Mechanical Behavior and Radiation Effects

Portfolio Description

This activity supports 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 deformation of ultra-fine scale materials, radiation-resistant material fundamentals, and intelligent microstructural design for increased strength, formability, and fracture resistance in energy relevant materials. The goals are to develop predictive models for the design of materials having superior mechanical properties and radiation resistance. Capital equipment funding is provided for microstructural analysis, nanoscale mechanical property measurement tools, and ion-beam processing instrumentation.

Unique Aspects

The ability, from a fundamental basis, to predict materials performance and reliability 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 component 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 – researchers are now beginning to develop unified, first-principles models of deformation, fracture, and damage. The compelling need for understanding deformation mechanisms is related to the fact that virtually all structural metals used in energy systems are fabricated to desired forms and shapes by deformation processes. In radiation effects, the compelling need for valid predictive models to forecast the long-term degradation of reactor components and radioactive waste hosts is expected to become increasingly critical over the next decade. Radiation tolerance of structural metals and insulating ceramics is also of great concern for fusion energy systems.

Relationship to Other Programs

This activity interacts closely with the DOE programs in fossil energy, fusion energy, nuclear energy, , environmental management, and defense programs, especially in the areas of materials performance and reliability. 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 and Electron and Scanning Probe Microscopies. Similarly, radiation effects projects on radiation-tolerant materials complement BES Heavy Element Chemistry research on actinide and heavy element chemistry. Principal investigators use BES scientific user facilities for x-ray and neutron scattering, electron beam microcharacterization and the Nanoscale Science Research Centers (NSRCs). Nanoscience-related projects in this activity are coordinated with the NSRC activities and reviews in the BES Scientific User Facilities Division. BES further coordinates the nanoscience activities with other federal agencies by participating in the National Science and Technology Council's Nanoscale Science, Engineering, and Technology subcommittee, which leads the National Nanotechnology Initiative.

Significant Accomplishments

New Materials for Radiation Environments – Materials capable of resisting damage from intense radiation are essential for advanced nuclear energy systems. The primary radiation-damage mechanism in materials involves the creation and accumulation of structural defects such as dislocations, point defects, and other anomalies. Multiple defects could lead to the collapse of the ordered crystalline structure of the material, adversely affecting the integrity of material components used in nuclear energy systems. Recent studies have shown that materials can be made radiation-damage resistant by creating structures that actually accommodate radiation-induced structural disorder on the atomic scale. Complex oxides are candidate materials for these structures because they exhibit strong tendencies for natural atomic disordering. As a result, the formation of radiation-induced defects causes very little structural change, allowing the crystal structure to remain mechanically intact. The materials exhibit good radiation tolerance after high-level radiation exposure. Similarly, radiation damage can be accommodated in composite materials containing a high volume fraction of nanoscale interfaces. The interfaces are found to possess a strong affinity for defects, thereby catalytically removing them from the bulk of the material. The research has provided fundamental insight into tailoring the atomic structure of materials to achieve substantial improvements in radiation damage tolerance.

Learning from Nature to Make Tough Ceramics – Nature generates strong materials, such as mother-of-pearl, with orders of magnitude more fracture resistance than any man-made materials. These strong materials are made by the formation of hybrid composites in which a hard, brittle mineral is combined with soft, organic molecules. Recently, researchers have developed a new fabrication process that mimics nature. The results are hybrid materials composed of aluminum oxide (strong, but brittle) and polymers (soft, organic materials) with toughness 300 times higher than either component alone. The processing involved controlled freezing of a suspension of aluminum oxide ceramic particles in water (which drives the particles into layered structures), sublimating the ice, and then infiltrating the remaining ceramic framework with a polymer. The layer orientation and spacing were designed to ensure that a crack that forms in the brittle mineral is shielded from stress and actually stops growing, thereby resulting in the combined high strength and facture resistance.

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; 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 A key challenge is the development of a fundamental understanding of the influence of large magnetic or electrical fields, chemical reactions and environmentally driven phase changes on the mechanical response of materials, and the influence of stress or strain on their physical properties. It is increasingly recognized that there is a strong linkage between physical and mechanical behavior. This is particularly apparent in processes such as magnetoplasticity, but has also been observed in metal forming, processing and sintering. Externally applied or internally generated magnetic and electric fields have been observed to influence the deformation response in a number of materials. This opens a new avenue for controlling the mechanical properties of materials.

Cooperative phenomena – What is missed when observing or modeling individual defects or processes? 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. These processes include strain hardening, grain boundary sliding, and grain growth.

Bridging length and time scales – 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 to years) in a unified manner.

Projected Evolution

Research opportunities that can be realized by the application of mechanics fundamentals to the general area of self-assembly, physical behavior, and behavior under extreme environments will constitute an increasingly significant part of the development of devices that harvest energy, sense trace amounts of matter, and manipulate information. 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, taking advantage of more powerful parallel computational platforms and new experimental tools.

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 US energy production, these are issues that need to be addressed at a fundamental level.

New initiatives in the Energy Frontier Research Centers and the Single-Investigator and Small Group Research program include materials under extreme environments as well as advanced nuclear energy systems. Both of these topics were subjects of Basic Research Needs workshops and are expected to have a large impact on the portfolio of this CRA.