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-related 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:

This activity closely interacts with all other sister programs under BES, and also, it is linked to the Center of Excellence for Synthesis and Processing of Advanced Materials and Computational Materials Sciences Network, Solid State Lighting/Building Technologies Program, Office of Energy Efficiency and Renewable Energy, Nuclear Energy Research Initiative, Energy Materials Coordinating Committee and Hydrogen Coordinating Committee. Additionally, this program interacts with the NSTC Materials Technology Subcommittee (MatTec) Interagency Working Groups on Metals, Structural Ceramics, Nondestructive Evaluation, and Nanotechnology and the OSTP Interagency Taskforce on Hydrogen R&D.

Significant Accomplishments:

This activity has had broad and significant impact in many classes of materials and phenomena. Some of the recent accomplishments include: experimentally resolving a single individual magnetic spin on an atom, using $KNbO_3$ nanowires that combines fluorescence and force microscopies; exploitation of structural bistability in liquid crystals for low energy consuming optical switches; development of predictive tools for phase stability and structure in transition-metal oxides for fuel cells; observation of "superplastic deformation" (280% of their original length) of single wall carbon nanotubes; realization of the smallest feature size (100 nanometer Gold) 3D metallic photonic crystal materials; observation of giant magnetoresistance in Mn-based full Heusler alloys; measuring thermoelectricity of a single individual molecule; and demonstration of 50-fold improvement in thermoelectric properties in silicon nanowires.

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 the Experimental and Theoretical Condensed Matter Physics program, 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 2007	FY 2008	FY 2009
25,964	25,960	33,539

Performer	Funding Percentage*
DOE Laboratories	68%
Universities	32%

*Based on FY2007
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. This program also 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.