Research Activity: **Structure and Composition of Materials**

Division: Materials Sciences and Engineering
Primary Contact(s): Jane G. Zhu (jane.zhu@science.doe.gov; 301-903-3811)
Team Leader: Helen Kerch (Acting)
Division Director: Harriet Kung

Portfolio Description:

This activity supports basic research in condensed matter physics and materials physics using electron scattering and microscopy and scanning probe techniques. Research includes experiments and theory to understand the atomic, electronic, and magnetic structures of materials. Increasingly important are the nanoscale structures and the structure and composition of inhomogeneities including defects, interfaces, surfaces, and precipitates. Advancing the state of the art of electron beam and scanning probe techniques and instrumentation for quantitative microscopy and microanalysis is an essential element in this portfolio.

Unique Aspects:

This activity is driven by the need for quantitative characterization and understanding of materials structure and its evolution over atomic to micron length scales. It is a major source of research in the United States that is focused on structure and defects 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 the BES three electron microscopy user centers. The portfolio includes characterization and analysis of materials by transmission and scanning transmission electron microscopy, atom-probe field ion microscopy, scanning probe microscopies, spin polarized low energy electron microscopy, electron beam holography and tomography, convergent beam electron diffraction, ultrafast electron diffraction and microscopy, and other state of the art 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 structure and Composition of Materials program interfaces with other programs in BES, other offices in DOE, and other federal agencies.

BES:

- Coordinated with activities under Mechanical Behavior and Radiation Effects, Physical Behavior, Synthesis and Processing, X-Ray and Neutron Scattering, Condensed Matter Physics, Materials Chemistry and Biomolecular Materials, Catalysis, Electron-beam Microcharacterization Centers, and Nanoscience Centers
- Linked with the Computational Materials Sciences Network

Other offices in DOE:

- Hydrogen Fuel Initiative (HFI)
- Energy Materials Coordinating Committee (EMaCC)

Interagency:

- Interagency Coordination and Communications Group for Metals (NSTC/CT/MatTec)
- Interagency Coordinating Committee on Structural Ceramics (NSTC/CT/MatTec)
- National Nanoscience Initiative (NNI)

Significant Accomplishments:

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

- The successful correction of electron microscope lens aberrations has 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 through analysis of the fine structure of the spectroscopic absorption edge.
- 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 advanced computer processing methods for a through-focus series of electron microscope images to achieve an "information limit" that exceeds the resolution of the best-ever single optimal image. This method enabled the first imaging of the light non-metallic elements-carbon, nitrogen, and oxygen.
- 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.
- Conceived and constructed the first three-dimensional, energy compensated, position sensitive atom microprobe that permits compositional imaging and depth analysis with atomic resolution.
- Refined Atomic Location by Channeling Enhanced Microanalysis in an electron microscope to precisely define locations of various atomic elements and reveal an unprecedented level of information in a variety of technologically important alloys.
- 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.
- Incorporated a controlled nanoindentation apparatus within a transmission electron microscope for the first time, permitting the simultaneous atomic-scale observation and mechanical testing of nanoscale sample regions.
- Developed the "Embedded Atom Method" that revolutionized the field of computational materials science by permitting large-scale simulations of atomic structure and evolution. It is currently being 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 fundamental properties of materials used in all areas of energy technology depend upon their structure and composition. Performance improvements for environmentally acceptable energy generation, transmission, storage, and conversion technologies likewise depend upon these characteristics of advanced materials. This dependency occurs because the spatial and chemical inhomogeneities in materials (e.g., dislocations, grain boundaries, interfaces, magnetic domain walls, and precipitates) determine and control critical behaviors 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 program is also relevant to the DOE HFI through the structural determination of nanostructured materials for hydrogen storage and solar hydrogen generation.

Scientific Challenges:

Major scientific challenges in the Structure and Composition of Materials program are: quantitative analysis of nanoscaled structures in nanomaterials, including the atomic, electronic, and magnetic structures; understanding nanoscale interactions and phenomena; understanding correlation between electrons and spins at nanoscale; determination of interface structures between dissimilar materials; understanding the role played by the interface structure in the evolution of microstructures; determination of local inhomogeneity and structure disorder; understanding the link between interface/surface/defect structures and materials properties; understanding of the structure and dynamics of amorphous materials, especially the short- and long-range order effects; development of ultrafast electron microscopy with high resolution both spatially and temporally to study the atomic level mechanisms during structural transformations; developing the ability to measure the distribution of valence electrons with sufficient accuracy; 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 structure.

Funding Summary:

Dollars in Thousands

FY 2005	**FY 2006**	**FY 2007 Request**
24,907	16,943	22,245

Performer	**Funding Percentage**
DOE Laboratories	77%
Universities	23%

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:

In the near term, program evolution builds upon recent accomplishments that span a wide range of areas including advances in microcharacterization science, the characterization of nanostructured materials, and detailed models of magnetic and structural phenomena. 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 characterizing and understanding the microstructure and microchemistry of materials are being opened with the creation of novel characterization techniques.

Development of advanced electron microscopy techniques will be continued, which will be partnered with the three electron-beam microcharacterization centers that were built up in this program and are now in the Electron Beam Microcharacterization activity. The enormous improvement in sensitivity will provide an array of opportunities for groundbreaking science. These include the possibilities of atomic-scale tomography, single-atom spectroscopic detection and identification, and increased experiment volumes within the microscope and consequently greater 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 detailed understanding of the mechanisms by which grain boundaries, interfaces and defects in metals, ceramics, semiconductors, and polymers influence the properties and behavior of these materials. Implementing nanostructural control over these mechanisms will revolutionize the fundamental principles of materials design.