Synthesis and Processing Science

Portfolio Description

This program supports research to understand the physical phenomena and unifying principles in different classes of materials that underpin their synthesis, including diffusion, nucleation, and phase transitions, often using *in situ* diagnostics, and development of new techniques to synthesize materials with tailored structure and desired properties. An important element of this activity is the development of real-time monitoring tools, diagnostic techniques, and instrumentation that can provide information on the progression of structure and properties as a material is formed, in order to understand the underlying physical dynamic mechanisms and to gain atomic-level control of material synthesis and processing. The emphasis is on fundamental research to enable discovery of new functional materials, and development of new crystal growth methods and thin-film deposition techniques to create complex materials with targeted structure and properties.

Scientific Challenges

With recent developments toward high-precision, *in situ*, dynamic, real-time, ultra-fast and ultra-small characterization tools and with increased accessibility of computational resources, synthesis and processing materials can be transformed to a science with a higher level of understanding. The time is ripe to address many open challenges 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? Can experiment and theory be bridged to construct accurate models of the evolution of materials away from equilibrium, and thus pave the way for new states of matter?
- How can we enable the fabrication and understanding of artificially structured materials with hierarchical arrangement and attain novel functionality?
- Can we more deeply characterize and understand the non-idealities that inevitably occur during synthetic processes for model materials? How can we effectively utilize these defects to synthesize useful structures, and thereby strengthen our ability to deal with the complexity of systems operating under more realistic conditions?
- *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, BES Basic Research Needs workshop reports (https://science.energy.gov/bes/community-resources/reports), especially the *Basic Research Needs for Synthesis Science for Energy Relevant Technology* due this year and the BES Advisory Committee's report, *Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science*, provide additional discussion on these and other challenges.

Projected Evolution

The Synthesis and Processing Science activity continues to focus on the area of predictive design and synthesis of materials across multiple length scales, with particular emphasis on the mesoscale, where functionalities begin to emerge. Proposals to accelerate progress in understanding synthesis pathways and in the discovery of new materials through coupling creative physical experimental synthesis and processing techniques, computational approaches, and/or *in situ* diagnostic tools and characterization techniques developed in the laboratory or at DOE-BES user facilities, are encouraged. The program has an increasing focus on understanding the kinetics and mechanisms of materials growth, including bulk material processes, organic and inorganic film deposition, plasma synthesis, and the organization of mesoscopic assemblies across a range of length scales, especially underpinning many energy-related technological areas.

Projects aimed at engineering scale-up, properties optimization, device fabrication, and device development are not encouraged.

Significant Accomplishments

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

- A new rapid processing method was developed for consolidating ceramic materials that stabilizes the processing temperature by applying an external pressure on the material through a press, equalizing the distribution of temperature. The uniform temperature resulted in almost instantaneous densification of the ceramic with only limited grain growth, confirming theoretical calculations.
- A new material that displays electrically controlled magnetism at room temperature was created by assembling alternating atomic layers of two oxide materials by exploiting geometric factors and atomic lattice distortions between the alternate materials.
- A new reversible chemical conversion reaction mechanism, similar to what powers lead-acid car batteries, was discovered and used to successfully manipulate the chemical balance in manganese oxide and zinc system. The battery could be charged-discharged over 5,000 cycles, while retaining 92 percent of its initial storage capacity, demonstrating its potential for ultra-low cost rechargeable batteries.
- A new fabrication method takes disordered (amorphous) solid glass and turns it into crystals with a single orientation (single crystals). A focused laser is used to heat the glass that allows controlled nucleation as the temperature increases from room temperature to the temperature at which a crystal is formed (below the melting temperature). The method suppresses excessive nucleation and allows for a single crystal seed to grow until the entire line or surface has a single orientation.
- Organic glasses were shown to have substantially increased photostability (resistance to changes in their molecular structure when exposed to light) when prepared by vapor deposition. The vapor deposited glasses are more densely packed in comparison with the more loosely-packed liquid-cooled glasses.
- Thousands of lanthanum strontium copper oxide compound samples were prepared by molecular beam epitaxy and characterized to reveal that the mechanism for high temperature superconductivity depends on the density of electron pairs that challenges the standard theory that superconductivity depends on the strength of electron pairing interactions.

Unique Aspects

Basic research supported in this activity underpins DOE’s mission to develop future, transformative energy technologies in areas such as energy conversion, transduction, and storage; high-efficiency electronic devices; advanced photonic materials; and light-weight, high-strength materials. 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. Current scientific thrusts balance grand challenge and use-inspired basic research, and require strong interactions among engineering, chemistry, physics, and computational science disciplines. This activity emphasizes physical control of material structure and properties, and bulk synthesis, crystal growth, and thin-film deposition to obtain new materials. The research is complementary to the Materials Chemistry research activity that focuses on chemistry-based formation and control of new materials and morphologies and the Biomolecular Materials research activity that emphasizes discovery of materials and systems using concepts and principles of biology.

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 by uncovering the mechanisms and kinetic factors for synthesis and by configuring materials through prediction, thus enabling the study of unique properties. Some examples of basic materials synthesis that support DOE's mission in energy include 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 to probe the atomistic basis for materials properties.

Relationship to Other Programs

The Synthesis and Processing Science 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 Centers program, and the Joint Center for Energy Storage Research (JCESR), as appropriate—program reviews, principal investigators' (PI) meetings, and programmatic workshops. Research efforts in this program are closely coordinated with other core research activities in BES, including the Physical Behavior of Materials on theory of formation in the nanoscale, Experimental Condensed Matter Physics on single crystal and thin film growth, and Electron and Scanning Probe Microscopies for studies on the growth phenomena at the nanoscale.
- There are active interactions with the DOE Offices of Energy Efficiency and Renewable Energy (EERE) and Fusion Energy Sciences (FES) through workshops, program reviews, PI meetings, and communication of research activities and highlights.
- Within the larger federal research enterprise, program coordination is through the Federal Interagency Materials Representatives (FIMaR), the Federal Interagency Chemistry Representatives (FICR), and the Interagency Coordination Committee on Ceramics Research and Development (ICCCRD).
- Nanoscience-related projects in this activity are coordinated with the Nanoscale Science Research Center activities and reviews in the BES Scientific User Facilities Division. BES further coordinates nanoscience activities with other federal agencies through the National Nanotechnology Coordination Office (NNCO), which provides technical and administrative support to the National Science and Technology Council (NSTC) Subcommittee on Nanoscale Science, Engineering, and Technology (NSET) for the National Nanotechnology Initiative (NNI).
- 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 (MGI).
- There are particularly active interactions with the National Science Foundation (NSF) through workshops, joint support of National Academy studies in relevant areas, and communication about research activities.