Advanced Photon Source

5 year Strategic Plan 2007 - 2011

X-ray Operations and Research and Collaborative Access Teams

March 7, 2007

The Advanced Photon Source is a world-class 3rd generation high-energy x-ray synchrotron source serving more than 3000 scientists per year. With the APS already a world leader, the focus of this strategic plan is on delivering the highest level synchrotron science well into the future by making critical choices regarding research directions, new and upgraded beam lines, leveraged APS-CAT interactions, and bringing it all together with the exciting upgrade of the APS to an ERL. Today, thirty sectors of the APS are either operational or under construction. The X-ray Operations and Research Section of the X-ray Science Division, is responsible for approximately half of the beam lines at the facility, and the remaining sectors are under the auspices of Collaborative Access Teams (CATs). In addition, there are 4 uncommitted insertion device ports. We propose to implement 6 highest-priority new capabilities by completing the four remaining uncommitted insertion device ports, and by reconstructing two existing sectors, which would lead to a fully built-out APS. A seventh new capability, implementation of a picosecond-pulse, is already currently underway. Each of these new developments reaches toward satisfying a highly compelling scientific need for a new user capability with leading-edge equipment. Having anticipated the need to generate high-quality proposals for the remaining sectors at the APS several years ago, we hosted numerous workshops and competitive reviews over the past few years, overseen by our own Scientific Advisory Committee. The APS plan is responsive to our user community and to the DOE Office of Science priorities, providing access to unique and reliable research instruments and offering strong scientific and technical support in a safe, rewarding and productive environment.

The success of the Advanced Photon Source depends upon the quality of users that it attracts, and on the ability of those users to perform first-rate research once they get here. Our focus in this plan is on the steps we need to take for maximum scientific impact and optimal utilization of the APS. To do this, we have identified areas of excellence upon which we plan to build, and compelling opportunities for new areas of research that address scientific and technological challenges uniquely suited to development at the

APS, and which will reach complete fruition with the completion of the future ERL. Implementation of these initiatives will enable APS users to perform leading-edge synchrotron x-ray research and to produce world-class scientific results well beyond the next decade. Areas of excellence at the APS today include high-pressure geophysics and condensed matter physics, biology and the life sciences, strongly correlated electron systems, nanomagnetism, and surface and interface science. Emerging and developing areas of excellence in the next few years are dynamics, coherence and imaging, chemistry and catalysis, and soft-x-ray angle-resolved photoemission and magnetism, high-field magnetism, and scattering.

Section 1 describes the scientific opportunities at the APS that will be addressed by the new capabilities. While all the proposed capabilities would be built and operated by the APS and supported by DOE-BES, in some case we would leverage construction funds from other agencies or parts of the DOE, and in all cases we have outstanding external science drivers who will work with us to develop the instrumentation that will maximize the scientific impact. Section 2 outlines the completion of current construction, upgrades and optimization. Section 3 describes essential developments in detectors, scientific software and optics in support of the scientific capabilities. Section 4 outlines leveraging between the CATs and the APS in future developments, and finally Section 5 provides a brief description of planned accelerator upgrades and new insertion devices.

1. Scientific opportunities at the Advanced Photon Source

1.1 Picosecond pulse

Fundamental chemical events can occur in nanoscale semiconductor materials, in proteins such as DNA, in polymers, in supramolecular complexes, and in molecular machines. X-ray pulses on the picosecond time scale provide access to structural and chemical information about such fundamental processes. We have determined that the APS can implement a ps-pulse capability that offers high x-ray flux and provides a unique bridge for hard x-ray science between the capabilities of current storage rings and future x-ray FELs. This capability, to be implemented in two phases on sector 7, will turn the Advanced Photon Source into a unique resource in the world for supporting time resolved x-ray research.

1.2 Intermediate-energy x-ray

One of the scientific grand challenges of the 21st century is to understand materials with competing interactions. These materials exhibit a remarkable array of electronic phases and a heightened sensitivity to extrinsic perturbations such as temperature, applied electric or magnetic fields, pressure or nanopatterning. To investigate the complex electronic excitation spectrum and the new electronic length scales we propose to develop a high-brilliance intermediate-energy x-ray (0.2 - 2.0 keV) beam line for high-energy angle-resolved photoemission spectroscopy (ARPES), which is a *bulk* probe of the low energy excited states in condensed matter, and resonant x-ray scattering (RXS), which is a direct probe of electronic ordering. ARPES and RXS are scientifically complementary, they are of interest to the same scientific community, and they have highly compatible source and beam line technical requirements. The new facility will provide full angular flexibility, access to T < 10 K, polarization selectivity, fluorescence rejection optics, and a factor of 50 more intensity than the most powerful sources available today.

