Mechanical Behavior and Radiation Effects

Portfolio Description

This activity supports hypothesis-driven basic research to understand defects in materials and their effects on the properties of 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. Topics include fundamental studies of deformation of ultra-fine scale materials, radiation resistance of structural materials, and intelligent microstructural design for increased strength, formability, and fracture resistance in energy relevant materials. The goals are to develop the scientific underpinning for predictive models for the design of materials having superior mechanical properties and radiation resistance. This program will support research in these areas as well as research on unique synergistic effects of multiple environments on the strength, structural development, or failure of materials.

Unique Aspects

The ability to predict materials performance and reliability from a fundamental basis and to address service life extension issues is important to the Department of Energy (DOE) missions in fossil energy, fusion energy, nuclear energy, energy efficiency, renewable energy, radioactive waste storage, environmental management, and defense programs. Among the key materials performance issues for these technologies are load-bearing capability, failure and fatigue resistance, fracture toughness and impact resistance, high-temperature strength and dimensional stability, ductility and deformability, and radiation tolerance. This activity represents a major fraction of federally supported basic research in mechanical behavior and is the sole source of 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.

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 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 Energy Frontier Research Centers program as appropriate, program reviews, contractor 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 the interagency coordination groups such the Interagency Coordination Committee on Ceramics Research and Development.
- Nanoscience-related projects in this activity are coordinated with the Nanoscale Science Research Center activities and reviews in the BES Scientific User Facilities Division. BES further coordinates nanoscience activities with other federal agencies through the National

Science and Technology Council (NSTC) Nanoscale Science, Engineering, and Technology Subcommittee that leads the National Nanotechnology Initiative.
- 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.

Significant Accomplishments
The Mechanical Behavior and Radiation Effects research 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:
- Based on a fundamental understanding of the role of fine-scaled precipitates, a new class of materials has been developed that can be used at relatively high operating temperatures without losing strength by microstructural evolution;
- Precise measurements of stress distribution during twinning of hexagonal close-packed materials, utilizing 3D x-ray diffraction to illustrate how these stresses are accommodated during compression;
- Developing a model for how specimen size and free surfaces affect the shape memory transitions in NiTi alloys using density functional theory;
- Demonstrating the effects of combined pressure and radiation on structural stability of ceramics such as $Gd_2Zr_2O_7$, in which irradiation under extreme pressures of a diamond anvil cell stabilized a non-equilibrium phase;
- Developed computational tools, along with synthetic and experimental capabilities, to design hybrid glasses with outstanding mechanical properties.

Mission Relevance
The ability to predict materials performance and reliability and to address service life extension issues is important to the DOE mission areas of robust energy storage systems; fossil, fusion, and nuclear energy conversion; radioactive waste storage; environmental cleanup; and defense. 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.

Scientific Challenges
Irradiation and deformation can push materials out of equilibrium, creating a dynamic system that has unexpected behaviors. Examples include severe plastic deformation that leads to non-equilibrium and highly radiation-resistant particles in oxide-dispersion-strengthen alloys, and radiation flux that creates 3-dimensional patterns or unexpected phase separations/morphologies. 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 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.

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

Research opportunities that can be realized by the application of mechanics fundamentals to the general areas of self-assembly, physical behavior, and behavior under extreme environments (primarily environments that are experienced in current or future fission reactors) of structural materials will be emphasized. With the emerging importance of nanoscale structures with high surface-to-volume ratios, it is appropriate to take advantage of the new, unprecedented capabilities to fabricate and test tailored structures down to the nanoscale. Another area of emerging interest is evaluation of the impact on mechanical behavior of using nanoscale building blocks to fabricate longer length scale structures. In all topical areas, new opportunities arise by taking advantage of more powerful parallel computational platforms and new experimental tools. 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, electrodes) so this will become an increasing part of the portfolio.

Radiation is increasingly being used as a tool and a probe to gain a greater understanding of fundamental atomistic behavior of materials. Incoming fluxes can be uniquely tuned to generate a materials response that can be detected *in situ* over moderate length and time scales. Materials also sustain damage after long times in high-radiation environments typical of current and projected nuclear energy reactors and in geological waste storage. As nuclear energy is projected to play a larger role in U.S. energy production, these are issues that need to be addressed at a fundamental level.