

Materials Science and Technology at the Renewed Advanced Photon Source

1. Executive Summary

Developing new materials is both the ultimate practical goal of the directions epitomized by the DOE's 5 grand challenges,¹ and a scientific challenge in itself. Materials have tremendous impact in energy, information technology, health, transportation, and defense. The fundamental challenges in each of these technological areas are in many cases defined by the capabilities of present materials and the potential to develop new ways to process materials. In energy, for example, the development of materials for applications in high temperature, solar photovoltaics, and light emission is the key to new energy technologies. Similarly, the development of new materials and the potential to process existing materials with nanometer precision have driven information technology and will continue to do so. Structural materials with longer fatigue lives, higher strengths, and better wear characteristics likewise have great promise across a number of applications.

New concepts in the way materials are processed have emerged as greater capabilities in theory, synthesis, and characterization have been developed. New directions in crystal growth, processing far from equilibrium, nanopatterning, and hierarchical self-assembly present challenges in fabrication, characterization, and in the basic theoretical description of materials. The science of new materials depends on advanced characterization techniques at length scales ranging from the positions of single atoms, to structures and defects at nanometer scales, to the overall organization of materials at large scales. In addition, the creation and transformation of materials is inherently a dynamic process that is greatly influenced by rare events. The properties and structure of materials evolve during these times, leading to the need for a fundamentally new approach to studies of random processes.

Techniques using synchrotron radiation have had a unique role in materials science and are rapidly evolving at the Advanced Photon Source (APS) and other facilities to keep pace with developments in the way that materials are designed, studied, and produced. In addition to these synchrotron radiation-based characterization tools of the end-products of materials processes, increasing access to synchrotron light sources will make them more valuable tools. This will be particularly valuable in areas of materials science and technology in which subtle changes in processing conditions can have large effects. Crystal growth, and the self-assembly of mesoscopic structures faces similar challenges will benefit tremendously from *in situ* instrumentation.

The medium-term renewal of the experimental facilities at the APS will enable a fundamental shift in the way that synchrotron radiation is used in materials science and technology. There are opportunities to develop new techniques, to use existing techniques more intelligently, and to combine scattering and imaging techniques with the revolutionary advances in information technology.

2. Introduction

Scientific Opportunities: One of the most important achievements in synchrotron x-ray characterization has been the development of techniques that provide unparalleled insight into the atomic structure of bulk materials, surfaces and interfaces, nanoparticles, nanostructures, and

nanodomains. Within these structures, x-rays have unique sensitivity to atomic positions, correlation and order, defects, and crystallographic distortion. Characterization techniques now allow the structure of individual nanostructures to be probed routinely. With new facilities, diffraction, scattering, and spectroscopy techniques can be widely applied to samples and processes that have been out of reach to the present generation of tools. Advances in detectors and sources promise to build on existing techniques by allowing existing techniques to be applied with great advances in speed and sensitivity, with reduced radiation damage.

Recent developments allow these x-ray scattering techniques to be applied to systems driven far from equilibrium. This is critical to materials science and technology from a fundamental perspective because the dynamic response of materials, the principles underlying the structure of materials and its evolution, and the dynamics of defects and domains are all fundamentally driven by non-equilibrium phenomena. In this sense, the structural, dielectric, and magnetic response to applied fields provides fundamental insight into the physics of materials. The relevant timescales range from femtoseconds to microseconds, and there are now opportunities to probe materials dynamics at a renewed APS at times as short as 1 ps. The processing of materials also inherently occurs away from equilibrium, and the emerging capability to probe non-equilibrium systems will be a powerful addition in systems for which there is presently no detailed *in situ* characterization. The dominant phenomena in non-equilibrium systems are often irreversible and rare, as in nucleation, crack initiation, and hysteresis in magnetic or electrical response. These non-equilibrium phenomena often occur in magnetic, optical, and pressure conditions for which conventional microscopies and characterization tools are not available.²

The transition from large-scale systems to nanoscience involves emergent phenomena that have no parallel in bulk systems. Electronic and magnetic phenomena are vastly different in confined systems and emergent and critical phenomena take new forms at small scales and at surfaces and interfaces. Defining the electronic effects relevant to doping in nanocrystals, for example, involves different statistical assumptions and electronic boundary conditions than in bulk semiconductors.³ These changes, and their dependence on size, composition, and how similar effects are manifested in nanoscale semiconductor devices are only beginning to be understood.

