Research Activity: Structure and Composition of Materials

Division: Materials Sciences and Engineering
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Portfolio Description:

Structure and composition of materials includes research on the arrangement and identity of atoms and molecules in materials, specifically the development of quantitative characterization techniques, theories, and models describing how atoms and molecules are arranged and the mechanisms by which the arrangements are created and evolve. Increasingly important are the structure and composition of inhomogeneities including defects and the morphology of interfaces, surfaces, and precipitates. Advancing the state of the art of electron beam microcharacterization methods and instruments is an essential element in this portfolio. Four electron beam microcharacterization centers are operated at ANL, LBNL, ORNL, and the Frederick Seitz MRL at the University of Illinois.

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 U.S. that is focused on structure and defects in atomic configurations over all length scales and dimensionalities. The cornerstone is the operation of four complementary, network-interfaced Electron Beam Microcharacterization Centers. They develop instrumentation for characterizing the spatial organization of atoms from the Ǻngstrom to the micron scale, and make such equipment and the associated knowledge, methods, software, and other resources available to the broad scientific community. 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, convergent beam electron diffraction and other state of the art methods. Recent unique advances within this CRA include: incorporation of a nanoindenter within a transmission electron microscope to observe the micromechanisms of deformation in real time; the determination that softening of lattice vibrations presages phase transformations, using a novel thermal diffuse scattering approach at a synchrotron light source; development of an understanding of how quantum dots can cause local substrate stresses which alter electronic band structure; and discovery of a new type of nanoscale crystalline "defect" structure at the intersection of a grain boundary and a surface.

Relationship to Others:

BES:

- Closely linked with activities under Core Research Activities on *Mechanical Behavior and Radiation Effects, Physical Behavior,* and *Synthesis and Processing*
- Linked with Computational Materials Sciences Center

Other Parts of DOE:

- Nuclear Energy Research Initiative
- Energy Materials Coordinating Committee

Interagency:

- Interagency Coordination and Communications Group for Metals
- Interagency Coordinating Committee on Structural Ceramics
- Nanoscale Science, Engineering, and Technology (NSET) subcommittee of the National Science and Technology Council (NSTC) – coordinating body for the National Nanoscience Initiative (NNI)

Significant Accomplishments:

This activity is responsible for the operation of four user centers for electron beam microcharacterization. They represent the Nation's only centralized facilities in electron beam scattering and related techniques that are available to outside users from the physical science community in academia, government laboratories, and industry. They have been the location of many world class scientific achievements in characterizing the structure and composition of materials. They 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. The following breakthroughs have collectively enabled the highest spatial resolution and the lowest limit in elemental detectability to be accomplished in electron beam microcharacterization.

- Demonstrated 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. The advance is made possible by correction of lens aberrations to give a smaller, brighter beam, approximately 1 Ångstrom (0.1 nanometer) in diameter.
- 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.

Other achievements under this activity include

- 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.
- Developed the "Constrained Local Moment" model for electron spin dynamics that won the Gordon Bell Award of the IEEE, presented at the High Performance Networking and Computing Conference, for the fastest real application. These calculations represented major progress towards a first principles understanding of finite temperature and non-equilibrium magnetic structure.
- Developed a new X-ray synchrotron method for directly measuring the ways atoms vibrate in a solid.

Mission Relevance:

The fundamental properties of all materials depend upon their structural arrangements and compositional distributions. 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, magnetic domain walls, precipitates, etc.) 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.

Funding Summary:

Dollars in Thousands

FY 2003	FY 2004	FY 2005 Request
28,915	32,954	32,183

Performer	Funding Percentage
DOE Laboratories	68%
Universities	31%
Other	1%

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 approaches supported by this program have higher spatial resolution than most other materials characterization techniques and are thus nearly unique in their ability to characterize discrete nanoscale and nanostructured regions within the interiors of samples. Characterization of semiconducting, magnetic, and ferroelectric materials benefits greatly from these abilities and from other research supported in this CRA. Concurrently, new frontiers in characterizing and understanding the microstructure and microchemistry of materials are being opened with the creation of novel characterization techniques.

The keystone of this activity is the set of capabilities to investigate structure and composition that is embodied in the four electron beam microcharacterization centers. Significant upgrading of equipment suites, acquisition of new capabilities, and commitment to adequate staffing levels will be required in the coming years to maintain these facilities as world-class user centers.

In the mid to long term, development of advanced characterization techniques is planned. The focus will be on aberration-corrected electron microscope designs, which 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, chemical environment).

Finally, sophisticated and highly integrated synthesis, characterization, and modeling efforts will lead to development of unique new analysis tools and breakthroughs in materials. We see opportunities to understand how nature produces model materials with desired structures and to utilize this understanding for the biomimetic synthesis of desired atomic arrangements and organizations. Further opportunities are likely to be discovered in self-assembled nanostructured materials, interfacial control, magnetic materials, and computational and modeling approaches to understanding atomic arrangements. At the same time, we anticipate that significant advances will be made in the detailed understanding of the mechanisms by which grain boundaries and interfaces 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.