Research Activity: Synthesis and Processing Science

Division: Materials Sciences and Engineering
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Portfolio Description:

The Synthesis and Processing Science Core Research activity develops atomic- to nano-scale scientific understanding using physical principles to enable reliable, reproducible and innovative production of novel materials. This knowledge is developed through research efforts conducted in a safe and environmentally responsible manner that: (1) further our *fundamental understanding of atomistic behavior* for predictive rational design of complex (spatially and dissimilar) materials with controlled defects and architectures ranging from the atomic and molecular scales to the continuum scale; (2) revolutionize reproducible physical *synthesis strategies or techniques* (principally using bottom-up approaches) and creative processing paradigm shifts; and (3) develop *diagnostic tools* to probe synthesis, *in situ* and in real-time, with multi-technique probes that push the limits of both spatial and temporal resolutions.

Synthesis of novel materials is not limited to the atomic scale but also includes nanoscale construction of novel metamaterials, as well as complex and frustrated materials. The physical processes that are used for the synthesis of bulk crystals and thin films may include self assembly, directed assembly, layer by layer deposition, atomic probe 3-D assembly, directed or templated growth, parallel printing, nanoscale rapid prototyping, nanolithography, electrodeposition, ion beam irradiation, vapor deposition, sputtering, laser deposition, molecular beam epitaxy, pattern formation, rapid solidification, microwave synthesis or sintering. In general the program supports research efforts that advance molecular level understanding of processes based on thermodynamics, kinetics, and mechanisms, in particular nucleation and crystal growth, solidification/vitrification/devitrification, and interphases and interfaces. In addition, we seek scientific enablers to the development of new tools for synthesis of materials using a cadre of physical principles including those developed under extreme conditions of temperature, pressure, electric/magnetic field, and radiation whether under equilibrium or non-equilibrium conditions.

Unique Aspects:

Basic research supported in this activity underpins many energy related technology areas. A focus of this activity is on the exploration of physical principles and concepts in synthesizing and processing new materials that is complementary to the emphasis on: (1) chemical synthesis and chemical control of material properties in the Materials Chemistry activity and (2) biomimetic/bioinspired design and synthesis in the Biomolecular Materials activity. Significant interactions and collaborations exist between the investigators in this program and the 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 the high resolution characterization of atomic scale structure at BES supported microscopy 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.

The program supports projects in research areas that are relevant to synthesis and processing science such as ion beam irradiation, molecular beam epitaxy, pulsed laser deposition and metal organic chemical vapor deposition, thermochemistry, nucleation and growth kinetics of nanorods and nanotubes, controlled nanoparticle morphology, polymer structure morphology, thin films as substrates for quantum dots and for preparing nanostructures, thin film growth for complex interfaces and superlattice growth, single crystals growth of novel materials, modeling of metallurgical processes, and colloidal assembly. In addition, the program supports the Materials Preparation Center (MPC) at the Ames Laboratory which has responded to 4,100 requests for preparation, fabrication and purification, and characterization of materials placed by customers worldwide as of FY 2007.

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.

- This research activity participates in DOE's Energy Materials Coordinating Committee (EMaCC). EMaCC is a forum for information exchange and coordination with representatives from the Offices of Science (SC), National Nuclear Security Administration (NNSA), Fossil Energy (FE), Environmental Management (EM), Nuclear Energy Science and Technology (NE), Energy Efficiency and Renewable Energy (EERE), and Electricity Delivery and Energy Reliability (OE).
- This research activity holds joint programmatic workshops and joint solicitation panel reviews and contractor review meetings with other divisions within BES and other DOE offices. For example, the Workshop on Basic Research Needs for Materials under Extreme Environments (June 2007) involved the coordination with NNSA, FE, EERE as well as participation from many national and international laboratories, universities, and companies. Another example was the Hydrogen Program Annual Review (May 2007) held jointly with the programs within BES and EERE.
- The program also participates in the interagency coordination groups such as the NSTC MatTec Communications Group on Metals, MatTec Communications group on Structural Ceramics, and National Nanotechnology Initiative.