Key Areas: This report focuses on six specific scientific areas that serve examples of the areas where the development of advanced experimental facilities at the APS will have a huge impact.

- a. **Crystal growth:** What phases and processes are relevant to crystal growth?
- b. **Dynamic compression:** What are the properties of materials under transient pressures far higher than those available in static experiments?
- c. **Imaging random events:** How can we understand the rare stochastic events behind nucleation and crack initiation and other seemingly random incidents?
- d. **Atomic positions in semiconductor devices, ultimate strain:** What are the positions of atoms in devices with sizes on the order of tens of nanometers? How do the concepts of strain, composition, and concentration apply at this scale?
- e. **Dynamics in applied fields:** What is the structural response of materials to applied electric and magnetic fields?
- f. **Interfaces in biomaterials:** How can interfaces between engineered materials and complex biological systems?

Progress in these areas must be accompanied by simultaneous advances in materials theory and in efforts that link theory and the results of new experiments. Advances in density functional theory, for example, now allow the properties of insulators and semiconductors in high electric fields to be predicted.⁴ Similar advances in multiscale techniques, in electronic properties predictions, and in models of materials growth are now required.

3. Key Science Drivers

a. Crystal Growth

The design, discovery, and growth of new materials underpin the success of future materials-driven science and technologies. New energy conversion and storage systems will require breakthroughs in materials design. The end of the silicon roadmap demands both new materials and processing paradigms to fuel the engine of information technology. The APS, by embracing a paradigm of ‘bringing the laboratory to the beamline’ can advance the fundamental understanding of complex materials chemistry and physics and in the process significantly advance our options for answering these and other materials-driven science and technology challenges.

Single crystals are extremely valuable as the gateway to intrinsic physical behaviors and anisotropies, be they electronic, mechanical or thermal. The opportunity here is for the APS to provide a platform for elevating crystal growth from an art form to a science by harnessing the power of *in situ* growth characterization in ways not possible using laboratory-scale instrumentation. A strategic plan will be to energize both targeted synthesis of known materials and the discovery and exploratory synthesis of new materials. In keeping with the facilities mission of providing unique capabilities, we identify several high-impact *in situ* approaches that will advance the state-of-the-art of crystal growth, addressing the needs of a growing the materials chemistry and physics community.

i. Floating-zone Growth: Many of the highest quality crystals of oxide superconductors and of heavy Fermion compounds derive from containerless floating-zone (FZ) crystal growth (Figure 1). The quality of FZ crystals would be vastly improved through real-time knowledge of (a) the melt composition in the zone, particularly at the solid-liquid interface where effects such as segregation, diffusion and convection presently result in great uncertainty and (b) the microstructure of the growing crystal boule; i.e., how are crystallites nucleating and growing toward the single crystal limit. These needs can be met by application of spatially-resolved element-specific probes using fluorescence and resonance scattering and x-ray radiography techniques. The latter has been used to map dendritic growth in two-dimensions at synchrotron facilities,^{5,6} but a real 3D picture of the growing crystal is actually what is needed. For doped crystals, knowledge of the dopant profile (or equivalently the effective distribution coefficient) could be addressed by spatial composition mapping during the growth. The overall goal should be more than just characterization, however. A more powerful outcome will be to couple such

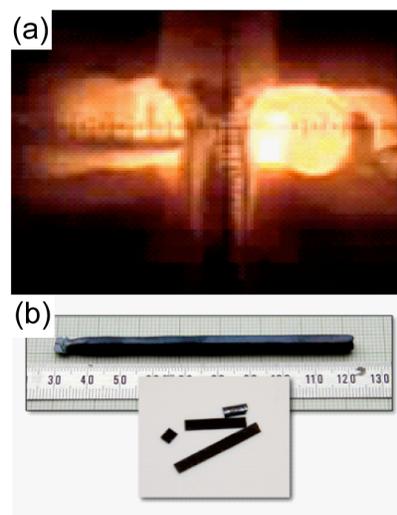


Figure 1 (a) Floating zone (FZ) crystal growth. (b) FZ-grown oxide crystals

information into a feedback mechanism for real-time adjustment of growth parameters, optimizing the growing crystal in response to the chemical and physical state during the growth.

