Synthesis and Processing Science

Portfolio Description

This program supports scientific research on materials to understand the physical phenomena and unifying principles that underpin materials synthesis, including diffusion, nucleation, and phase transitions often using *in situ* diagnostics, and development of new techniques to synthesize materials with tailored structure and properties. An important element of this activity is the development of real-time monitoring tools that probe the dynamic environment and the progression of structure and properties as a material is formed. This information is essential to understand the underlying physical mechanisms and to gain atomic level control of material synthesis and processing. The emphasis is on the synthesis of complex thin films with atomic control; preparation techniques for high-quality single crystal and bulk materials with novel physical properties; understanding the contributions of the precursor states to the processing of bulk materials; and mild processing techniques for the assembly of nanostructured materials into larger scale structures.

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 activities 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. The focus on materials discovery and design by physical means is complementary to the BES Materials Chemistry and Biomolecular Materials research activities, which emphasize chemical and biomimetic approaches.

Relationship to Other Programs

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

- Within BES, this research activity sponsors – jointly with other core research activities, the Energy Frontier Research Center 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 Offices of Energy Efficiency and Renewable Energy (EERE) and Fossil Energy (FE) 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 Ceramics Research and Development.
- 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

The Synthesis and Processing Science Research activity has many notable accomplishments. Some have already made an impact of scientific and technological significance:

- The discovery of superconductivity at the interface between metals and insulators was assisted by careful layer-by-layer defect controlled thin-film growth of superconducting oxide by molecular beam epitaxy.
- The evidence that even the thinnest silicon membranes are conductive provided the proper surface is present was supported through novel processing of silicon nano-membrane on insulator.
- The materials design of a tungsten photonic crystal opal structure used for thermal emission was enabled through first modeling and then fabrication.
- A newly developed theory of nanorod growth has guided experiments to realize the smallest well-separated metallic nanorods that can be used as air-tight glue for use in organic solar cell packaging.
- A liquid-crystalline dielectric fluid was shown for the first time to display a large electrocoloric effect near room-temperature that will enable efficient and environmentally friendly refrigerators to replace the vapor compression coolers.
- For the first time, high energy protons were used for real-time imaging of a large metal sample during melt and solidification without destroying the sample.
- For the first time, the design and discovery of new sulfur-rich highly ionic compounds as cathodes and electrolytes have enabled all-solid-state lithium-sulfur rechargeable batteries with high energy densities.
- Using a self-assembly process, porous graphene was developed into an electrode with high energy storage capacity for a lithium-air battery.

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 a wide range of semiconductors for solid state lighting and photovoltaics; light-weight metallic alloys and nanocomposites for transportation applications; novel, designer materials for electrical energy storage; and ceramics processing including high-temperature superconductors for near zero-loss electricity transmission. The research activity aims at providing new 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 high-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 advance understanding for the many challenges presently open in this field, including:

- Developing robust predictive thermodynamic and kinetic tools – How do we accurately incorporate dynamic processes and near-equilibrium phenomena into new or existing tools?
- Multiscale modeling of multi-phase functional materials – What new modeling approaches will enable us to accurately incorporate length scales of functional materials?
- Materials design and fabrication at the atomic scale to achieve tailored properties – How do we manipulate atoms at the atomic scale to achieve new functionality?
- *In situ* characterization of materials synthesis from the atomic to the micron scale – How do we measure *in situ* processes at their relevant length and time scales?

Finally, the BES Basic Research Needs workshop reports and the BES Advisory Committee's Grand Challenge report, *Directing Matter and Energy: Five Challenges for Science and the Imagination*, provide additional discussion on these and other challenges.

Projected Evolution

The Synthesis and Processing Science activity is encouraging hypothesis-driven proposals that integrate a creative experimental methodology with a first-principles theory-based approach that will accelerate progress in understanding and unifying principles for design, synthesis and discovery of new materials. Over the past few years, the activity has evolved an increasing interest in understanding nanoscale morphology, defect and dopant control in deposition processes, and complex chemical and structural materials growth. Over the next several years, these directions are expected to continue with a stronger focus on investigating fundamental mechanisms for bulk materials growth, new deposition techniques for organic and inorganic films, and organization of mesoscopic assemblies across a range of length scales, especially related to use-inspired clean energy research.