The Advanced Photon Source and the Advanced Photon Source Upgrade
Report to BESAC Facilities Review
February 27, 2013

The Advanced Photon Source (APS) plays a vital role in advancing the U.S. scientific enterprise, enabling fundamental discoveries in the physical and life sciences and supporting world-leading applied and industrial research. More than 5,000 users conduct research at the APS each year, performing experiments that yield groundbreaking results across a wide range of disciplines. As the keystone component of Argonne's suite of scientific facilities, the APS provides extraordinary research tools that address many of the most pressing scientific challenges of our time.

The APS characterization capabilities make it possible for materials scientists to study samples *in situ*, observing chemical processes and materials function in real time and under realistic conditions. Biologists use the APS to better visualize and understand fundamental protein structures; in 2009 and again in 2012, the Nobel Prize in Chemistry recognized pioneering discoveries in structural biology based in important part on research carried out at the APS. Geoscientists use APS diamond anvil cells to understand the behavior of minerals beneath the earth's mantle. Industrial researchers use the APS to design life-saving pharmaceuticals and develop revolutionary energy systems. Through the APS, talented researchers are gaining knowledge and making discoveries that promise to improve our health, protect our environment, strengthen our economy and expand our fundamental understanding of our world.

As we move forward, the APS Upgrade will equip this vital facility for scientific leadership in the 21st century. The APS Upgrade will offer researchers orders-of-magnitude improvements in spatial, time, and energy resolutions, detection efficiency, and beam brightness, stability and pulse width. These new capabilities will dramatically improve scientists' ability to observe, understand, synthesize and ultimately control chemical processes and advanced materials, creating valuable new opportunities for interdisciplinary, cross-platform grand challenge research. Notably, given the central importance of APS to a large and growing user community, the APS Upgrade project will not interrupt continuing operations and full user access.

The APS Upgrade project is proceeding through the rigorous review process established by DOE and is entering the construction phase. When the APS Upgrade is complete, the hard x-ray capabilities of APS will be unsurpassed within the constellation of BES x-ray facilities and will effectively complement other research tools throughout the National Laboratories.

Overview

The APS and its sister facility, the Advanced Light Source, were the first U.S. synchrotron facilities designed specifically to produce x-ray beams using undulators – magnet structures that produce quasi-monochromatic radiation with much higher brightness than previous sources. The APS storage ring was optimized to produce very bright x-rays in the medium (2-15 keV) and hard (>15 keV) energy ranges. (Figure 1 at right shows the brightness vs. x-ray energy at the top beamlines among the constellation of BES synchrotron facilities.) X-rays in the medium and hard energy ranges are powerful characterization tools, revealing atomic-scale structures via diffraction and their chemical nature via spectroscopy. These x-rays readily penetrate samples to allow imaging of internal structures and materials *in situ*. Additionally, the APS generates intense 100 ps x-ray pulses with flexible timing, offering excellent capabilities for studies of ultrafast dynamics in scientifically diverse systems. The high-quality, reliable x-ray beams at the APS have led to important discoveries in materials structure across multiple disciplines, including condensed matter physics, materials science, chemistry, geoscience, structural biology, and environmental science.

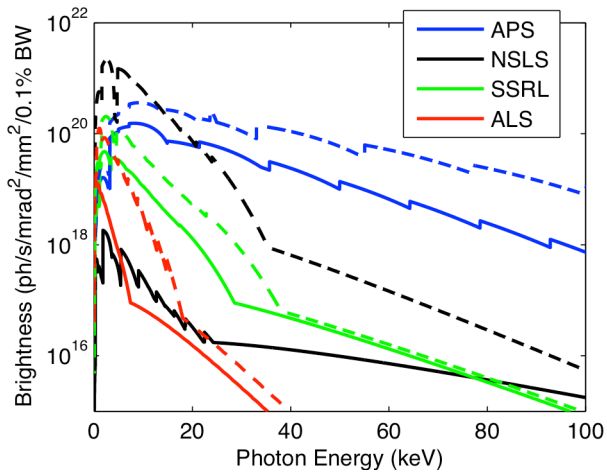

Fig. 1. Average spectral brightness vs. x-ray energy provided by optimum beamlines at current (solid) and future (dashed) BES rings.