ii. High-Pressure Crystal Growth: The frontier of new materials discovery and crystal growth lies at extreme conditions such as high pressure. New phases, extended solubility limits, metastable compositions, crystals that cannot be grown at ambient conditions – with concomitant new properties – have been and will continue to be found at high pressure. Synchrotrons are not new to this arena, with several important single crystal growth successes (e.g., GaN,⁷ oxide superconductors,⁸ low-dimensional magnets,⁹ as well as a number of other materials) depending on understanding solid-liquid phase relations at high pressure via *in situ* powder diffraction. An APS long-term vision could be to advance high pressure crystal growth by going beyond phase diagrams toward *in situ* identification of nucleating crystallites. The crystallization pathway is essential information, particularly for incongruently melting compounds. Simultaneous advances in techniques for obtaining 3D crystallographic data from samples in the pressure cell are also essential.

iii. Hydrothermal Synthesis: Significant inroads have been made already in the area of crystallization kinetics using *in situ* techniques.¹⁰ Rapid screening approaches, presumably by diffraction, would allow the grower to take either a combinatorial approach or to control products in real-time.

iv. Flux Growth: Molten fluxes (metals, salts) can be used to let equilibrium phase diagrams ‘compute’ the stability of new phases. As in high-pressure synthesis, interrogation of the melt composition, knowledge of the stepwise crystallization products, and the ability to modify process parameters in real-time would be distinct advantages for exploratory and targeted crystal growth. An opportunity for synchrotrons would be highly focused, high intensity beams that could identify the first nucleating crystals rather than having to wait hours or days to collect a specimen suitable for ex-situ analysis.

v. Biological/Protein Crystal Growth and Self-Assembly: The opportunities and concepts associated with the precision of crystal growth can be extended to longer length scales using self assembly techniques.^{11,12} The repeating units of these materials are at the scales of nanometers to hundreds of nanometers, but pose a similar set of fundamental challenges in the control of the resulting structure. The larger scale of these materials presents a different set of characterization challenges in small-angle scattering and coherent scattering, that should be addressed as part of a comprehensive effort in characterizing materials synthesis.

b. Dynamic Compression

Dynamic compression experiments (shock wave and shockless compression) subject materials to extreme conditions (very large compressions, high temperatures, and large deformations) on very short time scales (ps to μ s) resulting in a rich array of physical and chemical changes. Because our scientific focus is on the condensed state, only pressures to 500-1000 GPa (5-10 Mbar) and temperatures to 0.5 eV are considered here. The extreme conditions encountered under dynamic compression provide a unique opportunity to explore the delicate balance between mechanical ($P\Delta V$) and thermal ($T\Delta S$) energies by examining how this balance governs a wide variety of physical and chemical phenomena. The short times inherent in dynamic experiments result in the kinetics playing an important role in determining the governing mechanisms and the attainment of metastable states, beyond thermodynamic constraints. Dynamic compression can be used to examine fundamental scientific issues and

questions related to the following condensed matter phenomena: structural changes including electronic transitions; chemical reactions including bonding and energetics; and deformation and fracture.

Irrespective of the phenomena being examined, dynamic compression experiments are ideally suited to probe, in a time-resolved manner, physical and chemical changes as they occur. Such information is essential to a mechanistic understanding of condensed matter phenomena. Knowledge gained from dynamic loading experiments will have a broad impact on condensed matter sciences, well beyond dynamic loading. Dynamic compression experiments, because of the potential to probe physical and chemical changes as they occur on ps to μ s time scales, are ideal for understanding condensed matter response at extreme conditions.

