Research Activity: Physical Behavior of Materials

Division: Materials Sciences and Engineering
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Portfolio Description:

This activity is a fundamental research program focusing on the functional properties of materials. The major emphasis is on the behavior of complex materials in response to external stimuli often encountered in energy-intensive applications. This basic research program focuses on physical responses (such as optical, electronic, or magnetic changes) to temperature, electro-magnetic fields, chemical environments, and the proximity effects of surfaces and interfaces with an emphasis on the relationships between physical behavior and the microstructure and defects in the material. Included within the activity are research in aqueous, galvanic, and high-temperature gaseous corrosion and their prevention; photovoltaics and photovoltaic junctions and interfaces for solar energy conversion; the relationship of crystal defects to the semiconducting, superconducting and magnetic properties; phase equilibria and kinetics of reactions in materials in hostile environments, such as in the very high temperatures in energy conversion processes; and diffusion and transport phenomena in ceramic electrolytes for improved performance in batteries and fuel cells. Basic research is also supported to develop new instrumentation, including in-situ experimental tools, to probe the physical behavior in real environments encountered in energy applications.

Unique Aspects:

Research in this activity provides the primary support of the fundamental understanding and identification of detailed mechanisms responsible for the physical behavior of materials, 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. Some specific examples include: new levels of magnetic properties from nanoscale clusters, compound semiconductors that can remove excess CO_2 from the atmosphere, highly desirable phases of ferroelectric materials that can be formed through novel processing techniques, and a breakthrough in understanding of the chemistry of friction enabling the tuning of lubrication layers.

Relationship to Other Programs:

BES:

- Closely linked with activities under Engineering Physics, Structure and Composition, Mechanical Behavior and Radiation Effects, Synthesis and Processing Sciences, X-ray and Neutron Scattering, and Condensed Matter Physics
- Linked with Center of Excellence for Synthesis and Processing of Advanced Materials
- Linked with Computational Materials Sciences Network

Other Parts of DOE:

- Solid State Lighting/Building Technologies Program, Office of Energy Efficiency and Renewable Energy
- Nuclear Energy Research Initiative
- Energy Materials Coordinating Committee
- Hydrogen Coordinating Committee

Interagency:

- Interagency Coordination Group on Metals (NSTC/CT/MatTec)
- Interagency Coordination Group on Structural Ceramics (NSTC/CT/MatTec)
- Interagency Coordination Group on Nondestructive Evaluation (NSTC/CT/MatTec)
- Interagency Working Group on Nanotechnology (NSTC/CT/MatTec)
- OSTP Interagency Coordination Group on Hydrogen

Significant Accomplishments:

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 have led 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 the use of any refrigerant. This technology completely eliminates ozone depleting chemicals (e.g., Freon) used by conventional refrigeration and has the potential to develop into 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 in improved 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, major research accomplishments in silicon-based and other compound semiconductors are:

- Developed a biocompatible semiconductor laser for the rapid detection and analysis of chemical agents, such as anthrax spores. The device was based on recent advances in the surface chemistry of semiconductors and the concept of quantum squeezing of light emitted through a spore flowing at high speed in the laser's microcavity. This field-deployable biolaser should be able to identify different types of spores (e.g., anthrax) within a large population of harmless spores rapidly and effectively.
- Through research in wide band-gap semiconductors achieved 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.
- Developed a new dielectric technology for capacitors, based on high dielectric constant ceramic perovskites oxides. The new technology overcomes the conventional silicon dioxides thickness limitation of two to three nanometers (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, faster field effect transistors leading to faster and more versatile computers.
- Achieved a tenfold increase in the electrical conductivity of the semiconductor gallium arsenide which is now attracting market interest for application in electronic devices, diode lasers, reading compact discs, and ultra-high speed transistors.
- Achieved a new milestone towards light-emitting silicon through the identification of oxygen atoms as the mediator of silicon energy states. The result suggests possible ways to enhance light emitting efficiency of silicon, and hence easier and cheaper ways to integrate optoelectronic components with silicon-based technology.

Other major accomplishments supported by this activity are:

- A "direct" visualization of the three-dimensional rearrangements of atoms in a crystal lattice triggered by a magnetic field was realized by an *in-situ* x-ray diffraction technique. The observation sheds light on the mechanism governing the magnetocaloric effect and paves the way to designing advanced materials for improved environmentally-friendly cooling technologies.
- Two-dimensional (2D) photonic band gap crystals in the visible wavelength have been fabricated based on the self-assembled periodic arrays of aligned carbon nanotubes. These aligned periodic carbon nanotubes are unique as they exhibit a "tunable" photonic bandgap not previously observed in the visible region and demonstrate the feasibility of fabricating large areas of 2D photonic crystals without sophisticated electron lithography procedures. These photonic crystals may find wide applications in optical signal processing and switching.
- A synergistic approach of combined photoelectron spectroscopy and quantum chemical calculations has provided crucial insights on the origin of the loss of nobility and the catalytic properties of nanoscale gold particles.
- An innovative visualization tool has provided new insights in the corrosion behavior of aluminum and its alloys. The results show that the "noise" from electrical signals is dominated by the pit growth processes as opposed to the initiation and re-passivation of protective oxides speculated previously and observed in stainless steels.
- Strong coupling and giant magnetic moments were predicted in manganese atom clusters in the presence of nitrogen. The predictions are consistent with recent experimental results and the finding will aid the design of new magnetic materials and novel spintronic devices.
- Novel zinc oxide nanostructures, including hierarchical structures with different symmetries, nanobridges, and nanowalls have been synthesized by an innovative vapor transport and condensation technique. The results