The superb capabilities of the APS have attracted a strong and growing research community [1], making it the nation's largest user facility. At present, the facility's 66 simultaneously operating endstations are oversubscribed, on average, by a factor of 2. In 2012, ~5,600 APS users carried out some 4,900 experiments, producing 1,500 publications – 20% of them in high-impact journals. Researchers at the APS are the greatest contributors to the global Protein Data Bank, solving and depositing more than 3,800 protein structures since 2011. The APS user community also includes industrial researchers from more than 150 companies. Recently, the APS has implemented canted undulators, which allow two undulator beamlines in every sector, potentially doubling capacity. This expanded capacity, combined with increasingly mature and efficient experimental methods, will allow the numbers of annual users and experiments to approach 10,000 by 2024, as shown in Figure 2.

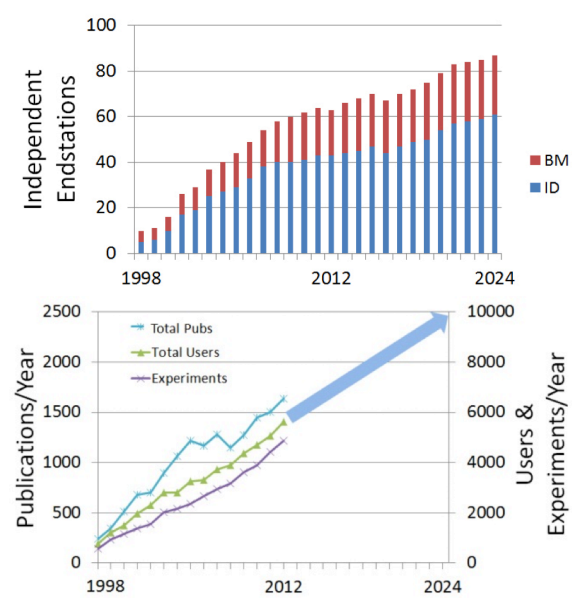

Fig. 2. Historical and projected simultaneously operating undulator (ID) and bending-magnet (BM) beamlines and yearly APS users, experiments, and publications.

Worldwide, synchrotron facilities are developing rapidly, driven by improvements in sources, optics, and detectors. In particular, new state-of-the-art hard x-ray beamlines are being deployed through the upgrade of the European Synchrotron Radiation Facility and the construction of the new PETRA-III facility at DESY. To assure that the APS will continue to offer world-class capabilities, we held a series of workshops with our user community to define the scientific themes for the future of APS: *"Real materials under real conditions in real time,"* and *"Mastering hierarchical structures through imaging."*[2] These themes guided development of a technical strategy for the APS Upgrade and beyond – a decadal plan to maximize the capacity and transform the capability of the APS for breakthrough science across disciplinary lines.

The APS Upgrade (APS-U) project will empower researchers to meet new scientific needs and to find breakthrough solutions to address the ultimate problems in materials, chemistry, energy, medicine and national security. The APS-U will provide orders-of-magnitude improvements in spatial, time, and energy resolutions. Increased detection efficiency and major advances in brightness, stability, and pulse width will make it possible to observe and image – in real time – important fast and ultrafast processes, including fuel sprays, shock compression, chemical transformations and biological processes in living organisms. These capabilities will enable new generations of experiments, ranging from studies of unconventional superconductors, nanoscale heat transport, and materials microstructures under extreme stresses, to imaging – and ultimately synthesis and control – of complex hierarchical structures. The impacts of the APS-U will be amplified by researchers' ready access to the other user facilities in the Argonne suite: the Center for Nanoscale Materials, the Electron Microscopy Center, and the Argonne Leadership Computing Facility. APS-U also will create synergies with scientific initiatives throughout Argonne, such as materials for energy, computing and big data, transportation and the new Joint Center for Energy Storage Research. Additionally, the expanded capabilities of APS-U will complement those being developed in other BES x-ray projects: NSLS-II, LCLS, and NGLS.

