features of letters as small as 0.3 nm. The feasibility was demonstrated for a new approach capable of achieving sub-atomic data storage. Imaging of electronic self-organization by atomic-resolution, tunneling-asymmetry scanning tunneling microscopy provided understanding of copper oxide electronic transport mechanisms for high-temperature superconductivity.

Mission Relevance

The nation’s long-term energy needs present many fundamental challenges, especially the need for 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 structural characteristics of advanced materials. Electron and scanning probe microscopies are among the primary tools for characterization of the atomic, electronic, and magnetic structures of materials. Quantitative analysis of nanoscale structure and phenomena is crucially important for materials used in energy technologies. The processes on the surface and interior of nanostructures and the functionality of materials can be imaged and analyzed by using *in situ* microscopy techniques under various environments. The activity is relevant to materials research and energy technologies through the structural and functionality determination of nanostructured materials for energy storage and solar energy/fuels.

Scientific Challenges

Major scientific challenges are: imaging functionality at the atomic or nanometer scale; correlation of structure and function at nanometer or atomic scale; fundamental understanding of electron scattering and nanoscale ordering phenomena in matter; understanding the atomic or nanoscale origin of macroscopic properties to enable the design of high-performance materials; quantitative analysis of nanomaterials; understanding correlation between electrons and spins at nanoscale and spin structure, dynamics and transport properties; determination of interface structures between dissimilar materials and understanding the link between interface/surface/defect structures and materials properties; understanding the role played by individual atoms, point defects, and dopant in materials; understanding surface reactions at the atomic level in real space and imaging site specific reactivity; combination of electron and scanning probes to study complex properties; probing the local properties of materials at the atomic scale with *in situ* microscopy in extreme energy environments; understanding the physics at the convergence of continuum and atomic phenomena; development of time-resolved microscopy with high resolution both spatially and temporally to study the atomic level mechanisms during structural transformations; and the application of first principles theory to understand and predict the structures of real materials. To address these challenges, new state-of-the-art experimental and theoretical techniques will need to be developed. It is our long term goal to invent multiscale characterizations tools and be able to link structural evolution, dynamics, and electronic behavior with first principles understanding of materials.

Projected Evolution

This program will build upon the tremendous advancements in electron and scanning probe microscopy capabilities in the last decade and use scattering, imaging and spectroscopy methods to understand functionality and fundamental processes at the atomic or nanometer scale. Characterization of semiconducting, superconducting, magnetic, and ferroelectric materials benefits greatly from these abilities and from other research supported in this program. Concurrently, new frontiers in fundamental understanding of materials are being opened with the creation of novel characterization techniques.

Development of advanced electron and scanning probe microscopy techniques will be continued in order to meet our energy and basic science challenges. Significant improvements in resolution and sensitivity will provide an array of opportunities for groundbreaking science. These include the possibilities of understanding and controlling nanoscale inhomogeneity, new phenomena emerging at nanoscale, atomic-scale tomography, probing magnetism at the atomic scale with spin excitation spectroscopy, imaging spin density and spin waves, imaging functionality at the atomic scale, combination of multiple probes, and *in situ* analysis capabilities (under perturbing parameters such as temperature, irradiation, stress, magnetic field, and chemical environment). New methods and approaches addressing the scientific challenges will lead to the development of unique new analysis tools and breakthroughs in materials. The combined new experimental and theoretical capabilities will enable the fundamental understanding of atomic origins of materials properties. Significant advances will be made in the fundamental understanding of the mechanisms by which electrons, individual atoms, surface/interfaces and defects influence the properties and behavior of materials.