demonstrate the feasibility of joining two different nano-components into a hierarchical structure. The nano-composites exhibited superior electrical and thermal conductivities.

- Russian doll models for the stabilization of silicon cage structures found that unfavorable energetics in the stretching of silicon to silicon bonds were responsible for previous failed attempts to synthesize the 60-atom silicon structure.
- A new epitaxial liquid-assisted growth method, which involves a fluoride compound in precursor films, has been developed to grow thick films of superconducting YBCO. The study yielded an understanding of the complex and unconventional growth process, which involves reactions of precursor films to form the desired compounds in several sequential steps. The understanding can be extended to other technologically important oxides that are of critical importance in solid-state electronic devices.
- 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, recognized by another 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.
- A new wetting model was constructed and validated by recent AFM observations of the interfacial structures between molten metals and ceramic surfaces. The model takes into account diffusion of the solid substrate under the molten metal and successfully explains why the contact angle differs for droplets that are growing versus those that are evaporating. Understanding the behavior at these metal-ceramic interfaces is critical to improving various industrial processes including soldering, brazing, coating, and composite processing.
- An innovative approach enabled the first direct observation on how water behaves near a hydrophobic surface. Measurements made by the surface force apparatus revealed the thrashing and rippling behavior of water near hydrophobic surfaces. These insights open doors to understanding a wide range of biological dynamic processes from protein folding and enzyme reactivity.
- A new study confirms the theoretical analysis that molecules of hydrogen, oxygen, and even water can travel across conducting membranes in opposite directions from what would normally be expected from chemical potential gradients. The new analysis shows that the behavior is a result of the simultaneous, coupled transport of multiple conducting species. The understanding of membrane transport is important in the development of advanced materials for energy storage such as fuel cells.

Mission Relevance:

Research underpins the DOE missions by developing the basic science necessary for improving the reliability of materials in chemical, electrical, and electrochemical applications and for improving the generation and storage of energy. With increased demands being placed on materials in real-world environments (extreme temperatures, strong magnetic fields, and hostile chemical conditions), understanding how their behavior is linked to their surroundings and treatment history is critical. Research in mission-relevant topics in this activity include corrosion, which annually consumes 4.2 percent of the Gross National Product; photovoltaics; fast-ion conducting electrolytes for batteries and fuel cells; novel magnetic materials for low magnetic loss and high-density storage; and magnetocaloric materials for high-efficiency refrigeration. The photovoltaic research supported is complementary to Experimental and Theoretical Condensed Matter Physics, whose emphasis is on the electronic structure of solar conversion processes and systems. Significant interactions and collaborations exist between this activity and Materials Chemistry and Biomolecular Materials program in surface chemistry and electrochemistry as related to oxidation and corrosion research.

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 program encompasses efforts aimed at understanding the behavior of organic and inorganic electronic materials, magnetism and advanced magnetic materials, manipulation of light/photonic lattices, corrosion/electrochemical reactions, and high-temperature materials behavior through intimately connected experimental, theory, and modeling efforts leading to a-priori design of new materials.

Funding Summary:

Dollars in Thousands

FY 2005	FY 2006	FY 2007 Request
25,551	24,677	29,756

Performer	Funding Percentage
DOE Laboratories	77%
Universities	23%

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:

In the near term, four central topics define the current program: electronic and magnetic behavior of materials; corrosion and electrochemistry science; nano-scale phenomena; and multiscale modeling of materials behaviors. Major efforts in these areas will continue. Increased investment in organic electronic materials will be considered. In addition, focus in theory and modeling at universities and national laboratories, taking advantage of the vast advances in computing speed and power, 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, with emphasis at the atomic level, and to understand the response of the nanometer and larger features of the material to those external stimuli. Studies of the physical response of a single nanometer-scale feature needs 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 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. In addition, tremendous advances in organic-based electronic materials applications have been reported recently. This program seeks to foster theory, modeling and simulation activities that address the following key topics in organic electronic materials: charge and energy transfer; electronic structure calculation; exciton dynamics and transport; and spin dynamics.

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 and multiple time scales. In particular, bridging models covering the mesoscale (covering phenomena in the range of 0.1 to 10 microns) will be developed. This is vital to linking disparate length scales and creating a scientifically rigorous understanding of materials performance and behavior. It is also vital to link the time scales that correspond to fast reactions and relaxation processes in materials.