Physical Behavior of Materials

Portfolio Description

This activity supports basic research on the physical behavior of materials in response to electric, magnetic fields, electromagnetic fields, chemical environments, thermal excitation, size effects and the proximity effects of surfaces and interfaces. Emphasis is on bringing a better understanding to fundamental processes taking place between electric charges, photons, lattice vibrations, and other collective excitations in materials. Included within the activity is research to understand the role of crystal defects to semiconducting, superconducting, and magnetic properties; phase equilibria and kinetics of reactions in materials in unusual environments; and diffusion and transport phenomena. 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

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, superconductors, ferroelectrics, and magnetocaloric materials. Some specific examples include: the stability and morphology of materials in solution as function of pH and oxidation environment are investigated and methods are developed to understand and predict how structure selection can be modified by environment in aqueous solutions as in Li-ion batteries; a 3D metallic carbon that is stable under ambient conditions is predicted to exist that has building blocks of interlocking hexagonal carbon rings; a general analytical expression relating equilibrium fluctuations of the grain boundary shape and position to key parameters governing its motion coupled to a shear deformation is proposed for metals.

Relationship to Other Programs

This activity closely interacts with other programs in BES as well as other DOE activities and interagency coordination groups:

- Within BES, this research activity sponsors – jointly with other core research activities, the Energy Frontier Research Centers program, and the Joint Center for Energy Storage Research (JCESR), as appropriate – program reviews, principal investigators (PI) meetings, and programmatic workshops.
- There are active interactions with the DOE Office of Energy Efficiency and Renewable Energy (EERE) through workshops, program reviews, PI meetings, and communication of research activities and highlights.
- Nanoscience-related projects in this activity are coordinated with the Nanoscale Science Research Center user facilities and reviews in the BES Scientific User Facilities Division. BES further coordinates nanoscience activities with other federal agencies through the National Science and Technology Council (NSTC) Nanoscale Science, Engineering, and Technology Subcommittee that leads the National Nanotechnology Initiative.

- Predictive materials sciences activities and the associated theory, modeling, characterization and synthesis research are coordinated with other federal agencies through the NSTC Subcommittee on the Materials Genome Initiative.
- The program also participates in the interagency coordination groups such the Interagency Coordination Committee on Hydrogen.
- Active interactions with the National Science Foundation through workshops, joint support of National Academy studies in relevant areas, and communication about research activities.

Significant Accomplishments

This activity has had broad impact in many classes of materials and phenomena. Some of the recent accomplishments include:

- A giant photonic Spin Hall effect was discovered when light is propagated through a metamaterial comprised of V-shaped antennas that follows a curved trajectory and drags light with different circular polarization in opposite transverse directions.
- The a.c. conductivity of a perfect dielectric was increased by more than 18 orders of magnitude within 1 femtosecond, allowing electric currents to be driven, directed and switched by the instantaneous light field without any material damage opening the way to ultra-high speed electronic signal processing in the petahertz (10^{15} hertz) domain range.
- An accurate magnetometer device was invented, based on a thin-film organic semiconductor diode, that is very low cost and yields better accuracies than existing sensors devices.
- Magneto-optical images have shown that high angle grain boundaries are the key critical current limiting factor in a superconductor $YBa_2Cu_3O_7$ film and enables future superconducting magnet energy storage.

Other accomplishments include: a technique to experimentally resolve a single individual magnetic spin on an atom using $KNbO_3$ nanowires that combine fluorescence and force microscopies; realization of the smallest feature size (100 nanometer gold) 3D metallic photonic crystal material; measuring thermoelectricity of a single individual molecule; and demonstration of 50-fold improvement in thermoelectric properties of silicon nanowires.

Mission Relevance

The research supported by this activity is necessary for discovery of novel material properties and improving materials reliability in chemical, electrical, and electrochemical applications, including 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 physical properties behavior is linked to these surroundings and exposure history is critical to the understanding of photovoltaics, fast-ion conducting electrolytes for batteries and fuel cells, corrosion, 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 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 photon-matter interactions, plasmonics, metamaterials and novel organic electronic materials will be considered. In addition, theory and modeling, taking advantage of the vast advances in computing speed and power, will be emphasized.

The long term goal of this program is to develop an atomistic understanding of 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-property relationship over multiple length scales, with emphasis at the atomic level, and by understanding the response of the nanometer and mesoscale 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 behavior of collections of these features at the mesoscale and onward 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. This program seeks to foster theory, modeling, and simulation activities that address charge and energy transfer; electronic structure calculation; exciton dynamics and transport; and spin dynamics in energy relevant materials. Developing and applying novel experimental techniques to these problems will be emphasized in coordination with the investment in theory and modeling.