Research Activity: **Electron and Scanning Probe Microscopies**
Division: Materials Sciences and Engineering
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Portfolio Description:

This activity supports basic research in condensed matter physics and materials science using electron scattering and scanning probe microscopy and spectroscopy techniques. Research includes experiments and theory to understand the atomic, electronic, and magnetic structures and properties of materials, especially the interplay between structural, electronic and magnetic properties at the atomic and nanometer scale and the effects of structural and compositional inhomogeneities including defects, surfaces, interfaces, and precipitates. This activity also supports the continual development and improvement of novel microscopy techniques and the next-generation instrumentation including high spatial- and temporal-resolution imaging, and high energy-resolution spectroscopy techniques to enable new discoveries in materials and nanoscience based on the ability to image the structure and functionality of materials at the nanometer or atomic scale.

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. It is a major source of research in the United States that is focused on structure and properties in atomic configurations over all length scales and dimensionalities and is the nation's only investment in large-scale, comprehensive microscopy research groups which bring together science-driven investigators whose focus is the development and implementation of a wide variety of electron scattering and scanning probe techniques. Therefore, it supports the facility stewardship role of the Department of Energy (DOE) by enabling full exploitation of BES' Electron Beam Microcharacterization Centers and Nanoscale Science Research Centers. The portfolio includes fundamental understanding, characterization, and analysis of materials by various electron scattering and scanning probe microscopy and spectroscopy methods. Research results are increasingly coupled with first-principles theory, which offers quantitative insights into the atomic origins of materials properties.

Relationship to Other Programs:

The Electron and Scanning Probe Microscopies program interfaces with other programs in BES, including the activities under Condensed Matter Physics, Mechanical Behavior and Radiation Effects, Physical Behavior, Synthesis and Processing, X-Ray and Neutron Scattering, Materials Chemistry and Biomolecular Materials, Catalysis, Electron-beam Microcharacterization Centers, and Nanoscience Centers; in the Office of Science through the Computational Materials Sciences Network; in DOE through the Hydrogen Fuel Initiative (HFI) and the Energy Materials Coordinating Committee (EMaCC); and in other federal agencies through the Interagency Coordination and Communications Group for Metals (NSTC/CT/MatTec), the interagency Coordinating Committee on Structural Ceramics (NSTC/CT/MatTec), and the National Nanoscience Initiative (NNI).

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Significant Accomplishments:

World class scientific achievements in this program represent the leading U.S. capabilities for materials characterization at atomic length scale, coupled with advances in detectability limits and precision of quantitative analytical measurement for fundamental understandings of materials. Accomplishments include:

- Imaging of electronic self-organization at atomic scale was achieved through the development of atomic resolution tunneling asymmetry scanning tunneling microscopy focusing on the locations of electrons, which will help, for example, to unlock the atomic-scale gridlock within copper oxide electronic transport system and to better understand the high temperature superconductivity.
- Using the state-of-art local probes, combining electron microscopy and scanning tunneling microscopy, the cooperative action of electron and lattice and the formation of a ferroelectric state in doped manganites were analyzed, which established the connection between colossal resistance effects and multiferroci properties, i.e., the coexistence of ferroelectric and antiferromagnetic ordering.
- A combination of first-principle theoretical calculations and atomic-resolution electron microscopy techniques provided a new understanding of the role of impurities in superconducting material, which indicates controlled impurities could further enhance the superconductivity of practical superconductors.

