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

Division: Materials Sciences and Engineering

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Portfolio Description:

This activity supports basic research to understand the deformation, embrittlement, fracture, and radiation damage of materials with an emphasis on the relationships between mechanical behavior and radiation effects and defects in the material. This research builds on atomic level understanding of the relationship between mechanical behavior and defects in order to develop predictive models of materials behavior for the design of materials having superior mechanical behavior such as at very high temperatures. The mechanical behavior of materials under repeated or cyclic stress, high rates of stress application, and over a range of temperatures and stress conditions are relevant to present and projected energy conversion systems. The focus on radiation effects is to achieve atomic level understanding of radiation damage mechanisms and subsequent materials property changes to design radiation-tolerant materials for advanced energy systems. Important radiation induced materials property changes include embrittlement, stress-corrosion cracking, amorphization (transition from a crystalline to a non-crystalline phase), and ion irradiation-induced surface modification.

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, 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 a matter 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 Structure and Composition of Materials 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. Principal investigators use BES national 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:

Atomic Scale Revelations of Brittle Fracture. A molecular dynamics study has revealed for the first time how fracture processes at the atomic scale affect bulk behavior, such as dynamic fracture toughness and crack propagation rate. Using an interatomic potential derived from the modified embedded atom method, atomistic calculations showed that at low crack propagation rates, silicon fractures via perfect cleavage on atomic planes, but at higher crack propagation rates, atomic lattice defects, uneven crack surfaces, and phonon vibrations are produced leading to an increase in the energy consumed during fracture. This increased energy consumption reduces the

energy that would otherwise be available to drive cracks to even higher propagation rates and limits the maximum crack propagation rate to significantly less than the theoretical maximum crack propagation rate. The results demonstrate that molecular dynamics can be used to accurately reproduce bulk experimental results, while simultaneously capturing the atomic level details of the fracture process. The added significance of this method is that it can be easily extended to other materials and incorporated into models of large dynamic systems.

Silicon Carbide: Going Where Silicon-based Technology Cannot Go. Major breakthroughs in understanding atomic defects and nanostructures in silicon carbide enable this semiconductor material to be used in a new generation of devices for severe environments where silicon-based devices cannot operate. This new understanding can be used to overcome materials degradation problems that hinder advanced device development. Atomistic computational methods have determined critical defect formation and diffusion properties and accurately predicted evolution of nanostructures, phase transformations, and changes in volume and mechanical properties. The excellent agreement between computational predictions and experimental measurements provides the scientific confidence to use the computational methods to predict properties and behavior under extreme conditions that cannot be tested in the laboratory. It allows the use of defect engineering to minimize degradation, enhance materials reliability, and design materials that allow the remarkable physical properties and biocompatibility of silicon carbide to be fully used for energy-saving devices, advanced optoelectronics, improved sensors, medical devices, advanced-energy components, and chemically-challenging environments.

Mechanical Properties Affected by Magnetic Interaction - A New Fundamental Principle. Quantum effects involving magnetic interaction have been discovered to be responsible for unexpected solid solution hardening/softening in intermetallic alloys, thus resulting in their superior mechanical properties. This new phenomenon was discovered by careful coordination between theory and experiments: first-principle quantum-mechanical calculations coupled with polarized neutron diffraction and electron energy-loss spectroscopy (EELS). Experimental studies have revealed unusual interatomic spacing and resultant solid solution softening in nickel-aluminum alloys induced by iron, manganese and chromium solute atoms, which cannot be explained by current hardening theories. Quantum mechanical calculations revealed the development of a large electron-spin polarization when these solute atoms substitute for aluminum in nickel-aluminum alloys. The spin polarization results in a large magnetic moment that dilates the lattice parameter and strongly affects mechanical properties of nickel-aluminum alloys. The calculated values are unambiguously supported by EELS and polarized neutron diffraction. These studies have led to the discovery of a new concept in the design of strong and tough intermetallic and metallic alloys for advanced heat engines and energy conversion systems. This new principle is expected to appear in textbooks illustrating cross-fertilization between two disciplines which have had no connection.

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 at high operating temperatures. 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. For example, a recent study to understand environmental cracking of metallic alloys on the atomic scale has strong implications in pressurized water reactors.

Scientific Challenges:

Amorphization of materials occurs at the atomic scale when oxides are irradiated with neutrons or positive ions, adversely affecting its physical and chemical properties. By understanding the mechanism and the parameters contributing to radiation tolerance, it will be possible to predict or engineer materials that are less susceptible to amorphization by radiation damage. Dislocation theory for deformation and fracture is typically valid for length scales less than 0.1 micron. Continuum elasticity and constitutive equations derived from it are typically limited to macroscopic length scales greater than 10 microns. These models do not converge in the interval often referred to as “mesoscale” between these limits. It is often possible, however, to control or "tune" microstructural features in this mesoscale regime by suitable adjustment of synthesis and processing parameters. Thus a unified model is sought

that will quantitatively describe mechanical behavior (including strength, deformation parameters, and fracture toughness) over all length scales. Such a model could be used to design microstructures as well as synthesis and processing parameters leading to optimized materials properties and behavior. Many metals and metallic alloys, including common steels, undergo a profound ductile-to-brittle transition over a small temperature interval, without detectable structural or chemical change. The understanding of the origins of this transition remains elusive and represents an on-going challenge. Investigating and understanding nanoscale materials, their response to mechanical stress and radiation damage, will reveal previously inaccessible realms of materials behavior as well as paving the way to novel applications.

Funding Summary:

Dollars in Thousands

FY 2005	FY 2006	FY 2007 Request
14,008	13,037	18,195

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, directed self-assembly, and fluidics will constitute an increasingly significant part of the technology that mass-produces 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 hostile environment of energy systems. With the emerging importance of nanoscale structures with high surface-to-volume ratios, many of the old unresolved topics, such as fragmentation and shear instabilities, need to be revisited from a multi-disciplinary perspective, taking advantage of more powerful parallel computational platforms and new experimental tools.

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.

Unified models will be developed covering all length scales that will provide significant insights into deformation and fracture. Concurrent advances in microstructural characterization will be exploited to understand the ductile-to-brittle transition and permit this understanding to be exploited for the design of embrittlement-resistant materials. The origins of radiation tolerance will continue to be pursued including exploitation of parameters, which feed into the phenomena of radiation tolerance, such as structure, stoichiometry, and ionic (or atomic) size. Mesoscale and nanoscale modeling efforts will be extended to include nanostructured materials.

With high-end computational capability now a reality, computational materials science will play a pre-eminent role in predicting radiation-damage evolution in materials. Specific research for materials relevant to future fusion and Generation-IV fission reactors will examine methods to examine structural materials performance issues. The need to predict material behavior under exposure conditions (irradiation, temperature, and mechanical loading) that represent a significant extrapolation beyond our existing knowledge base will also be addressed.