Mechanical Behavior and Radiation Effects

Portfolio Description

This activity supports basic research to understand defects in materials and their effects on properties such as strength, structure, deformation, and failure. Defect formation, growth, migration, and propagation are examined by coordinated experimental and modeling efforts over a wide range of spatial and temporal scales. The program supports research on deformation of ultra-fine-scale materials, fundamental studies of radiation resistance, and research that would lead to microstructural design for increased strength, formability, and fracture resistance in energy-relevant materials. In addition to traditional structural materials, it is also becoming increasingly important to understand deformation and failure mechanisms in other materials used in energy systems (e.g., membranes, coating materials, electrodes). Within these areas, research on topics such as driven systems, mesoscale science, and non-linear cooperative phenomena (multiple inputs, e.g., radiation + stress + corrosion) are of interest.

The long-term goal of this program is to develop the scientific underpinning of defect behavior that will allow the development of predictive models for the design of materials having superior mechanical properties and radiation resistance. Towards this goal, research will be emphasized that takes advantage of the new capabilities to fabricate and test tailored structures down to the nanoscale, as well as utilizing newly developed and more powerful parallel computational platforms and experimental tools to evaluate and measure behavior at a wide range of time and length scales.

Scientific Challenges

Irradiation and deformation can push materials out of equilibrium, creating a dynamic system that has unexpected behaviors. Examples include the type of severe plastic deformation that leads to non-equilibrium and highly radiation-resistant particles in oxide-dispersion-strengthened alloys, and 3-dimensional patterns and unexpected phase separations/morphologies developed by radiation damage. These are challenging to study because of the non-equilibrium nature, but can have profound influence on the development of new understanding and superior materials.

Cooperative phenomena: What is missed when observing or modeling individual defects or processes in a linear fashion? Often it is found that there are synergistic and system-level effects to mechanical behavior, as a number of deformation processes rely on cooperative movement of defects or microstructural components, or application of more than one driving force. These processes include strain hardening, stress corrosion cracking, grain boundary sliding, and chemo-mechanical response. Investigation of mechanical behavior emphasizing cooperative phenomena could yield greater insight into material behavior. It should be emphasized that complexity alone is not of interest, but rather synergy in behavior leading to unexpected phenomena.

Bridging the length and time scales, modeling, and measurement from atomic to continuum: The formation and motion of defects take place over a wide range of length and time scales. In order to fully understand response of the materials, it is necessary to successfully model and measure defect motion and interactions over this range of length (from sub-nanometer to millimeter) and time scales (picoseconds to seconds) in a unified manner. This includes not only improved computational methods but also improved measurement techniques for full 3-dimensional analysis of microstructures.

Projected Evolution

Systems that are driven away from equilibrium, or studies that focus on dynamic equilibrium, are of increasing interest. Important characteristics to be understood, for example, are the complex behaviors of interfaces (e.g. diffuse, dynamically re-arranging). This can affect the response to being driven by stress and strain (grain boundary sliding, segregation, particle-dislocation interactions, strain transfer across boundaries) and the response of the material to irradiation. One can also imagine systems resistant to being driven from equilibrium, or utilizing new strategies to provide equilibrium structures.

In addition to traditional structural materials, it is also important to understand deformation and failure mechanisms in other materials used in energy systems (e.g., membranes, coating materials, and electrodes), so this is an area of potential growth.

Areas that are not part of the core program and are therefore not encouraged for future research are studies that focus on mechanics of materials rather than materials science, high-strain-rate deformation, and high-dose irradiation response.

Significant Accomplishments

The Mechanical Behavior and Radiation Effects activity has resulted in a variety of scientific accomplishments, including the discovery of new materials that resist radiation damage; the understanding of new, tough ceramic materials; and the discovery of new analytical techniques and test methods that have impacted a number of research projects. Recent accomplishments include:

- Developing an understanding of ionization-induced healing in irradiated structural ceramics;
- Use of experimental methods and atomistic modeling to elucidate the mechanisms by which radiation resistance in silicon carbide is influenced by the proximity of grain boundaries;
- Discovering and defining unexpectedly high chromium mobility and selective oxidation during grain-boundary corrosion in Ni-Cr alloys;
- Measuring of rare and potentially harmful microstructural features during abnormal grain growth, by refinement of an x-ray diffraction technique; and
- Gaining an overarching picture of nano-indentation response in small structures, including the influence of stochastic events at length scales intermediate between “nano” and “bulk” behavior.

Unique Aspects

This activity represents a major fraction of federal support for basic research in mechanical behavior and is the sole source of federal support for basic research in radiation damage. In the science of mechanical behavior, cutting-edge experimental and computational tools are bringing about a renaissance, such that researchers are now beginning to develop unified, first-principles models of deformation, fracture, and damage.

Mission Relevance

The ability to predict materials performance and reliability and to address service life extension issues are important to the DOE mission areas of robust energy storage systems; fossil, fusion, and nuclear energy conversion; radioactive waste storage; environmental cleanup; and defense programs. Among the key materials performance goals for these technologies are good load-bearing capacity, failure and fatigue resistance, fracture toughness and impact resistance, high-temperature strength and dimensional stability, ductility and deformability, and radiation tolerance. Since materials from large-scale nuclear reactor components to nanoscale electronic switches undergo mechanical stress and may be subjected to ionizing radiation, this activity provides the fundamental scientific underpinning to enable the advancement of high-efficiency and safe energy generation, use, and storage as well as transportation systems.

Relationship to Other Programs

The research in this activity has, at its heart, the influence of defects on properties of materials and as such underpins, or interacts with, a number of BES, DOE, and other Federal government programs. Particularly, through its focus on atomic-level understanding of defect-property relationships, it is complementary to the emphasis on behavior of complex materials in the BES Physical Behavior of Materials activity, and to Electron and Scanning Probe Microscopies research, whose focus is on the relationship of structure to physical properties.

- Within BES and DOE, this research activity sponsors—jointly with other core research activities and the Energy Frontier Research Centers program as appropriate—program reviews, principal investigators' meetings, and programmatic workshops. Important links have been made with DOE research on nuclear energy, fusion energy, lightweight materials, defense programs, and radioactive waste storage.
- The program also participates in interagency coordination groups such the Interagency Coordination Committee on Ceramics Research and Development and the Federal Interagency Materials Representatives (FIMaR).
- Some nanoscience-related projects in this activity are performed using capabilities in the Nanoscale Science Research Centers managed by the BES Scientific User Facilities Division. BES further coordinates nanoscience activities with other federal agencies through the National Nanotechnology Coordination Office (NNCO), which provides technical and administrative support to the National Science and Technology Council (NSTC) Subcommittee on Nanoscale Science, Engineering, and Technology (NSET) for the National Nanotechnology Initiative (NNI).
- Predictive materials sciences activities and the associated theory, modeling, characterization, and synthesis research are coordinated with other federal agencies through the NSTC Subcommittee on the Materials Genome Initiative (MGI).