A full description of the APS Upgrade is available in the Preliminary Design Report completed in 2012 [3]. In summary, the APS Upgrade project includes:

- 20 undulator beamlines, including high-energy diffraction, resonant inelastic scattering, ultrafast diffraction and spectroscopy, *in situ* studies of materials synthesis and function and wide-field imaging, each with orders-of-magnitude performance improvement through optimized accelerator systems, undulators, beamline optical systems, and detector systems,
- Development and deployment of critical accelerator technology:
  - Short-pulse x-ray system (SPX) to open the time window from 100 to 2 ps for high rep-rate pump-probe studies of dynamics;
  - Higher brightness undulators (superconducting and revolver) and extended straight sections;
  - Increased stability and beam current.

Scientific Impacts of APS and the APS Upgrade

As the recent BESAC report [4] on Next Generation Photon Sources for Grand Challenges in Science and Energy made clear, advanced x-ray sources are crucial to our ongoing efforts to solve the grand challenges of sustainable energy, climate change, information technology, biological complexity, and medicine. The APS-U will transform the universe of experimental capabilities available to researchers, creating new opportunities to answer pivotal scientific questions: How does the collective behavior of strongly correlated electrons give rise to fundamentally new properties? How do materials transform under planetary core pressures? Can

we understand the dynamics and manipulate the hierarchical structures of life, from molecules to cells to organisms? Can we create new structural materials that will withstand harsh, extreme conditions? How do electronic and atomic configurations interact during chemical reactions – and can we control their outcomes?

Understanding the origins of excitations in strongly correlated electrons

A grand challenge of 21st century science is *to understand the fundamental excitations that produce the striking properties of materials with strongly correlated electrons*. Many of these properties – such as superconductivity, magnetic, charge and orbital order, localized electronic transport – are realized as delicate low-energy phenomena, disrupted on the scale of thermal energies. However, their origin lies in strong Coulomb forces that operate at high energy scales over long distances with strengths in many electron volts. The emergence of delicate broken symmetry phases out of strong interactions is a paradigm for all of physics, but there exists very little detailed understanding of how the low-energy phenomena appear. The most direct probe of these scenarios would be to measure charge- and spin-fluctuation spectral functions over the full range of momentum in the Brillouin zone, and over an energy range from several eV (a typical bandwidth) down to energies of 0.1 eV. This would reveal the origin of collective modes, which themselves mediate interactions between quasiparticles on lower energy scales, and which in weak-coupling approximations bootstrap the broken symmetries.

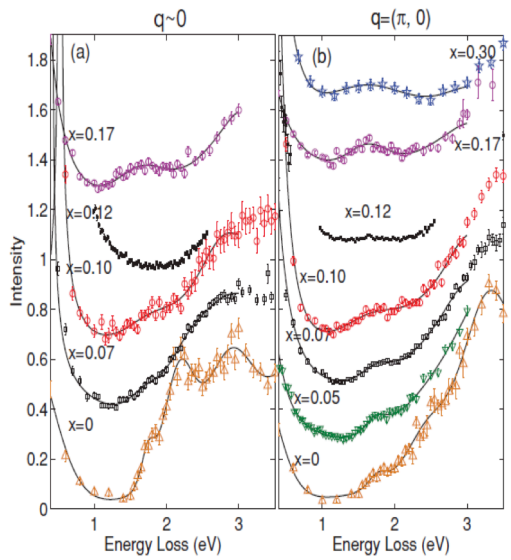

Fig. 3. Low-energy part of the RIXS spectra of mid-IR excitations in $La_{1-x}Sr_xCuO_3$ [5], demonstrating that fluctuations related to charge order increase with doping. APS-U will deliver higher intensity and resolution, allowing systematic study of these mid-IR excitations for the first time.

Resonant inelastic x-ray scattering (RIXS) is a powerful probe that offers a full measurement of charge fluctuations over the relevant energy and momentum range, and the critical mid-IR regime below 2 eV has remained a terra incognita. Recently, however, RIXS instrumentation at APS has achieved the resolution required for excitations in the mid-infrared band [5]. Moreover, recent progress in the theory of RIXS indicates that its cross-section has a term proportional to the loss function $\chi''(q,\omega)$ [6]. Unfortunately, the RIXS intensity at APS today is too low, requiring roughly 24 hours to measure one spectrum and thus a full week of beam time to perform a complete momentum-dependent experiment. This limitation will be eliminated by the APS-U. In addition to greatly improved source and optics, APS-U will provide a multi-analyzer assembly capable of measuring many momenta simultaneously. Hence, APS-U will allow – for the first time – a measurement of the loss function in the critical regime of energies where quasiparticles emerge.

