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 time-resolved and ultrafast materials science are an integral part of the portfolio.

Scientific Challenges

Ultrafast excitation and exploration of dynamic pathways to metastable states provides another path 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). Optical, IR, and THz pumped probes can excite materials away from equilibrium through different mechanisms; and ultrafast probe measurements are capable of capturing the short-lived and elusive physics in a unique regime of matter. Recent and foreseeable advances in high-brightness x-ray sources create an unprecedented opportunity to image interactions at nanometer spatial dimensions and ultrafast time scales. Understanding how ultrafast 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 samples, facilitating rapid experiments and in-place 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-place studies are entering the ultrafast time domain by coupling laser pumped ultrafast electronic excitations to atomic strain-driven processes. There also exists the possibility of selectively studying the dynamics of such phenomena through designed and driven excitations of quasi-particles and 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 supporting research that pushes instrumentation and technique development to address frontier scientific challenges. A continuing theme will be the integration and support of materials preparation and complex data analysis development, as these are vital to carrying out and understanding 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 and THz radiation probes created by conventional tabletop laser sources. The program does not support research considered “mature use” of existing x-ray or ultrafast techniques.

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 and coherent diffraction imaging, 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 were made, as well as measurements of distortions in the atomic ordering resulting from the interfacial constraints on perovskite oxide films that 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.

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 phase transformations and the nucleation of defects in materials that result in the degradation of their properties. Time-resolved fundamental investigations of the dynamic shifts in electronic structure and the flow of energy in new materials, such as two-dimensional films and surface states on topologically constrained quantum materials with strong spin-orbit coupling, are supported by this activity. Potential applications involve coherent control of surface chemical reactions and structures, creation of non-equilibrium phonon distributions with ultra-short lifetimes or transient and metastable phase structures, dynamic control of magnetic spin physics and ferroelectric polarization ordering, and excitation driven separation of degeneracies in materials with competing states of quantum ordering.

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.

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, layered hetero-structures, and catalytic surfaces under realistic chemical environments and in actual engineering designs such as those found in batteries and electronic devices. Extending into the ultrafast regime, there is the promise of expanding understanding across the full range of chemistry and materials sciences by allowing femtosecond stroboscopic investigations of the earliest stages of dynamic phenomena critical to energy conversion.

The x-ray scattering portfolio contributes to other program elements as they seek to understand atom and electron structural behavior relevant to the unique materials configurations supported by those programs. This is particularly true of the Experimental and Theoretical Condensed Matter Physics programs in BES because charge, spin, orbital and atomic structure and dynamics determination play a critical role in understanding materials behavior at the level of strong quantum interactions and emergent quantum coherence. There is close coordination with the BES Scientific User Facilities Division and with other agencies, including the National Science Foundation.

Within the larger federal research enterprise, program coordination is through the Federal Interagency Materials Representatives (FIMaR).