X-ray Scattering

Portfolio Description

This activity supports basic research on the fundamental interactions of photons with matter to achieve an understanding of atomic, electronic, and magnetic structures and excitations and their relationships to materials properties. The main emphasis is on x-ray scattering, spectroscopy, and imaging research, primarily at major BES-supported user facilities. Instrumentation development and experimental research in ultrafast materials science, including research aimed at generating, manipulating, and detecting ultrashort and ultrahigh-peak-power electron, x-ray, and laser pulses to study ultrafast physical phenomena in materials, is an integral part of the portfolio.

Unique Aspects

The DOE history and mission have played important roles in BES' current position as the nation's steward of major x-ray facilities. As part of its stewardship, BES maintains strong fundamental research programs at these facilities in materials and related disciplines. This includes the research that has motivated the BES-supported construction of the Linac Coherent Light Source (LCLS) and National Synchrotron Light Source-II (NSLS-II). The unique properties of synchrotron and free electron laser radiation – high flux and brightness, tunability, polarizability, and high spatial and temporal coherence, along with the pulsed nature of the beam – afford a wide variety of experimental techniques whose development and early application to materials science are supported by this program.

Ultrafast materials science involves time domain investigations examining, for example, the early stages of materials transformation through electronic structure excitation and subsequent energy transfer through various quantum mechanical structural pathways involving competing modes of ordering and energy dissipation. The aim of such ultrafast research is to investigate the details of dynamic events at the most fundamental time scales, leading to the understanding of emergent phenomena such as chemical reactions, the nucleation of defects in materials that result in the degradation of their properties, and the flow of energy in devices engineered with attention to novel nanoscale property effects. Potential applications involve the coherent control of surface chemical reactions and structures, switching and control of magnetic spin and ferroelectric polarization domains, and non-equilibrium optical processing during material synthesis.

Relationship to Other Programs

Within the various DOE science and technology programs, x-ray techniques play a key role in the investigation of materials and processes related to energy conversion and use by providing atomic- and molecular-level information on the structure of nano-particles and catalytic surfaces under *in situ* realistic chemical environments and in realistic device structures. Extending into the ultrafast regime, there is the promise of expanding understanding across the full range of chemistry and materials sciences by allowing femto-second stroboscopic investigations of the earliest stages of dynamic phenomena critical to energy conversion. The x-ray scattering portfolio contributes to other program elements, including:

- BES Energy Frontier Research Centers (EFRCs) benefit from the significant involvement of synchrotron x-ray researchers and their techniques. *In situ* characterization and nanoscale tracking of active materials in realistic energy conversion environments enhances the activities of several EFRCs.

The scattering program interfaces with other programs in BES dealing with scattering theory and models:

- Soft matter and biophysical materials interrogation through techniques such as grazing incidence small angle scattering and resonant soft x-ray scattering;
- Geosciences research through high pressure x-ray scattering techniques; and
- Spectroscopy applied to heavy element chemistry.

Coordination with other agencies includes:

- Joint funding (with NNSA) of the HPCAT beamline at the Advanced Photon Source optimized for high pressure condensed matter science.
- Predictive materials sciences activities and the associated theory, modeling, characterization and synthesis research are coordinated with other federal agencies through the National Science and Technology Council Subcommittee on the Materials Genome Initiative.
- Active interactions occur with the National Science Foundation through workshops, joint support of National Academy studies in relevant areas, and communication about research activities.

Significant Accomplishments

This program supports groups that have contributed to the development of such powerful techniques as inelastic x-ray scattering, x-ray absorption structural spectroscopy, x-ray microscopy, nanoscale focused beam diffraction, time-resolved spectroscopy, and resonant x-ray scattering providing specific chemical, magnetic, and excitation contrast.

Recent accomplishments include:

- Sensitive measurements of surface segregated atomic and electronic structure in new catalysis alloys and nano-particles, as well as measurements of distortions in the atomic ordering resulting from the interfacial constraints on perovskite oxide films which exhibit unique magnetic and electron transport behavior.
- Progress in understanding the rich magnetic and electronic structure of correlated electron materials continues in terms of mapping out phase boundaries and determining the nature of the competing quantum interactions behind transitions in physical properties.
- Refined *in situ* techniques have become more adept at probing small samples, surfaces, and interfaces under extreme processing environments of temperature, pressure, and reactive gases.
- When a material is excited by light or thermal energy to non-equilibrium states, different pathways back to equilibrium often have different time scales. Recent experiments in ultrafast science have employed multiple probes with different sensitivity to various relaxation mechanisms. Fresh results are beginning to tease out the faster dynamics of electronic structure from the slower recovery of atomic motion and lattice strain.

Mission Relevance

The increasing complexity of DOE mission-relevant materials such as superconductors, semiconductors, and magnets requires ever more sophisticated scattering techniques to extract useful knowledge and to develop new theories for the behavior of these materials. X-ray scattering probes are among the primary tools for characterizing the atomic, electronic, and magnetic structures of materials in relevant processing and energy conversion environments.

Scientific Challenges

The ultrafast excitation and exploration of dynamic pathways to metastable states provides another knob to explore the subtle energetic phase space of correlated electron materials, (much like ultra-high pressure techniques access new states along that not fully explored dimension.) Optically pumped excited states may be far from equilibrium and short lived, but the probe measurements are ultrafast and capable of capturing the elusive physics in a unique regime of matter. Recent and foreseeable advances in high-brightness x-ray sources create an unprecedented opportunity to image the primary event at nanometer spatial dimensions and ultra-fast time scales. Understanding how ultra-fast coherent radiation can manipulate condensed matter and how matter relaxes back to its unperturbed state may ultimately lead to novel materials synthesis techniques, especially at the nanoscale.

Recent advances in both sources and instrumentation have yielded gains in intensity on sample, facilitating rapid experiments and *in situ* configurations. Smaller samples can be probed with unprecedented temporal and spatial resolution, accuracy, and sensitivity under various parametric conditions. Such information aids the development of novel processing techniques and the search for new exotic materials. *In situ* studies are entering the ultrafast time domain through coupling laser pumped ultra-fast electronic excitations to atomic strain driven processes. There also exists the possibility of selectively studying the dynamics of such phenomena through the photo-doped creation of metastable states that would not necessarily be thermally accessible.

Projected Evolution

Advances in x-ray scattering and ultrafast sciences will continue to be driven by scientific opportunities presented by improved source performance and optimized instrumentation. The x-ray scattering activity will continue to fully develop the capabilities at the DOE facilities by providing support for instrumentation, technique development, and research. A continuing theme will be the integration and support of materials preparation (especially when coupled to *in situ* investigation of materials processing) as this is vital to careful x-ray structural measurements related to materials properties. New investments in ultrafast science will focus on research that develops and uses radiation sources associated with BES facilities and beam lines, but also includes ultra short pulse x-ray, electron beam and THz radiation probes created by conventional tabletop laser sources.