Expanding the frontiers of high-pressure science

There are good reasons to believe that most of the unknown materials in the world can be found at high pressure. Materials under high pressure display unexpected properties, transform into

new phases and even form new states of matter. Pressure is an increasingly important dimension in experimental science, making it possible *to use high pressure to understand the nature of matter itself*. As we reach ever-higher pressures in experiments, surprising and exotic phenomena reveal themselves: molecular solids can become atomic solids, and quantum effects can come into play.

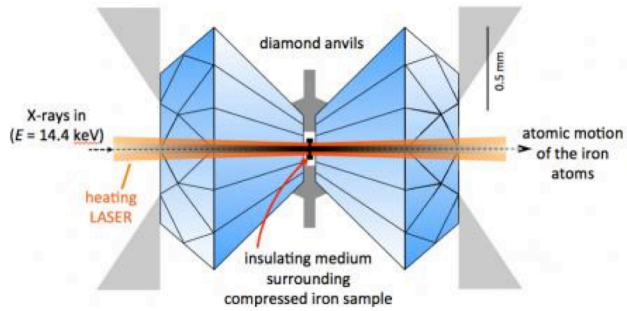

Fig. 4. Diamond anvil cell with laser heating, used for Mossbauer spectroscopy study of Fe melting at >3000K and >800 kbar. Smaller focal spots with APS-U will allow studies at conditions found in the Earth's core. [7]

Experiments at APS combine high-pressure cells with a number of x-ray techniques to investigate the myriad impacts of pressure on molecular interactions. For example, researchers at APS subjected an iron sample to laser heating in a diamond-anvil cell, as shown in Fig. 4. Mössbauer spectroscopy indicated that iron melts at ~3025 K at 820 kbar [7] – significantly warmer than previous estimates, a finding with important implications for Earth science. With APS-U, higher brightness and smaller spot sizes will enable experiments across the full array of x-ray techniques at a new range of pressures, reaching multi-Mbar conditions approaching conditions at planetary cores.

Exploring the hierarchies of living structures, from molecules to cells to organisms

Although the use of synchrotron facilities for x-ray crystallography of protein structures has revolutionized structural biology, researchers have not yet been able *to fully comprehend the ways in which proteins and other macro-molecules determine function at every level, from molecules to cells to organisms*. In particular, the rich dynamics of these hierarchical structures remain largely unexplored.

INDUSTRIAL IMPACT
Conquering disease through drug design

A strong community of pharmaceutical companies – including Eli Lilly, Abbott, Bristol-Meyers Squibb, Merck, Novartis and Pfizer – rely on the APS to provide the highest quality crystallographic data for structure-guided drug design, leading to therapies targeting cancer, diabetes, Alzheimer's, HIV and chronic pain.

Lilly now has a dozen experimental compounds developed with the aid of APS that are now in Phase I and II clinical trials. The APS plays a key role in a third of Lilly's discovery portfolio and daily crystallographic experiments are integrated directly into the drug discovery process. Robotics and automation now allow Lilly to process more than 200 crystals in 24 hours.

In the future, focused beams of high stability provided by APS-U will extend structure-based drug discovery to membrane proteins, such as G protein-coupled receptors, which are increasingly targeted by modern pharmaceuticals.

Today, APS is the world leader in macro-molecular crystallography because its high-brightness x-ray source enables rapid screening of crystals and collection of high quality datasets from even very small crystals. Current work focuses on solving the structures of these molecules and has allowed researchers to address numerous critical questions. For example, the 2012 Nobel Prize in Chemistry was awarded to Kobilka and Lefkowitz for their studies of G protein-coupled receptors (GPCRs), membrane proteins that allow the internal processes of cells to respond to external hormones and other small molecule signals. Using the APS, Kobilka was able to image these proteins in complexes with partner molecules and thus discover how transmembrane signaling is initiated.

As described in a recent report [8], the APS-U will provide leading-edge x-ray capabilities to the biological sciences community. APS-U will significantly extend the ability to probe protein

structure and dynamics and to image nonperiodic soft structures, from tissues to cells to subcellular structures. This new capability has the potential to transform our understanding of biological structures; it will allow researchers to use a single imaging tool with increasing resolution – from mm to 10 nm – to view samples cryogenically preserved in their native state.