In recent years, there have been major experimental advances, mainly at the DOE- NNSA Laboratories to vary the loading conditions of interest (compression, temperature, deformation, and loading times) in a controlled manner. These advances provide new opportunities for examining and understanding condensed matter phenomena. However, the experimental measurements to date are almost exclusively at the continuum scale. As such, the ability to address fundamental scientific issues related to mechanistic understanding at the microscopic level is limited.

Simultaneously with the major advances in dynamic compression technology, the extraordinary developments in computational capabilities (starting with the ASCI efforts) over the past 10–15 years have added a new dimension to scientific research. The pace in modeling and simulations will continue at this or even a higher rate for the foreseeable future. Despite the impressive advances in modeling and simulations of condensed matter phenomena, the following question continually arises: how valid are the predictions from these simulations? The third element of dynamic compression research, measurement capabilities, has lagged behind significantly in comparison to advances in dynamic loading technologies and computational developments. The principal need at the present time is for time-resolved, in-situ microscopic measurements. Without comparable advances in measurement capabilities, the full scientific potential of investments and advances in dynamic loading and computational capabilities will not be achieved.

Time-resolved, *in situ* microscopic measurements constitute the most important need for achieving a fundamental understanding of condensed matter phenomena and processes under dynamic loading. Such measurements will lead to revolutionary scientific advances well beyond dynamic compression. Although the need for the above indicated measurements is clear, obtaining such data in single event experiments is a formidable challenge and requires special measurement capabilities.

c. Imaging Random Events

A number of problems in materials science and engineering derive from statistical origins. These include the initiation of fatigue cracks in metals,¹³ brittle failure in ceramics, intermetallics and network polymers,¹⁴ pitting by corrosion,¹⁵ and grain boundary environmental corrosion.¹⁶ To gain a fundamental understanding of these processes, experiments are contrived in a way to eliminate their statistical nature. In fracture experiments, for example, pre-cracks or notches are placed in specimens to provide focus for the experiment. While affording useful information in assessing the steady state phenomena of crack growth, these experiments risk the loss of crucial information regarding the nucleation or initiation event. Of even greater concern, from a

technological perspective, is that lifetime predictions based continuum or fracture mechanics treatments for long, artificial cracks are not well suited for short or just nucleated cracks.¹³ Hence, *in situ* experiments of defect-free samples are particularly promising, not only helping to elucidate fundamental mechanisms of nucleation events, but also to provide grist for lifetime models which more accurately simulate reality.

The random nature of these events poses serious challenges for observation. Firstly, real-time imaging is essential. Dendritic growth during the solidification of aluminum alloys has been observed using real-time X-ray imaging.¹⁷ However, the technique relies on a sharp difference in X-ray attenuation between separate phase domains, e.g. a crack (void space) in a fatiguing metal or a corrosion product surrounded by non-corroded material. Secondly, observation volumes must be of the order of the sample size to “catch” the nucleation event. Large detector arrays would be required to afford sensing over the entire sampled volume in real time. Analogous screening has been done in the field of acoustics for seismic and biomedical imaging of random incidents¹⁸ and in structural health monitoring,¹⁹ using “time-reversal imaging.” The technique affords both spatial and temporal focusing on regions of interest in inhomogeneous environments, as for the solid oxide fuel cell in Figure 2.²⁰ Finally, environmental control must be uniform over the entire observation volume. This may require elevated temperatures, corrosive environments, applied loads, or some combination of these.

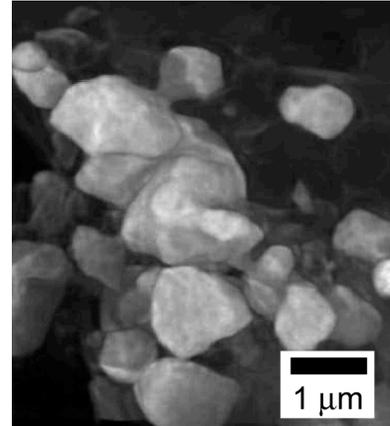


Figure 2 Transmission x-ray microscope image of Ni grains in a solid oxide fuel cell, ref. 20.

