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 user 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 keystone is the operation of four complementary, network-interfaced Electron Beam Microcharacterization Centers. They invent and expand the usability of instrumentation for characterizing the spatial organization of atoms from the angstrom to the micron scale. The portfolio includes characterization and analysis of crystalline defects by atom-probe field ion microscopy, scanning probe microscopy, spin polarized low energy electron microscopy, and other state of the art methods. Unique advances within this CRA include: the ability to image light elements (such as nitrogen) within a matrix of heavy elements; a high resolution method for mapping the spatial distribution of valence electrons in high temperature superconductors, utilizing electron holography to image grain boundary potentials in a dielectric; and development of a three-dimensional atom probe to study impurities and precipitation.

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 Center of Excellence for Synthesis and Processing for Advanced Materials
- Linked with Computational Materials Sciences Center
- Linked with Defense Programs via Nanoscience Network

Other Parts of DOE:
- Nuclear Energy Research Initiative
- Energy Materials Coordinating Committee

Interagency:
- MatTec Communications Group on Metals
- MatTec Communications Group on Structural Ceramics
- MatTec Communications Group on Nondestructive Evaluation
- Interagency Working Group on Nanotechnology

Significant Accomplishments:

This activity is responsible for the operation of four user centers for electron beam microcharacterization. They represent the Nation's only facilities in electron beam microcharacterization 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 spatial resolution for structural and compositional characterization, 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.

- 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 new method enabled the first ever 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. This world-class achievement has thus far been recognized with the 1998 Burton Award of the Microscopy Society of America and the 2001 Presidential (U.S.A.) Early Career Award.
- 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 the electron microscope to highly coherent electron waves to an applied electric field, which has led to unparalleled understanding of these highly complex and technologically significant materials.
- 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.

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 1998 Gordon Bell Award, 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.
- Discovered and developed bulk metallic glasses which exhibit extraordinary mechanical, tribological, corrosion resistant and magnetic behaviors. This work was honored with the 1996 Sir William Hume-Rothery Award presented by the Minerals, Materials and Metals Society, the 1998 Gold Medal presented by the Materials Research Society, and the 1999 election of the scientific investigator to the National Academy of Engineering.

Mission Relevance:

The properties and performance of all materials applied in all areas of energy technology depend upon their structure. Performance improvements for environmentally acceptable energy generation, transmission, storage, and conversion technologies likewise depend upon the structural characteristics of advanced materials. This dependency occurs because the spatial and chemical inhomogeneities in materials (e.g. dislocations, grain boundaries, magnetic domain walls, and 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 2000	**FY 2001**	**FY 2002**
$ 34,293	$ 33,767	$ 36,292

Performer	**Funding Percentage**
DOE Laboratories	78.0%
Universities	22.0%

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 nano-structured materials, and detailed models of magnetic and structural phenomena. Continuous progress is anticipated in characterizing nanostructured materials. Magnetic materials and bulk magnetic glasses also benefit from these and other research topics in this CRA. Concurrently, new frontiers in characterizing and understanding the structure of materials are being opened with the creation of novel microcharacterization techniques.

The keystone of the Structure of Materials activity is its microcharacterization capabilities in the four electron beam microcharacterization centers. Significant replacement equipment and staff will be required in the coming years to maintain these facilities.

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 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 the self-assembled nanostructured materials, bulk metallic glasses, and magnetic materials areas. At the same time, we anticipate that a detailed understanding of the mechanisms by which grain boundaries in metals and ceramics influence the properties and behavior of these materials will emerge. This should revolutionize the design of the structure of metals and ceramics in the same way that nanostructure control is currently changing the fundamental principles of materials design.

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