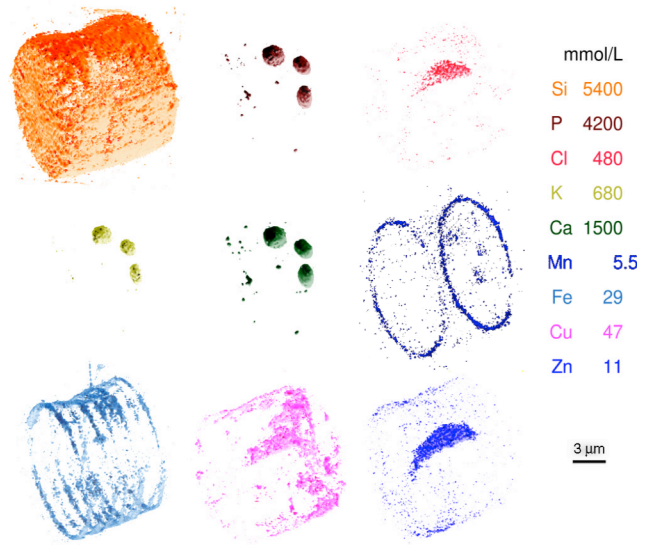

Fig. 5. Fluorescence nanoprobe images of trace elements in a diatom cell, at 400 nm resolution [9]. APS-U will improve resolution to 20 nm and sensitivity to 10 atoms, allowing structure of intracellular organelles to be observed.

Progress in biological crystallography is limited by the difficulty of obtaining sufficiently large crystals of many of the most interesting proteins and complexes, such as GPCRs. APS-U's improvements in beam stability are critical for high-quality crystallographic measurements of small crystals, reducing the smallest measurable crystal size from 5 to 1 μm. This benefit will be amplified by increased brightness. APS-U's higher x-ray energies also are needed for biological science: Higher x-ray energies cause less radiation damage, an important feature when using highly focused beams. The deeper penetration of higher-energy x-ray beams enables *in situ* observations essential for environmental science and whole-organism and tissue studies. For fluorescence microscopy, higher energies will provide access to all elements in the periodic table. The capabilities of APS-U will drive development of beamlines and yield expanded bioscience research capabilities, including phase-, absorption-, and fluorescence-contrast imaging; microfocus macromolecular crystallography; and combined small- and wide-angle scattering.

Although study of static biological structures has proven extremely powerful, the static approach alone is insufficient. All biological and chemical processes involve motion, on timescales from femtoseconds to seconds. The greater challenge in life science is to observe the dynamics of biological processes as they occur, in functional environments and on their natural timescales. APS-U's advanced detectors, combined with improved source brightness and stability and with shorter x-ray pulses in the few-picosecond range, will provide unprecedented time resolution. This will allow observation of real-time biological functions, from molecular dynamics on picosecond timescales to protein folding in solution on nanosecond to millisecond timescales, and to more complex functions in solution, in the cell and even in the organism, that occur on longer timescales.

Creating robust structural materials for use in extreme conditions

Our ability to develop innovative new low-carbon energy sources and energy-efficient technologies is currently constrained by the limits of materials performance. To reach our goals in developing more efficient automobile and jet engines, next-generation nuclear reactors and cost-efficient renewable energy sources, we must find new ways *to create robust structural materials that will perform without failure in extreme conditions*.

Underlying this fundamental challenge are a number of important scientific questions: Why do materials often fail at one-tenth of their intrinsic limits? What determines the critical strain for onset of plastic deformation? How can we control the formation of individual defects to make higher-performing materials? A path forward in answering these questions may be developed in conjunction with computational models linking materials processing, microstructure, and properties/performance.

Experimental research is needed to understand the physical processes that underlie evolution of internal microstructure and strain under realistic conditions, such as the agglomeration of voids, stacking faults, dislocations and ultimately larger structures that cause crack initiation and finally materials failure. At present, development of appropriate characterization techniques is being accelerated by coordinated efforts at high-energy synchrotron x-ray beamlines. Current high-energy diffraction microscopy (HEDM) allows simultaneous mapping of more than 100 grains in mm-sized samples. These studies allow monitoring of grain-interactions and anisotropy that convert 'simple' uniaxial loading to complex local strain.