Once the locations of nucleation events are established, taking advantage of further capabilities of the synchrotron could enhance mechanistic understanding. For example, using near-field grain mapping, the evolution of the dislocation structure in individual grains could be followed, and hence, related to crack nucleation. Grain orientations could be monitored to assess corrosion prone orientations. A SAXS detector would be useful in tracking the statistics of void formation during elevated temperature fracture experiments.

Several kinetic processes in materials would benefit from these studies:

- 1) Crack initiation and growth under monotonic loading in brittle materials. These experiments would be limited to materials that demonstrate stable crack growth, such as that seen in ceramic-matrix composites.
- 2) Fatigue crack initiation and growth in metals.
- 3) Pitting during aqueous or gas-phase corrosion.
- 4) Environmental-assisted or embrittlement of grain boundaries. These experiments would highlight which grain boundaries are more susceptible to embrittlement than others.
- 5) Vortices in superconductors and other nano-to-mesoscale phenomena in condensed matter systems.

Establishing the intrinsic or extrinsic causes for nucleation events would provide critical information for mechanistic models and life prediction strategies.

d. Atomic positions in semiconductor devices, ultimate strain

The presence of strain distributions within semiconductor features influences many aspects of their behavior. For example, microelectronic technology that incorporates strained silicon improves device performance by increasing carrier mobility in the Si channels. Because current semiconductor fabrication contains multiple levels of metallic and dielectric structures, an understanding of the mechanical response of the constituent elements is critical to the prediction of the overall device performance. In addition, the interaction of strain fields between adjacent structures becomes greater as feature sizes decrease and the corresponding feature density increases. Therefore, the mechanical response of the semiconductor and its environment is critical to assessing the true state of strain near these devices. We note that the continuum mechanics concept of strain may be inapplicable when the linear dimensions of the semiconducting regions are less than 10 nm or so. The equilibrium spacing between the atoms on such a small length scale cannot be assumed to be constant; there is no rigorous definition of normalized displacement at a point. X-ray diffraction from these small structures includes coherent effects which cause dramatic effects that cannot be understood with the rules of thumb developed for larger structures.²¹ As such, we need to measure the atomic coordinates of the atoms within the channel region, since the local symmetry will determine the effective masses, and hence the mobilities of the charge carriers.²²

While the modeling and verification of the electronic properties of regions on the nanometer length scale has been successful (for example, the effect of size quantization through modified local density approximations), the corresponding analysis of the mechanical behavior at these dimensions is incomplete. There are significant theoretical and experimental challenges to be addressed because the extension of continuum mechanics approaches to nanoscale volumes has not yet been verified. In addition to the intrinsic complexity associated with measurements at the relevant dimensions, the presence of local discontinuities (edges, free surfaces, interfaces, defects) can significantly modify the atomic positions within these domains. The presence of a single extended defect in these systems is already known to cause large deleterious electrical effects and characterizing the nature of defects remains a challenge.

Emergent effects at the new small length scale at which integrated semiconductor devices can now be produced include vastly different thermal properties, which can be the key to using semiconductor technology in new thermoelectrics and in other applications taking advantage of the large-scale processing of silicon.²³

e. Dynamics in applied fields

The structures and properties of materials can be dramatically changed by applied electric fields. The effects associated with the response of materials include polarization, piezoelectric distortion, and at high fields or strains the stabilization crystallographic phases that are structurally or electronically distinct from the ground state.²⁴ The transitions to these phases can be driven by piezoelectric strain or by charge carriers accumulated in the near-surface layer screening the applied field.²⁵ Despite the differences in these mechanisms, in broad terms, the coupling of the electric field to the polarization to effectively expands the phase diagram in much the same way as hydrostatic pressure or other thermodynamic variables. The problem of describing long-range polarization in first principles calculations has recently been solved, making available a range of predictions of materials properties that have yet to be tested.

The timescales associated with the structural response to applied electric fields range from domain wall motion in ferroelectrics, which spans a wide range of timescales from seconds to nanoseconds, to the development of the ionic contribution to dielectric polarization with timescales on the order of tens of picoseconds or less. X-ray scattering is unique in that it can provide structural information with essentially the same precision at these timescales as at any other. The transient strain developed in response to a short applied electric field pulse can be evaluated using diffraction, and can reach several percent.²⁶ There is now the opportunity to extend this type of approach to other, more subtle properties.

