## Research Activity: Mechanical Behavior of Materials and Radiation Effects

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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:

- 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.

Magnetism affects hardness? Experimental studies and first-principals theoretical calculations of a model intermetallic system have identified magnetic interactions as the cause of the unusually large lattice dilation and resultant solid solution softening in NiAl alloyed with Fe solutes. Solid solution hardening is an important element in the design of metallic materials as strength elements for structural use. The hardening behavior of random substitutional solid solution has traditionally been correlated with a mismatch in atomic size or elastic moduli, and/or difference in valence electrons between solute and solvent atoms. The solid-solution effect in ordered intermetallic alloys, however, is much more complex and not well understood because hardening behavior of intermetallics requires the consideration of both site occupancy and excess point defects induced by solute atoms.

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 radioactive plutonium for hundred thousands of years. Current materials proposed for plutonium immobilization become unstable in several decades and eventually the 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 scientific basis. The research in this area has contributed to a Guggenheim Fellowship Award, Canada's Hawley Medal, and a Distinguished Scholar Award from the Microbeam Analysis Society.

Materials Friendly to Nuclear Waste: The ability to predict the composition and structure of materials that are resistant to radiation damage, such as in nuclear waste storage, has been formulated on a firm scientific basis. Current nuclear storage materials cannot resist radiation damage for the required thousands of years, because radioactive emissions in a storage material jostle atoms out of their carefully ordered arrangements. These materials become unstable, and eventually leach into the environment. Computer simulations and experiments revealed that a special class of complex ceramic oxides called *fluorites* is able to resist this fate. This class of materials shares a basic chemical formula: two different pairs of metallic ions and seven oxygen atoms. The fundamental principle is rather simple: The configurations of atomic arrangements in these oxides are relatively disordered which explains why they can easily tolerate displaced atoms caused by radiation. Like an out-of-place object in a messy household, a misplaced atom into an anti-site is not all that conspicuous.

Dialing Friction? In the U.S. alone, an estimated $1.9 billion/year in energy is wasted to fight friction. The trick to controlling friction between microscopic moving parts is to coat them with molecules that spontaneously order into a single layer like the bristles on a brush. Experiments using a unique Interfacial Force Microscope to delicately rub together different layer combinations showed how chemical interactions both within the brush-like layer and across the moving interface determine friction. Alkanethiol molecules with chemically inert ends self-assemble into a passive, Teflon-like surface with remarkably low friction due only to the physical waving motion of the "bristles." Substituting chemically active ends on the same molecules introduces attractive forces that increase friction. These attractive forces can be fine-tuned by changing the molecule length, which effectively points the end group in a different direction and consequently "dials-in" the amount of friction.

## 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:

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 2002** | **FY 2003 Request** | **FY 2004 Request** |
|---|---|---|
| 14,530 | 14,530 | 14,510 |

| **Performer** | **Funding Percentage** |
|---|---|
| DOE Laboratories | 81.7% |
| Universities | 18.3% |

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:

Predicting the elemental, stoichiometric, and structural combinations that will yield radiation-tolerant materials by design is likely to make strong progress, thus ending an era of empirical and trial-and-error design. The Nanoscience Network project on “Tribology at the Nanoscale” leverages 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.

It is envisioned that nanomechanics will occupy the stage in the next decade. It will be impacted especially by the fundamental understanding of quasi zero-dimensional clusters of atoms. Nanoclusters involve small assemblies of atoms and can be envisioned as constituting the third dimension of the periodic table. Nanocluster research will evolve with its own spectroscopy and magic numbers. Such understanding is expected to have profound effects on sub-fields such as MEMS and NEMS.