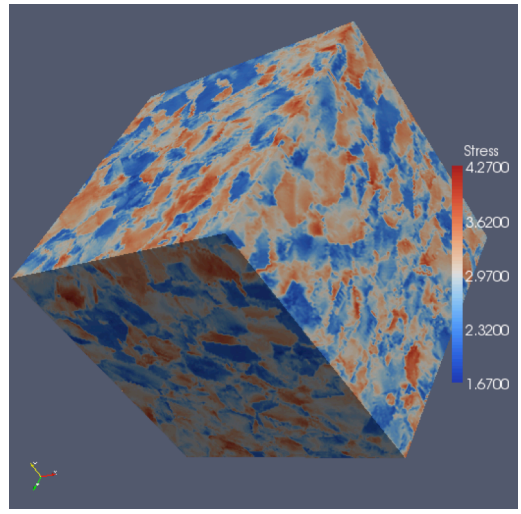

Fig. 6. Computational model of elastic response inside a polycrystalline metal [10]. The color distribution indicates that stresses on the internal crystallites are highly inhomogeneous. It is this heterogeneity that determines the onset of irreversible (plastic) deformation and, eventually, to void formation and materials failure in materials subjected to extreme environments of stress, temperature, and irradiation. APS-U will provide the first combined stress and orientation maps under realistic conditions for comparison.

APS-U will afford orders-of-magnitude improvement in volume and energy resolution, allowing simultaneous mapping of grain orientation and internal strains in samples under load and in extreme temperature conditions. The resulting data will allow researchers to test and validate computational models, potentially leading to replacement of current "trial and error" materials synthesis and testing with a new paradigm of materials testing by computational methods.

Developing innovative materials for energy systems

An overarching challenge in developing innovative energy systems is *to see materials structure and composition change in situ during synthesis processing or under functional conditions*. For example, to create the next generation of batteries, researchers need the ability to observe the structure of advanced electrode materials and electrolytes with nanoscale resolution in a variety of contrast modes, and to see the material evolve during cycling. To date, sub-millimeter imaging with hard x-rays at the APS has allowed researchers to observe the phase and microstructure changes that occur in novel battery electrode materials during

INDUSTRIAL IMPACT
Dow's Solar Shingles

Using *in situ* x-ray diffraction at APS to observe phase formation, Dow researchers were able to develop a successful process to form a semiconductor phase with optimal solar photovoltaic properties in the four-component CuInGaSe system.

This research has since been scaled up into a manufacturing process for the first commercial 'solar shingles', in which photovoltaics are built into the roofing materials. A manufacturing plant using this process will be opening in 2013.

charge/discharge cycles, as well as the mechanisms that eventually limit performance. APS-U will provide the additional hard x-ray tools needed for diffraction and phase contrast tomography and pair distribution function analysis of atomic-scale electrode structures, as well as interface scattering required to study electrochemistry at buried interfaces in model systems.

Materials dynamics in shock waves

Studies of materials under shock compression can yield results important both for security applications and for fundamental questions of materials science and high-pressure physics. *To understand fundamental questions about how atoms and defects evolve under extreme conditions,* researchers must answer a number of critical questions: What role does inelastic deformation play in governing phase transition kinetics? How does material strength factor into structural changes under dynamic loading? Can we tailor the transition path for shocked solids*?*

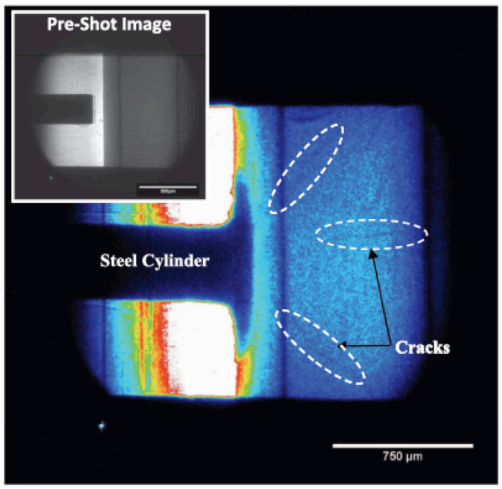

Fig. 7. Single-pulse (80 ps) white beam image just after impact of a 300-μ m diameter stainless steel cylinder into boron carbide plates. Researchers observed cylinder deformation during impact and the onset of cracking of the ceramic plates. [11]

