Synthesis and Processing Science

Portfolio Description

This activity supports basic research for developing new techniques to synthesize materials with desired structure and properties; to understand the physical phenomena that underpin materials synthesis such as diffusion, nucleation, and phase transitions; and to develop *in situ* monitoring and diagnostic capabilities. The emphasis is on the synthesis of complex thin films and nanoscale materials with atomic layer-by-layer control; preparation techniques for pristine single crystal and bulk materials with novel physical properties; understanding the contributions of the liquid and other precursor states to the processing of bulk nanoscale materials; and low energy processing techniques for large-scale nanostructured materials. The focus of this activity on bulk synthesis and crystal and thin films growth via physical means is complementary to the BES Materials Chemistry and Biomolecular Materials research activities, which emphasize chemical and biomimetic routes to new materials synthesis and design. Equipment funding is provided for crystal growth apparatus, heat treatment furnaces, lasers, chemical vapor deposition and molecular beam epitaxial processing equipment, plasma and ion sources, and deposition instruments.

Unique Aspects

Basic research supported in this activity underpins many energy related technology areas while balancing "use-inspired basic research" and "discovery-class research." Significant interactions and collaborations exist between the investigators in this activity and other BES research activities, e.g., the X-ray and Neutron Scattering activity for the characterization of new materials by use of advanced scattering/spectroscopic tools at BES supported synchrotron and neutron facilities and the Electron and Scanning Probe Microscopies activity for high-resolution characterization of atomic scale structure at BES supported microscopy facilities. Research in materials synthesis furthers our capabilities in single crystal growth and preparation of high quality specimens used by other investigators funded by BES, often at the DOE x-ray synchrotron and neutron facilities. Many of the scientists performing work on nano-materials sponsored by this activity are also leaders of corresponding science thrust areas at the BES Nanoscale Science Research Centers (NSRCs).

Relationship to Other Programs

The Synthesis and Processing program is a critical element of the materials sciences that has emphasis in the physical sciences. This connection results in especially active interactions.

- Within BES, this research activity sponsors – jointly with other core research activities and EFRCs as appropriate – individual projects, program reviews, contractor meetings, and programmatic workshops.
- Within DOE, program coordination is through the Energy Materials Coordinating Committee, with representatives from the Offices of Science, National Nuclear Security Administration, Fossil Energy, Environmental Management, Nuclear Energy Science and Technology, Energy Efficiency and Renewable Energy, and Electricity Delivery and Energy Reliability.

- Nanoscience-related projects in this activity are coordinated with the NSRCs activities 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, which leads the National Nanotechnology Initiative.
- The program also participates in the interagency coordination groups such as the NSTC MatTec Communications Group on Metals, and Interagency Coordination Committee on Ceramics Research and Development.

Significant Accomplishments

The activity supports fundamental research that has allowed for the unprecedented defect controlled thin-film growth of superconducting oxide by molecular beam epitaxy, which has enabled the discovery of superconductivity at the interface between metals and insulators. It has accomplished the synthesis of artificially structured thin-film semiconductors that has allowed the design of thin-film structures with desired opto-electronic properties and devices. Of significance is the accomplishment of novel processing of silicon nano-membrane on insulator, which has proven that even the thinnest silicon membrane can be conductive provided the proper surface is present. This activity has modeled and fabricated a tungsten photonic crystal opal structure that can be used for thermal emission. Most recently, the activity has allowed for the discovery of the polymer ferroelectric responsible for the colossal electrocolaric effect near room temperature, which can mean the next refrigeration devices can be bendable.

Mission Relevance

Synthesis and processing science is a key component in the discovery and design of a wide variety of energy relevant materials. In this regard, the activity supports DOE's mission in the synthesis of wide bandgap semiconductors for solid state lighting; light-weight metallic alloys for efficient transportation; novel materials such as metal organic frameworks for hydrogen storage; and ceramics processing, including high-temperature superconductors for near zero-loss electricity transmission. The research activity aims at providing synthesis and processing capabilities to enable the manipulation of individual spin, charge, and atomic configurations in ways to probe the atomistic basis for materials properties.

Scientific Challenges

With recent developments toward precision, *in situ*, dynamic, real-time ultra-fast and ultra-small characterization equipment and increased accessibility of computational resources, synthesis and processing has been transformed to a science with a higher level of understanding. The time is ripe to attempt to answer the many challenges presently open in this field.

- **Precision Processing**: Stochastic non-equilibrium processing that is predictable, reliable, and uniform over large scales used to control, tailor the number and distribution of defects.
- **Long- and Short-range Forces**: Better understand long- and short-range forces and their contributions to the growth of nanoscale objects and of nanoscale morphology development. Roles of electrostatics and electrodynamics, and how

these relate to the polar and acid/base approaches of the chemistry community. Roles of defects and long-range interactions on phase stability and interface motion.

- **Atomistic Deposition:** Oxide and non-oxide film deposition and growth with better control at low and high rates, better control of oxygen at high activities and *in situ* characterization improvements.
- **Synthetic Strategies**: New processing strategies to discover new classes of materials beyond the periodic table (compounds, architecture, unnatural elements).
- **Designing Interfaces**: Define the design rules for integrating soft with hard materials creating hybrid and dissimilar materials. Synthetic techniques to create tailorable hard materials and robust soft materials. Soft/hard/hybrid materials that can hierarchically organize in 3-dimensional architecture by self or through external stimuli and control the materials interfaces of heterostructures.
- **Theory**: Guide experiments beyond Edisonian approaches. Use reverse design by proposing a desired band structure and compute the thermodynamically most plausible synthetic route.

Finally, the Basic Research Needs workshop reports and the Basic Energy Sciences Advisory Committee (BESAC) Grand Challenge report *Directing Matter and Energy: Five Challenges for Science and the Imagination* provides additional discussion on these and other challenges.

Projected Evolution

Over the past few years, the activity has evolved an increasing interest in understanding nanoscale morphology through nucleation and growth kinetics and mechanisms, defect control in deposition processes, and complex chemical and structural materials growth. Over the next several years, these directions are expected to continue with strengthen research in bulk materials growth, deposition, and sintering and added emphasis in the fundamental understanding of the mechanisms for interfacing soft-hard hybrid materials and the organization of these structures. Expansion is planned in research for discovery of novel synthesis methods, especially using extreme environments of field and flux, and research to push the limits of our basic understanding in synthesis and processing related to use-inspired technologies including solid-state lighting, solar energy conversion, hydrogen storage, and electrical energy storage. This activity will continue to support hypothesis-driven fundamental science in synthesis and processing with a particular interest in high-risk, high-impact, innovative, and imaginative projects. The activity continues to support and encourages natural collaboration between theorists and experimentalists to address the opportunities described in the scientific challenges described above.