- The successful correction of electron microscope lens aberrations had doubled resolution in just a few years, allowing for the first time the direct imaging of materials at sub-Angstrom resolution.
- The first spectroscopic imaging of single atoms within a bulk solid using an aberration-corrected scanning transmission electron microscope. The ability to collect electron energy loss spectra from an individual atom allows not only elemental identification, but also the determination of chemical valence and its bonding configuration or local electronic structure.
- Combined scanning probes, electron microscopy, and theoretical calculations to reveal an unexpected behavior: ferroelectric ordering in a non ferroelectric compound ($SrTiO_3$) induced by a grain boundary.
- Invented new local probes: scanning impedance microscopy and nanoimpedance spectroscopy.
- Developed a new interferometric electron beam technique to measure atomic displacements in crystals with unprecedented picometer accuracy.
- Developed and demonstrated new quantitative methods to image and measure the distribution of valence electrons in solids, which have made significant contributions to the understanding of electronic transport in high temperature superconductors.
- Pioneered the application of electron beam holography to image and measure the grain-boundary potentials in vital ceramics such as superconductors, ferroelectrics, and dielectrics by exploiting the sensitivity of highly coherent electron waves to local electric fields.
- Developed the highest spatial resolution and lowest elemental detectability limit in-situ electron energy loss spectroscopy.
- Developed a new electron microscopy technique known as "fluctuation microscopy" that shows atomic arrangements in amorphous and glassy materials better than any alternative method.
- Developed the "Embedded Atom Method" that revolutionized the field of computational materials science by permitting large-scale simulations of atomic structure and evolution. It has been used by more than 100 groups worldwide and has resulted in over 1100 published works with over 2700 citations to the original work.

Mission Relevance:

The nation’s long-term energy strategy presents many fundamental materials challenges, especially the need for new materials and new tools to characterize them such as electron beams and scanning probes. Materials for power generation, energy storage and transportation, renewable energy, and catalysis are all affected by the structure, trace amount of specific elements and the presence of specific crystal defects. Performance improvements for environmentally acceptable energy generation, transmission, storage, and conversion technologies likewise depend upon the characteristics of advanced materials. This dependency occurs because the spatial and chemical inhomogeneities in materials (e.g., defects, dislocations, grain boundaries, interfaces, magnetic domain walls, and precipitates) determine and control critical properties such as fracture toughness, ease of fabrication by deformation processing, charge transport and storage capacity, superconducting parameters, magnetic behavior, and corrosion susceptibility. Quantitative analysis of nanoscale structures is crucial to the progress of nanoscale science–a major thrust in BES. The processes on the surface and interior of nanostructures and the functionality of nanomaterials can be imaged and analyzed by using i*n-situ* microscopy techniques under various environments. The program is also relevant to the DOE energy initiatives through the local property determination of nanostructured materials for hydrogen storage and solar hydrogen generation, and structural materials for nuclear energy applications.

Scientific Challenges:

Major scientific challenges in the Electron and Scanning Probe Microscopies program are: quantitative analysis of nanoscaled structures in nanomaterials, including the atomic, electronic, and magnetic structures; fundamental understanding of scattering phenomena of charged particles in matter; understanding the atomic or nanoscale origin of macroscopic properties to enable the design of high-performance materials; imaging structure and functionality at the atomic or nanometer scale; understanding correlation between electrons and spins at the 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 of the structure and dynamics of ordered and disordered materials, especially the short- and long-range order effects; 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 and properties of real materials. To address these challenges, new state-of-the-art experimental and theoretical techniques will need to be developed. The long term goal is to develop multiscale characterization tools for linking structural evolution, dynamics, and electronic behavior with first principles understanding of materials.

Funding Summary:

Dollars in Thousands

FY 2007	FY 2008	FY 2009
23,021	23,020	34,496

Performer	Funding Percentage
DOE Laboratories	69%
Universities	31%

*Based on FY2007
These are percentages of the operating research expenditures in this area; they do not contain laboratory capital equipment, infrastructure, or other non-operating components.

Projected Evolution:

This activity evolved from the program previously known as Structure and Composition of Materials and was formally renamed as Electron and Scanning Probe Microscopies in July 2007. 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. Electron scattering and scanning probe approaches supported by this program have higher spatial resolution than most other materials characterization techniques and are thus unique in their ability to characterize discrete nanoscale and nanostructured regions within the interiors of samples. 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 the basic science challenges, which will be partnered with the BES Electron-Beam Microcharacterization Centers and Nanoscale Science Research Centers. The enormous improvement in resolution and sensitivity will provide an array of opportunities for groundbreaking science. These include the possibilities of atomic-scale tomography, probing a single electron spin and its quantum dynamics, imaging spin density in multiple dimensions, single-atom spectroscopic detection and identification, 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.