The high flux at hard x-ray energies and the flexible pulse structure at APS are uniquely suited to examine time-dependent changes in materials subjected to single-event shocks over a broad range of peak stresses (50 kbar to 1 Mbar) and time durations (tens to several hundred nanoseconds). Today, researchers can make individual absorption images during a shock event using a single 80 ps x-ray bunch with 3 μ m spatial resolution. The future goal is to obtain real-time measurements, with nanosecond-scale time resolution, of the structure of materials undergoing ultra-high strain rates. We expect to observe elastic and plastic deformation and defect generation, followed by phase transitions that may lead to new stable or metastable states. APS-U will enable these experiments with improved flux per pulse using revolver-undulator technology as well as development of high-speed area detectors.

Controlling chemical dynamics in solution

Understanding and controlling the electronic and nuclear configurations during a chemical reaction is an enduring challenge in chemical sciences. The majority of reactions carried out by chemists take place in liquid solutions, and femtosecond optical and infrared laser spectroscopies are commonly used to observe the progress of reactions in solution. However, electronic and nuclear coordinates are entangled in optical spectra, which report only on optically active modes and yield an incomplete picture of the reaction. In contrast, x-ray spectroscopy and scattering report on all atoms, providing

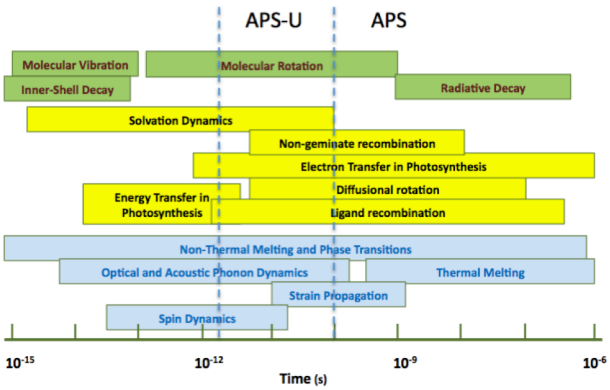

Fig. 8. Timescales of physical and chemical processes showing windows accessible now at APS (>100 ps) and at APS-U (>2 ps). Timescale provided by APS-U is well matched to nanoscale dynamics, which are often mediated by the speed of sound (~1 nm/ps), and to chemical dynamics in solution, which are mediated by solvent reorientation.

complementary atom-specific characterization of transient electronic and nuclear coordinates.

A pilot study on Fe spin-crossover complexes in aqueous solution at APS demonstrated that it is possible to obtain information on transient states with lifetimes greater than ~100 ps at precision comparable to conventional static studies. [12] This was enabled by a high-repetition-rate laser system that increased data acquisition rates by more than 1,000-fold. However, the 100 ps-duration pulses at APS cannot capture key transients associated with solution phase photochemistry, e.g. solvent reorientation and ligand replacement. These complex rearrangements of atoms in solutions typically occur on the 1-50 ps timescale and are fundamental to photocatalysis (as in the recently discovered "artificial leaf," a Co_4 oxygen-evolving complex that mimics the catalyst found in Photosystem II [13]). Access to the evolving structure of transient oxidation states in solar-driven catalysis will be enabled by the high-flux, tunable, polarized, short-pulse x-rays provided by APS-U.

Understanding nanoscale heat transport

The interaction of hot carriers with phonons is a fundamental problem with important technological implications. The bottleneck in the decay of certain phonon modes leads to increased electron scattering from the nonthermal phonons, directly affecting carrier mobility and heat removal in devices. A striking example is limitation in the efficiency of photovoltaics caused by energy loss from the photo-excited electrons (carriers) to phonons, such that the photon energy above the band-gap is lost to heat. Recent demonstration experiments on photoexcited InP [14] show the transition between longitudinal and transverse acoustic phonon modes on sub-nanosecond time scales. However, high optical driving power is necessary to massively populate the phonons, and the critical early time regime of the optical to acoustic transitions is inaccessible. APS-U will provide the short pulses and the high flux required to study electronic and vibrational dynamics with atomic-scale temporal and spatial resolution. For example, APS-U will allow researchers to perform momentum-resolved inelastic scattering in the time domain, which is particularly well suited for studying phonon dynamics, such as phonon-phonon and electron-phonon coupling. Thus, one can follow the non-equilibrium phonon population from the initial emission from the hot electrons through the subsequent anharmonic decay until the lattice thermalizes.