Strain and other properties are a result of the modification of the interatomic potential in the applied electric field. The phonon dispersion provides a direct measure of the interatomic potentials. The phonon dispersion can be determined quantitatively using thermal diffuse scattering.²⁷ With specific technical advances, thermal diffuse scattering can be adapted to provide the equilibrium and non-equilibrium elastic properties of nanostructures.

In multiferroic materials that are both ferroelectric and magnetic, applied electric fields can influence the magnetism of the material. X-rays are unique in providing a quantitative probe of magnetism that, unlike neutrons, can be focused to small sizes and used to study individual isolated devices and domains.²⁸ Magnetic scattering will provide a unique window into the coupling of the magnetic and electrical degrees of freedom in multiferroics. At interfaces, absorption spectroscopy, dichroism studies in applied fields will provide insight into the spin injection process in ferromagnetic semiconductor contacts.

More generally, the influence of applied fields on structural order has a wide influence in materials that are purely magnetic. Magnetic shape memory alloys such as Ni₂MnGa have a large structural response to applied magnetic fields that is influenced by structural, magnetic, and composition effects that are only beginning to be understood.²⁹ The physical fundamentals underlying the dynamics of this response are largely unknown, because there have been no structural probes available. It is possible now to traverse the thermal phase transitions relevant to similar materials rapidly using ultrafast laser techniques, and possible to create intense pulsed magnetic fields and spin polarized currents on a small scale.^{30,31} Applying these approaches to understanding how structural phases coexist as a function of applied magnetic field and strain would be an important advance.

The timescales associated with the response to applied field extend far below the times that can be resolved using the APS in its current form. Developing an ultrafast capability extending to the few-ps scale, and the capability to induce phase transitions and drive samples electrically and magnetically, would open a new range of possible experiments.

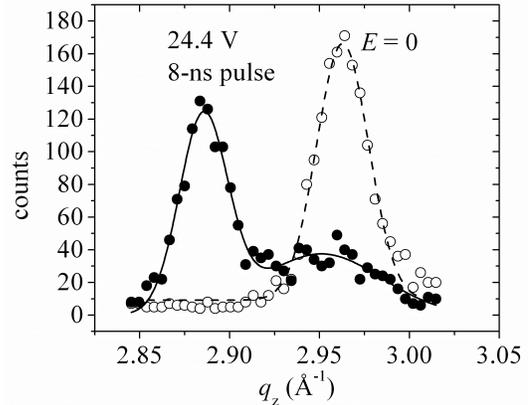


Figure 3 Transient strain of 2.7% in a 40 nm-thick PZT film in response to an 8 ns electric field pulse, ref. 26.

4. Significance of APS

The APS is uniquely suited to studies of materials using scattering and spectroscopy. Among U.S. light sources, only the APS has a large diameter and high electron energy. The large diameter of the APS allows it to be run in a mode in which the discrete electron bunches are widely spaced in time, which greatly simplifies time-resolved experiments. This bunch spacing is an excellent match for the capabilities of new detectors capable of single-bunch time resolution. Simultaneously, the development of new beamline-scale electron optics producing short pulses (as in the proposed APS-based Short-Pulse X-ray Source, SPX) requires the uniquely long time between bunches of the APS.³²

The high electron energy of the APS allows insertion devices to produce intense beams at high photon energy. High photon energies with brilliant stable sources are essential for *in situ* scattering and imaging experiments in which the beam must penetrate into the environments of high pressure, temperature, or high-fields. High photon energies also allow x-rays to be used to study the liquid-solid interface in crystal growth, where absorption lengths at lower photon energies would penetrate only a few microns.

The APS has an inherently low emittance and as a layout of the experimental floor that favors microscopy and imaging. Further developments in electron optics, insertion devices, and x-ray optics will solidify this advantage.