Significant Accomplishments:

This program is responsible for the unprecedented defect controlled thin-film growth of superconducting oxide by MBE which has allowed the discovery of photo-induced phase transitions in the films. It is also noteworthy for the mechanistic understanding of spontaneous formation of sputter ripple patterns by low energy ion beam bombardment. It has accomplished the synthesis of artificially structured thin-film semiconductors that has enabled the design of thin-film structures with desired opto-electronic properties and devices. And of significance is the accomplishment of novel processing of silicon nanomembrane on insulator which has proven that even the thinnest silicon membrane can be conductive provided the proper surface is present.

Mission Relevance:

The research in this portfolio, in support of the scientific discovery, scientific innovation, and energy security missions of the U.S. Department of Energy, not only underpins the fundamental science of synthesis and processing in general but also underpins many of the use-inspired energy-related technologies. These include the challenge of finding new superconductors, designed solid state lighting architectures and materials, catalysts, novel hydrogen storage materials, and electrical energy storage materials, photovoltaics, electrochromics, supercapacitors, fuel cells, and materials that can withstand or be prepared by extreme environments. Many of our Basic Research Needs Workshops sponsored by DOE-BES brought out a common theme of the scientific needs in materials synthesis and processing for these technologies.

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:* Often precision processing comes at a cost of time and expense and is small scale. Envision what scientific approach will lead stochastic non-equilibrium processing of materials to be predictable, reliable, and uniform over large scales? Can this process be used to control defects? Can we tailor the number and distribution of defects?
- *Long and Short Range Forces*: How may we better understand long and short range forces and their contributions to the growth of nanoscale objects and of nanoscale morphology development? What are the relative roles of electrostatics and electrodynamics, and how do we relate them to the polar and acid/base approaches of the chemistry community? What are the roles of defects and long-range interactions on phase stability and interface motion?

- *Atomistic Deposition*: Atomistically controlled oxide films deposition and growth continues to provide excitement to the synthesis and condensed matter communities. Continuing unanswered questions in the synthesis of oxides include better control of deposition at low and high rates, better control of oxygen at high activities and in situ characterization improvements. As interesting as these problems are, and as interesting as the emergent behaviors they can reveal, there is the consideration of what opportunities are beyond the oxides? What is the scientific case for investigating other systems? What synthesis techniques need further development in order to have atomistically controlled deposition in these other systems?
- *Synthetic Strategies:* Even if we only consider the elements on the periodic table (and exclude the materials structure, architecture, and unnatural elements) only a small fraction of possible compounds have been synthesized. What new processing strategies can we employ that are feasible to discover new classes of materials?
- *Designing Interfaces:* What are the design rules for integrating soft with hard materials creating hybrid and dissimilar materials? Can we use synthetic techniques to create hard materials that are tailorable and soft materials that are robust? How do we synthesize soft/hard/hybrid materials that can hierarchically organize by self or through external stimuli? Can we control the 3-D architecture of these materials? Can we control the materials interfaces of heterostructures?
- *Theory:* Theory, modeling, and simulation can often complement experimental efforts, predict trends, and provide design criteria for new materials and guide experiments beyond Edisonian or "Cook and Look" approaches. Can we reverse design by proposing a desired band structure and compute the thermodynamically most plausible synthetic route? What other scientific approaches can we take?

Finally, we refer you to the challenges reported in the Basic Research Needs workshop reports and the BESAC Grand Challenge report *"Directing Matter and Energy: Five Challenges for Science and the Imagination"* for more discussion on these and other challenges.

Funding Summary:

Dollars in Thousands		
FY 2007	**FY 2008**	**FY 2009**
15,592	**16,590**	**25,529**

Perfomer	**Funding Percentages***
DOE Laboratories	55%
Universities	45%

*Based on FY2007

Projected Evolution:

Over the past few years the program has evolved with 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 we expect to continue in these areas of interest, but with the added interest in the fundamental understanding of the mechanisms of interfacing soft-hard hybrid materials and the organization of these structures. We will expand our program towards the discovery of novel synthesis methods especially using extreme environments of field and flux and push the limits in our basic understanding in synthesis and processing of use-inspired technologies including solid-state lighting, solar energy conversion, hydrogen storage, and electrical energy storage.

This program will continue to support hypothesis driven fundamental science in the core research area of synthesis and processing with a particular interest in high-risk, high impact, innovative, and imaginative projects. The program continues to support and encourages natural collaboration between theorists and experimentalists to address the opportunities described in the "Scientific Challenges" above.