Electron and Scanning Probe Microscopies

Portfolio Description

This activity supports basic research in materials sciences using advanced electron and scanning probe microscopies and related spectroscopy techniques to understand the 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, to advance basic science and materials characterizations for energy applications. The goal is to develop a fundamental understanding of materials through advanced microscopy and spectroscopy.

Scientific Challenges

There are major scientific challenges in understanding quantum materials in order to harness their rich technological potential. Advanced, innovative imaging and spectroscopy are needed to solve forefront scientific problems in understanding materials properties and functionality, including quantum phase transitions, order and disorder in quantum materials, new types of topological order, spin transport and dynamics, and nano-structuring as a means of controlling relevant parameters of quantum materials systems. Relevant research challenges include: imaging functionality at the near-atomic to the 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 electronic structure, spin dynamics, magnetism, and transport properties from atomistic to mesoscopic scales; understanding the interplay between charge, orbital, spin, and lattice structures in complex materials; determination of interface structures and understanding the link between surface/interface/defect structures and materials properties; correlation of structure and properties of nano- and meso-structured materials for energy applications with quantitative *in situ* analysis capabilities; development of time-resolved microscopy with high spatial, temporal, and energy resolutions to understand and potentially control emergent phenomena at their natural time and length scales, under equilibrium and/or extreme conditions; 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

This program emphasizes basic research for the fundamental understanding of materials using advanced microscopy and spectroscopy techniques. The 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 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. A growing area in recent years is imaging functionality and correlating structure and properties at the atomic or nanometer scale. In addition to the high spatial and energy resolutions, recent research efforts also include ultrafast electron diffraction, spectroscopy, and imaging to understand the dynamics and behavior of matter under conditions far from equilibrium. 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. Research that is deemed “mature use” of microscopy techniques is not a programmatic priority.

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 sub-angstrom 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. Investigations by local probes have revealed new physics in two-dimensional materials, including an electron-hole asymmetric sequence of fractional quantum Hall states in bilayer graphene afforded via electronic compressibility measurements using a scanning single-electron transistor.

Recent accomplishments include:

- Precision measurements of the heavy-fermion band structure using quasiparticle interference imaging scanning tunneling microscopy, in combination with theory, shows that the mechanism of Cooper pair formation (and thus superconductivity) is magnetic interactions between the spins on the Ce atomic sites in a heavy fermion superconductor $CeCoIn_5$. This is the first direct verification for a magnetic Cooper pairing in a material.
- With improved energy resolution, vibrational spectroscopy is performed for the first time in an electron microscope with a subnanometer focused electron beam.
- Magnetoelectric Force Microscopy is developed to detect the local cross-coupling between magnetic and electric dipoles. Combined experimental observation and theoretical modeling provide understanding on how a bulk linear magnetoelectric effect can be realized in a new family of materials.
- Precise determination of the 3D coordinates of thousands of individual atoms in a material allows direct measurements of the atomic displacement and full strain tensor through advanced electron tomography.
- Femtosecond optical doping and electron crystallography reveal metastable and hidden phases in correlated electron crystals.
- Through the development of atomically resolved secondary electron imaging method, the

atomic structure of the surface of a material is resolved in addition to its bulk atomic structure.
- Elastic softening phenomena associated with the lattice instability at ferroelectric phase transitions are revealed at length scales of ~10 nm. A giant elastic tunability of stiffness (>30%) was discovered in $BiFeO_3$ epitaxial thin films through an atomic force microscopy study utilizing band-excitation piezoresponse spectroscopy.
- Direct imaging by electron microscopy shows that amphiphilic peptoid molecules form tubes with radii of about 4 nm wherein both hydrophilic and hydrophobic groups are exposed to water, revealing another design principle for building nanostructures in soft matter.
- One-dimensional conductive edges and characteristic flaws are revealed in atomically thin transistors using near-field microwave microscopy.

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 microscopies and spectroscopy provides unique opportunities to characterize atomic and mesoscale structures in technologically important materials. This activity supports comprehensive microscopy research in the development, implementation, and exploitation of a variety of electron beam and scanning probe techniques for fundamental understanding, characterization, and analysis of materials. These microscopy and spectroscopy tools have the highest spatial, energy, and time resolutions to address the forefront scientific questions in materials. Research results are increasingly coupled with first-principles theory, which offers quantitative insights on the atomic origins of materials properties.

Mission Relevance
This activity is relevant to materials research and energy technologies through the determination of structure and properties 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. A recent report from the Basic Energy Sciences Advisory Committee has identified “Exploiting Transformative Advances in Imaging Capabilities across Multiple Scales” as a transformative opportunity for discovery science. 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 multimodal or multiple-probe *in situ* and *in operando* microscopy techniques under various environments. Design and development of revolutionary tools and techniques are needed to accelerate discovery and technological deployment of advanced materials.

Relationship to Other Programs
This activity interfaces with other research programs in BES, including X-Ray and Neutron

Scattering, Condensed Matter Physics, Synthesis and Processing Science, Materials Chemistry, and Catalysis Science. In addition,

- BES Nanoscale Science Research Centers (NSRCs) user facilities have thrust areas that provide unique capabilities for electron and scanning probe microscopy.
- This activity produces research outcomes of relevance to programs of the Office of Energy Efficiency and Renewable Energy (EERE).
- Within the larger federal research enterprise, program coordination is through meetings of the Federal Interagency Materials Representatives (FIMaR).