Research Activity: Mechanical Behavior of Materials and Radiation Effects

Division: Materials Sciences and Engineering
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Portfolio Description:

This activity focuses on understanding the mechanical behavior of materials under static and dynamic stresses and the effects of radiation on materials properties and behavior. The objective is to understand the defect-behavior relationship at an atomic level. In the area of mechanical behavior, the research aims to advance understanding of deformation and fracture and to develop predictive models for design of materials having desired mechanical behavior. In the area of radiation effects, the research aims to advance understanding of mechanisms of amorphization (transition from crystalline to a non-crystalline phase), understand mechanisms of radiation damage, predict and learn how to suppress radiation damage, develop radiation-tolerant materials, and modify surfaces by ion implantation.

Unique Aspects:

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 utilized 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 Others:

This research activity forms the basis for:

- Several distributed centers for the Synthesis and Processing of Advanced Materials, which promote coordinated, collaborative research partnerships among various institutions.
- The activities of these centers include concerted outreach effort coordinating the science with Small Business Innovation Business (SBIR) program on topics such as surface modification by ion implantation, metal forming, oxide protective films on metals, high-temperature intermetallic alloys, and corrosion.
- This CRA also coordinates with DOE's Office of Defense Programs (DP) on the multi-institutional collaborative Nansoscience Network topic entitled "Mechanics and Tribology at the Nanoscale."

Other parts of DOE:

- Nuclear Energy Research Initiative (NERI)
- Energy Materials Coordinating Committee (EMaCC)

Interagency:

- MatTec Communications Group on Metals
- MatTec Communications Group on Structural Ceramics
- MatTec Communications Group on Nondestructive Evaluation
- Interagency Working Group on Nanotechnology

Significant Accomplishments:

Ordered intermetallic alloys based on aluminides and silicides have great potential for structural use at high temperatures because of their excellent mechanical strength and corrosion resistance. However, because they lack ductility, they are generally brittle and impossible to fabricate by conventional techniques such as rolling, forging, extruding, drawing or sheet forming at ambient temperatures. Clear evidence has now been developed over the past twenty years of work under this activity that many intermetallic alloys are intrinsically quite ductile; the observed poor ductility and inability to fabricate them is now understood to arise from moisture-induced embrittlement. The understanding of the embrittlement mechanism has led to the formulation of scientific alloying and processing principles that have now proved to be effective in the design of ductile intermetallic alloys for commercial use. This cumulative work has led to eight commercial licenses and has been recognized by the Department of Energy's E. O. Lawrence Award, the Acta Metallurgica Gold Medal, two Humboldt (Germany) awards and numerous other honors to the investigators that have been involved.

Another effort in this activity is focused on the understanding and development of radiation-tolerant materials, which have critical implications for environmentally acceptable and reliable nuclear-waste storage. Experiments have shown that a class of complex oxides, gadolinium zirconate, will lock plutonium in its structure and remain highly resistant to the radiation damage from the radioactive plutonium for hundred thousands of years. Current materials proposed for plutonium immobilization become unstable in several decades and eventually this plutonium will leach into the environment. In parallel studies, the ability to theoretically predict the composition and structure of radiation-tolerant materials has been formulated on a firm scientific basis.

Combined surface-sensitive synchrotron X-ray diffraction with *in-situ,* real-time electrochemical experiments has revealed the surprising discovery that the passive oxide films that form on pure iron or on stainless steel have a very fine-grained nanocrystalline structure. This startling conclusion overturned the long-term belief that stainless steel derives corrosion resistance from the non-crystalline nature of the film. This result is of critical importance to the development of improved corrosion materials in these widely used materials.

The principal restriction to the widespread use of structural ceramics in high temperature load bearing applications such as turbines, generators, transportation and other engines, and machine cutting tools is their brittleness or susceptibility to undergo brittle fracture under an impact load. A new silicon carbide based structural ceramic was developed as a consequence of a detailed understanding of the relationship of the precise chemical composition and impurity concentrations and processing parameters to the microstructure of the material. This understanding was then used to develop a silicon carbide based ceramic that has the largest resistance to brittle fracture or *fracture toughness* ever achieved for any structural ceramic. It also has mechanical strength at temperatures up to 1300C that exceed that of any commercial material, and excellent resistance to repeated stress-cycle fatigue, which is a critical concern for energy power-plant turbine blades and aircraft engines.

Mission Relevance:

The scientific results of this activity contribute to 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:

There are two grand challenges: (a) Understanding the mechanism of amorphization at the atomic scale when oxides are irradiated with neutrons or positive ions. Amorphization degrades a material and adversely affects 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. (b) A unified model covering all length scales that can successfully explain deformation and fracture. Dislocation theory 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. A unified predictive model that is valid in the mesoscale regime could be used to design microstructures that could then be achieved via appropriate selection of synthesis and processing parameters and thus lead to optimized materials properties and behavior. Other challenges are: (a) Many metals and metallic alloys, including common steels, undergo a profound ductile-to-brittle transition over a small temperature interval, without structural or chemical change. The understanding of the origins of this transition remains elusive and represents an on-going challenge. (b) 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 2000	FY 2001	FY 2002
$ 16,200	$ 15,286	$ 14,617

Performer	Funding Percentage
DOE Laboratories	83.0%
Universities	16.0%
Other	1.0%

Projected Evolution:

Predicting the elemental, stoichiometry, and structural combinations that will yield radiation-tolerant materials by design is likely to have made strong progress, thus ending an era of empirical and trial-and-error design. The Network project on "Tribology at the Nanoscale" should be leveraging both BES and DP investments. The materials-by-design approach at the nanoscale level, and the time-and-length scale of the experiments necessary to link with models, will require state-of-the-art microscopies and innovative techniques.

In the long term, we anticipate continued efforts to develop a unified model 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. Advanced computer simulations for modeling radiation-induced degradation developed during this time will also be essential to progress. During this time, the mesoscale and nanoscale modeling efforts will be extended to include nanoscale materials.

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