<u>Advanced synchrotron technology provided by APS-U</u>

The APS-U project significantly advances key technologies that are critical to the APS user community and necessary to support the nation's continued leadership in hard x-ray science.

A revolutionary component of APS-U is the short-pulse x-ray system (SPX), consisting of superconducting radiofrequency deflecting cavities with the capability to produce hard x-ray pulses more than an order of magnitude shorter than those currently at storage ring sources. The SPX will address the research community's need for intense, tunable, high-repetition-rate, few-picosecond x-ray pulses. As shown in Fig. 9, the MHz rep rate of SPX is ideally suited for high-rep-rate pump-probe

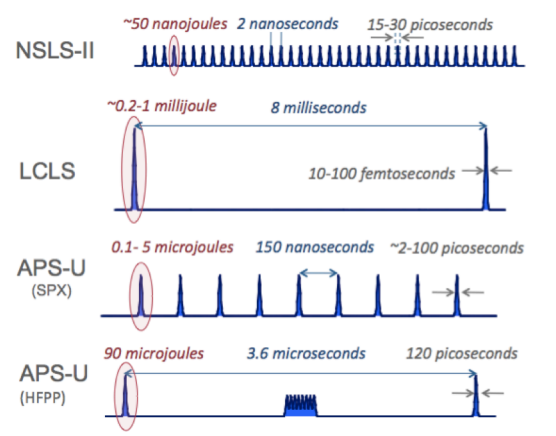

Fig. 9. Flux and time structure of various lightsources showing flexible MHz rep rate at APS, which provides unique capabilities for pump-probe measurements.

experiments and is complementary to the 120 Hz rep rate of LCLS.

The superconducting undulator (SCU) at APS-U will be the first-ever of its kind to provide highest-brightness beams in the hard x-ray range. This small-period, strong-magnetic-field device represents a breakthrough in undulator technology. In January 2013, APS successfully installed a prototype of the SCU that is now providing outstanding performance for users. The full version of this innovative device will allow the APS to deliver unsurpassed hard x-ray brightness.

Readiness of APS-U for construction

The APS-U project is proceeding through the rigorous review process established by DOE and is entering the construction phase. The mission need CD-0 was granted in April 2010, and the conceptual design [15] was approved with CD-1 granted in August 2011. Approval for start of early procurement CD-3a was granted in August 2012, and construction of the first beamline for early science (RIXS) has begun. The $391M construction cost estimate was reviewed in October 2012. The preliminary design [3] was favorably reviewed in December 2012; CD-2 is anticipated in Spring 2013. Regarding the need for R&D, 85% of the project consists of state-of-the-art beamline and accelerator components requiring no further R&D. A prototype SCU is now operating, and prototype RF cavities for SPX have shown very promising performance. Remaining R&D needed for these systems is proceeding according to plan. Operations costs of the additional beamlines and accelerator systems are understood and will add 15% to the operations cost of APS.

Summary

The Advanced Photon Source provides high brightness x-ray capabilities to an ever-growing range of scientific activities. Because of beamline construction at NSLS II, APS beamlines soon will account for more than half of the nation's available capacity at energies above 2 keV – making the APS facility's optimized reliability and availability even more critical. The APS Upgrade project will allow full ongoing user access while equipping this vital facility for the challenges of 21st century science. The comprehensive technological advances that make up the APS-U respond to the scientific community's increasing need to observe real materials under real conditions in real time, with spatial, energy, and temporal resolution far exceeding existing capabilities. As APS-U moves to completion, it will offer drastically improved capabilities in high-energy diffraction, *in situ* studies of material synthesis, imaging, ultra-fast diffraction and spectroscopy, driving an increase in both user numbers and user productivity.

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