Research Activity: Physical Behavior of Materials

Division: Materials Sciences and Engineering
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Portfolio Description:

Physical behavior refers to the electronic, chemical, microstructural or other response of a material to an applied stimulus. The research in this portfolio aims to understand, predict, and control physical behavior of materials by developing scientifically rigorous models for the response of materials to environmental stimuli such as temperature, electromagnetic field, chemical environment, and proximity of surfaces or interfaces. Basic research topics supported include modeling of materials behaviors, electrochemistry and corrosion, high-temperature materials performance, superconductivity, photovoltaics and fuel cells, and more.

Unique Aspects:

The research in this activity provides the primary support of the fundamental understanding and identification of detailed mechanisms responsible for materials behavior and the incorporation of this knowledge into reliable detailed predictive models. The understanding that has resulted from such modeling work has already led to the design of unique new classes of materials including compound semiconductors, tough structural ceramics, ferroelectrics, and magnetocaloric materials. For example, the predicted magnetic properties of nanoscale clusters have been verified by high fidelity measurements. New compound semiconductors have been developed that can remove excess CO_2 from the atmosphere. Highly desirable phases of ferroelectric materials can be formed using novel processing techniques. Breakthrough understanding of the chemistry of friction now enables the tuning of lubrication layers.

Relationship to Others:

BES:

- Closely linked with activities under Core Research Activities on *Structure and Composition* and *Mechanical Behavior and Radiation Effects*
- Linked with Center of Excellence for Synthesis and Processing of Advanced Materials
- Linked with Computational Materials Sciences Center
- Linked with Defense Programs via Nanoscience Network

Other Parts of DOE:

- Nuclear Energy Research Initiative
- Energy Materials Coordinating Committee

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:

Over the years, this activity has had broad and significant impact in many classes of materials and phenomena. In magnetic materials, continuous fundamental studies of bulk alloys and nanoclusters lead to the following breakthroughs:

- Discovery of the extraordinary giant magnetocaloric phenomena, which has led to the demonstration of high-efficiency refrigeration that does not require freon or any other refrigerant. This technology completely eliminates ozone depleting or other environmental impacts caused by conventional refrigeration, and is now developing a global market.
- Development of ferromagnetic bulk metallic glasses with dramatic reductions in hysteretic energy loss, which has the potential of leading to $30 billion dollars per year in savings from more energy efficient motors and transformers;
- The prediction and validation of extremely large magnetic moments in nanoclusters, which has the potential of leading to higher density nanomagnetic storage devices.

In semiconductors research, major accomplishments in silicon-based and other compound semiconductors are:

- Research in wide band-gap semiconductors has led to a succession of world records for energy conversion efficiency in solar photovoltaics, and been recognized by the 2001 John Bardeen Award from the American Physical Society.
- Breakthrough work in the understanding of the electronic properties of gallium nitride has led to much brighter and substantially more energy-efficient lighting sources using light emitting diodes. This work was recognized by the 1999 James C. McGroddy Prize from the American Physical Society, and is now being marketed for traffic light and a multitude of other applications by virtue of their greatly extended lifetimes, increased brightness and reduced energy consumption.
- A new dielectric technology for capacitors, based on high dielectric constant ceramic perovskites oxides, has been developed. The new technology overcomes the conventional silicon dioxides thickness limitation of two to three nanometers (i.e. about three to five atomic layers), and thus offers promise of further extending Moore's Law, which predicts the doubling of the performance/cost ratio for silicon-based devices every eighteen months. This breakthrough promises smaller and faster field effect transistors that will in turn lead to faster and more versatile computers.
- A tenfold increase in the electrical conductivity of the semiconductor gallium arsenide was achieved and is now an attracting market interest for application in electronic devices, diode lasers, reading compact discs and ultra-high speed transistors.

