Research Activity: **Mechanical Behavior and Radiation Effects**

Division: Materials Sciences and Engineering

Primary Contact(s): John Vetrano (john.vetrano@science.doe.gov; 301-903-5976)

Team Leader: James Horwitz

Division Director: Aravinda Kini, Acting

Portfolio Description:

This activity supports basic research to understand the formation and motion of defects in materials and their effect on strength, structure, deformation, and failure. Energy-relevant materials from large-scale nuclear reactor components to nano-scale switches undergo mechanical stress and may be subjected to ionizing radiation. It is therefore important to elucidate their response to these conditions to enable the advancement of high-efficiency and safe energy generation, utilization, storage, and transportation systems. The objective of this research area is to achieve a complete understanding of the relationship between mechanical behavior and defects in materials, including defect formation, growth, migration, and propagation. Research supported in this area includes understanding deformation of ultra-fine scale materials, understanding radiation-resistant materials, and intelligent microstructural design of materials for increased strength, formability and fracture resistance. This research aims to build on this understanding in order to develop predictive models for the design of materials having superior mechanical properties and radiation resistance. A key aspect of this area will also include the development of new techniques for studying mechanical behavior and radiation resistance using the major BES scientific user facilities such as the high-brightness light sources, neutron sources, and electron microscopes in both static and dynamic conditions. Research in this topical area underpins DOE research in areas such as nuclear energy, energy efficiency, and defense programs.

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 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. 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. The compelling need in radiation effects - 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, energy efficiency, radioactive waste storage, 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 Physical Behavior of Materials activity and Electron and Scanning Probe Microscopies research whose focus is on the relationship of structure to physical properties. Similarly, the radiation effects element's activity on radiation-tolerant materials complements Heavy Element Chemistry research whose focus is on actinide and heavy element chemistry. The radiation aspect of this activity interacts closely with a related Computational Materials Science Network project in the Theoretical Condensed Matter Physics program. Principal investigators use BES scientific user facilities for x-ray and neutron scattering and collaborate with the X-ray and Neutron Scattering activities. They also use the BES Electron Beam Microcharacterization Centers and the Nanoscale Science Research Centers.

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 atomic dislocations, vacancies, 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 accumulation of large numbers of defects would otherwise lead to embrittlement and loss of mechanical integrity. The research has provided fundamental insight into tailoring the atomic structure of materials to achieve substantial improvements in radiation damage tolerance.

Nanomechanics: Elasticity and Friction in Nano-objects. The development of new materials with the size of a few nanometers has opened a new field of scientific and technological research. Nanomaterials such as oxide nanobelts and semiconductor nanowires are promising building blocks in future integrated nano-electronic and photonic circuits, nano-sensors, interconnects, and electro-mechanical nanodevices. The goal is to develop faster and better communication systems and transports, as well as smarter and smaller nanodevices for biomedical applications. To reach these objectives it is crucial to answer some fundamental questions such as what are the effects that different bonding arrangements and chemical modifications have on the elastic behavior of a nano-object. In a recent study the investigators measured the Young's modulus of ZnO nanobelts with an atomic force microscope by means of the modulated nanoindentation method developed in their lab. The elastic modulus was found to depend strongly on the width-to-thickness ratio of the nanobelt, decreasing from about 100 to 10 GPa, as the width-to-thickness ratio increases from 1.2 to 10.3. This surprising behavior was explained by a growth-direction-dependent aspect ratio and the presence of stacking faults in nanobelts growing along particular crystalline directions.

Hierarchical Structures for Enhanced Properties. A method has been devised to fabricate materials that exhibit a unique combination of desirable properties: strength, toughness, and light-weight. These materials mimic the natural oyster-shell material nacre, whose strength and toughness are far in excess of those of its constituent materials. The enhanced properties result from the "hierarchical" architecture of the materials, an architecture that is extremely difficult to fabricate because it involves the overlay of structures of multiple length scales, from micrometers to nanometers. A path for the synthesis of hierarchical materials was developed by mimicking the formation of sea ice. As saltwater freezes, impurities are expelled to separate pure water from crystalline salt. Similarly, during the freezing of water-based ceramic suspensions, ceramic particles are expelled and concentrate in the spaces between the ice crystals. The ice is then sublimated away and the space between the remaining ceramic layers is filled with an inorganic (metal) material, or, as in nacre, with an organic (polymer). The technique could be used in the fabrication of composites for a myriad of applications in which strength and lightness are imperative: structural materials, armor, airplane parts, computer hardware or orthopedic implants.

Mission Relevance:

The scientific results of this activity contribute to the DOE mission in the areas of fossil energy, fusion energy, nuclear energy, transportation systems, industrial technologies, defense programs, radioactive waste storage, energy efficiency, and environmental management. In an age when economics require life extension of materials, and environmental and safety concerns demand reliability, the ability to predict performance from a fundamental basis is a priority. Furthermore, high energy-conversion efficiency requires materials that maintain their structural integrity under extreme conditions. It is also necessary to understand the deformation behavior of structural metals so as to fabricate them to desired forms and shapes. This activity seeks to understand the mechanical behavior of materials. It also relates to nuclear technologies including fusion, radioactive waste storage, and extending the reliability and safe lifetime of nuclear facilities.

Scientific Challenges:

Interaction between mechanical and physical behavior: How do large magnetic or electrical fields, chemical reactions and driven phase changes (amorphization under irradiation, for example) influence the mechanical response of materials, and how does stress or strain alter their physical properties? It is being 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. A more broad study of mechanical behavior at a level emphasizing cooperative phenomena would yield greater insight into how materials behave under stress.

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-D analysis of microstructures.

Funding Summary:

Dollars in Thousands

FY 2007	FY 2008	FY 2009
12,626	13,620	23,112

Performer	Funding Percentage*
DOE Laboratories	77%
Universities	23%

*Based on FY2007

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:

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. Mechanics plays a fundamental role in understanding functions in biological, bio-inspired, and bio-hybrid material systems at all length scales. Biology and biological techniques are just beginning to be used to develop new materials and devices that will have broad impacts on engineering. An understand is needed of how the hierarchical nano- and micro-structure of biological of soft materials controls the deformation and fracturing modes and behaviors of the biological systems. This understanding needs to be imported to the behavior of hard alloys and ceramics that are used in the extreme environment of energy systems. 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.

The accessibility of national user facilities for neutrons and photons enables a new dimension for the studies of mechanical behavior of materials. The advantages of using neutrons and photons, as compared to the more traditional electron scattering techniques, such as in transmission electron microscopy, are several including in-situ and non-destructive experiments on bulk samples, time-resolved studies, and three dimensional profiles.

With high-end computational capability now a reality, computational materials science will play a pre-eminent role in predicting and understanding the generation, migration and interactions of defects in materials while under stress and/or irradiation. Unified models will be developed covering all length scales that will provide significant insights into how materials react to extreme conditions at a fundamental level. Mesoscale and nanoscale modeling efforts will be extended to include nanostructured materials. With the increasing power of computers and computational codes, along with unprecedented capabilities to fabricate and test nano-scale structures under extreme conditions, the time and length scales of experiments and simulations are converging and allowing new insight into mechanical behavior and radiation effects of materials.