Physical Behavior of Materials

Portfolio Description

This activity supports basic research on the behavior of materials in response to external stimuli, such as temperature, electromagnetic fields, chemical environments, and the proximity effects of surfaces and interfaces. Emphasis is on the relationships between performance, such as electrical, magnetic, optical, electrochemical, and thermal performance, and the microstructure and defects in the material. Included within the activity are research to establish the relationship of crystal defects to semiconducting, superconducting, and magnetic properties; phase equilibria and kinetics of reactions in materials in hostile environments; and diffusion and transport phenomena. Basic research is also supported to develop new instrumentation, including *in situ* experimental tools, and to probe the physical behavior in real environments encountered in energy applications. Capital equipment funding is provided for items such as physical property measurement tools that include spectroscopic and analytical instruments for chemical and electrochemical analysis.

Unique Aspects

This activity is the primary supporter of research to develop a fundamental understanding and identification of detailed mechanisms responsible for the physical behavior of materials, and the incorporation of this knowledge into 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 other programs under BES, such as the Computational Materials Sciences Network. It also has contact with the Solid State Lighting/Building Technologies Program, Office of Energy Efficiency and Renewable Energy, Energy Materials Coordinating Committee and Hydrogen Coordinating Committee. Additionally, this program interacts with the National Science and Technology Committee's Materials Technology Subcommittee Interagency Working Groups on Metals, Structural Ceramics, Nondestructive Evaluation, and Nanotechnology and with the Office of Science and Technology Policy 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: a technique to experimentally resolve 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

The research supported by this activity is necessary for improving materials reliability in chemical, electrical, and electrochemical applications and for improving the ability to generate and store energy in materials. Materials in energy-relevant environments are increasingly being exposed to extreme temperatures, strong magnetic fields, and hostile chemical conditions. A detailed understanding of how materials behavior is linked to the surroundings and treatment history is critical to the understanding of corrosion, photovoltaics, fast-ion conducting electrolytes for batteries and fuel cells, novel magnetic materials for low magnetic loss power generation, magnetocaloric materials for high-efficiency refrigeration, and new materials for high-temperature gasification.

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.

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 plasmonics, metamaterials and 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.

The long term goals of this program to understand the macroscopic behavior of materials it is important to understand the relationship between a material's properties and its response to external stimuli. This can be achieved by determining structure over multiple length scales, with emphasis at the atomic level, and by understanding 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.