Other major accomplishments supported by this activity are:

- Nanocrystals of semiconductor cadmium selenide were demonstrated to successfully remove excess carbon dioxide from the atmosphere. The technology could potentially convert unwanted carbon dioxide into useful organic molecules with major environmental benefits.
- Experimental studies of interfacial forces have resulted in an atomic understanding of interfacial adhesion and the ability to tune frictional forces at the atomic level. The development of instrumentation that enabled this work was recognized by an R&D 100 award.
- Pioneering work in rare earth alloys, which was also recognized by an R&D 100 Award, has led to high performance phosphors that are now marketed in television tubes, and cheaper and more powerful permanent magnets including the development of a new market and the spawning of a private sector company that markets it.
- Discovery of a molecular coating that spontaneously self-assembles and orders into a single layer like the bristles on a brush. The coating permits remarkably low friction as a consequence of the physical waving motion of the oriented "bristles". This discovery could lead to energy savings in the U.S. where frictional energy losses are presently estimated as $1.9 billion dollars per year.

Mission Relevance:

Research in this activity underpins the mission of DOE in many ways by developing the basic science necessary to improve reliability of materials in mechanical and electrical applications and to improve the generation and storage of energy. With increased demands being placed on materials in real-world environments (extreme temperatures, strong magnetic fields, hostile chemical environments, etc.), understanding how their behavior is linked to their surroundings and treatment history is critical. Research in mission-relevant topics in this activity include corrosion (4.2% of GNP), photovoltaics, fast-ion conducting electrolytes for batteries and fuel cells, novel magnetic materials for low magnetic loss ($30 billion/year) and high-density storage, and magnetocaloric materials for high-efficiency refrigeration.

Scientific Challenges:

The challenge in this area is to develop the scientific understanding of the mechanisms that control the behavior of materials and to use that understanding to design new materials with desired behaviors. The CRA encompasses efforts aimed at understanding the behavior of materials including control of conductivity, magnetic response, corrosion resistance, and high-temperature performance through first principles modeling leading to *a-priori* design of new materials systems.

Funding Summary:

Dollars in Thousands

FY 2000	FY 2001	FY 2002
$ 14,667	$ 16,449	$ 15,832

Performer	Funding Percentage
DOE Laboratories	79.0%
Universities	21.0%

Projected Evolution:

In the near term, four central topics define the current program: physical behavior of electronic and magnetic materials, corrosion and electrochemistry science, nano-scale phenomena, and multiscale modeling of materials behaviors. Major efforts in these areas will continue. Increased investment in theory and modeling at universities will be emphasized.

In the mid to long term, in order to understand the macroscopic behavior of materials it is important to understand the relationship between the material's structure and its response to external stimuli. One needs to first study the structure over all length scales and in particular down to the atomic scale and to understand the response of the nanometer and larger features of the material to external stimuli. After studying the response of a single nanometer-scale feature, this has to be related to the macroscopic behavior of the material. This can often be done with modeling but further advances are necessary to fully couple the length scales from atomic to macroscopic. Currently, atomistic simulation methods can be used to study systems containing hundreds of thousands of atoms, but these systems are still orders of magnitude too small to describe macroscopic behavior. Continuum methods, typically using finite element methods, fail to adequately describe many important properties because they use phenomenology that has little connection to the real physical processes that govern physical interactions. Modeling at an intermediate length scale, the *mesoscale*, where many defects can be included and from which predictive models at the continuum scale can be developed is required for advances in materials science. At this intermediate length-scale it is necessary to model the *collective phenomena* that include well over a billions atoms. Developing and applying novel techniques to these problems will be emphasized in coordination with the investment in theory and modeling.

Finally, in order to understand the complex phenomena that are linked to both a material and its local environment, a long-term investment is needed. During this funding period, we anticipate supporting programs that apply advances in both experimental techniques and computational methodologies to understand the macroscopic behavior of materials by studying materials at all length scales. In particular, bridging models covering the *mesoscale* (covering phenomena in the range of 0.1 to 10 microns) will be developed over this time scale. This is vital to linking disparate length scales and creating a scientifically rigorous understanding of materials performance and behavior.

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