The APS is the home of emerging technologies on which the advances in the synchrotron radiation study of materials will be based, for example developments in multilayer Laue lens optics for x-ray focusing,³³ high-resolution primary beam monochromators and analyzers for inelastic scattering,³⁴ and high-pressure research,³⁵ as well as in a myriad of other areas. These efforts provide the APS with an important base on which future developments are based.

5. Scientific Community

There is a large scientific community of researchers, scientists, and technologists that will find new ways to connect to synchrotron radiation experiments using the developments described here. The scientific community will also be strengthened by these developments in that there will be new opportunities for one-of-a-kind experiments at the cutting edge of synchrotron radiation technology. These types of studies are the basis for future work with broad impact in the community. The challenges in these areas span all of the disciplines of materials science and involve communities of researchers in academia, industry, and government laboratories.

6. Requirements and Capabilities

Full-Field Microscopy and Tomography: The development of full-field imaging and diffraction enhanced imaging capabilities is essential in advancing areas of research that depend on surveying large areas of materials including **crystal growth** and **imaging random events**. In studying three dimensional phenomena including crystal growth, real-time or near real-time tomographic reconstructions with high rates of data acquisition and analysis are essential. The proposed long beamline for imaging will provide for larger fields of view.

Nanodiffraction: To address the questions associated with **atomic positions in semiconductor devices** we need a state-of-the art beamline with a beam-size around 10 nm or better, with energy resolution below 1 eV over 5-30 keV range. Large gradients in the strain distributions near the feature edges are convoluted by larger x-ray microbeam sizes. In order to capture the strain distributions at these critical regions, a smaller beam size is required. X-ray nanoprobe with

improved spatial resolution in diffraction, imaging, and spectroscopy will allow us to measure these strain distributions at a much finer length scale, which is commensurate with current Si device sizes (< 65 nm). We also need data analysis software that can be used to analyze the x-ray scattering from such small domains.

Short Pulse Sources: The Short Pulse X-ray (SPX) Source at the Advanced Photon Source will extend time-resolved capabilities to the important 1-ps timescale for to study **dynamic compression**, **dynamics in applied fields**, and **imaging random events** while retaining the user-controlled continuous tunability of energy, polarization and bandwidth combined with x-ray energy and pulse length stability over a wide energy range. The very high average flux ($\sim 10^{13}/\text{s}$) of the proposed SPX combined with high repetition rate excitation methods and year-round operation, will enable time-resolved studies with unprecedented precision – yielding joint resolution of picoseconds and picometers for a variety of atomic, molecular, chemical and material systems.

Environments: For **dynamic compression** experiments, the experimental challenge is to combine the dynamic loading capabilities (developed by groups at the DOE's NNSA laboratories) with the microscopic measurement capabilities at the APS. The development in this sense could parallel the precedent of HP-CAT and result in the establishment of a first-of-a-kind user facility dedicated for dynamic compression experiments. For **imaging random events** both elevated temperatures to 1500°C and controlled gaseous environments, e.g. water vapor or other corrosive species, coupled with dynamic loading, would be essential. **Crystal growth** requires a similar commitment to sample environments that can be integrated with imaging, scattering, and spectroscopy experiments.

Facility-wide improvements and Infrastructure: There are three facility-wide improvements that must accompany the critical upgrades in scientific capability.

- 1) Software to process the stream of data arising from these scattering and imaging tools. Advances in beamline control software are necessary to allow these experiments to take place routinely. This improvement in the information infrastructure will simplify use of the APS and allow its capabilities to reach wider groups of materials researchers.
- 2) Better stability in beamline software and hardware must be achieved to allow experiments with *in situ* components. The accelerator side of the APS has developed metrics for the availability of the beam that the allow progress being made in optimizing the facility to be quantified, and a similar push needs to be made for the beamlines.
- 3) Improved point and area detectors for scattering and fluorescence will be required to allow the diffraction and imaging experiments to proceed.
- 4) Infrastructure additions that enable the safe and usable installation of a variety of sample processing and synthesis environments. Access modes permitting long term installation of both complex user-designed environments optimized for a particular material system as well as general environmental chambers. Infrastructure needs include adequate ventilation and exhaust systems, ability for gas and chemical handling, cleaning, and sensing.

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