1.3 High magnetic field

X-ray scattering in a high magnetic field will make it possible to investigate previously inaccessible parameters of novel vortex matter in superconducting cuprates, metamagnetic structures, multipolar ordering in 4f and 5f compounds, fractional quantum Hall effects in 2D electron gases, quantum phase transitions of electronic matter, and Bose-Einstein condensation. In collaboration with the National High-Magnetic-Field Laboratory, we propose to combine the brilliant hard-x-ray beam at the APS with a high (30 - 40 Tesla) magnetic field to establish world-leading facilities for magnetism research. The APS is the ideal location for a high magnetic field beam line because the straight sections can easily be extended to 8.5 m for optimized insertion devices, further increasing the x-ray beam brilliance; these insertion devices operate with a 7 GeV electron beam, which allows continuous coverage of the entire spectral region; the APS beam has outstanding stability, necessary for long data acquisition times; polarization control and switching are efficiently implemented at the APS; and novel focusing optics deliver a small beam spot to the sample.

1.4 *In-situ* surface and interface scattering

Structure and chemistry at surfaces and interfaces play a vital role in many important scientific and technological areas ranging through environmental science, energy, communications, semiconductors, catalysis, lubrication, corrosion, nano-science, geo-science, and membrane science. In addition, many biochemical reactions that sustain life occur at surfaces and interfaces. X rays offer a unique opportunity to penetrate complex environments (gas, liquid, or solid thin-film overlayers) to probe the structure and chemistry of surfaces and internal boundaries from macroscopic lengths down to the atomic level. A new sector at the APS will enable these *in-situ* studies, permit real-time investigations to elucidate thin film growth mechanisms, and allow molecular scale studies of important chemical interactions at internal boundaries using scattering, diffraction, resonance & absorption, fluorescence, standing wave, and imaging techniques.

1.5 Intermediate energy x-ray magnetism

Many of the most compelling problems in contemporary magnetism research involve the measurement of extremely small magnetic moments in nanoengineered materials. Geometric confinement, physical proximity and self-organization in such nanosystems lead to competing interactions that result in a rich complexity giving rise to many new and unanticipated phenomena. Studies using polarized x rays at third generation sources are uniquely suited to provide invaluable insights into the physics of such systems due to their intrinsically high brilliance, magnetic sensitivity, time resolution, and elemental selectivity. Enabling such novel science, however, requires a dedicated polarized x-ray beam line in the energy range between 400 to 2000 eV, with x-ray pulse widths of 100 ps or less. This energy range covers both the transition metal L and rare earth M edges which probe the predominant magnetic electrons in nearly all magnetic materials. While this new beam line would probe magnetism at ~100 ps time-scales with the existing APS storage ring, the proposed upgrade to ERL would enable us to develop revolutionary new capabilities for the study of magnetic dynamics.

1.6 Advanced x-ray imaging

X-ray imaging has emerged as a key technique for the investigation of material structures on the nanometer to millimeter scales. Research areas include microstructure/properties studies, bone and cartilage growth and formation, small animal and soft tissue research, biomedical research such as tumor detection, structure and development of polymer and metal foams, and high-speed imaging of the dynamics of complex fluid flow and nanofluidics. Additional areas where x-ray imaging is expected to have significant impact include time-resolved imaging of electrodeposition, imaging of subcellular organelle structures in frozen-hydrated biological cells, and three-dimensional (3D) structure and strain analysis in nanocrystallites, nanoclusters and other nanostructures. We propose to continue the development of the 32-ID beam line for advanced x-ray imaging, with the goal of providing < 1 μrad detection of refractive angular deviations by any specimen, which would represent the state-of-the-art in x-ray phase-contrast imaging capabilities. With the APS upgrade to ERL in the future, this imaging beam line will offer "second to none" imaging capabilities.

1.7 BioNanoprobe

Metals and trace elements in living tissues are essential for the existence of life. In any organism, very few intracellular processes are independent of metals or other trace elements. With current developments in genomics and proteomics, our knowledge of the enormous number of pathways in which metals and trace elements are necessary for life is increasing. However, our knowledge about the actual (re)distribution of metals and trace elements that accompany development and differentiation and the beginning or advancement of different diseases is still lacking, as we do not have adequately sensitive approaches to follow fluctuations in metal homeostasis. The development of a hard x-ray BioNanoprobe (BNP) and supporting instrumentation at the APS is a critical contribution to answering these questions. Using characteristic x-ray fluorescence, excited by a hard x-ray beam focused down to ~20 nm, the BioNanoprobe will offer the ability to detect, quantify, and map metals at trace quantity levels and distinguish their chemical states at a spatial resolution smaller than the size of intracellular organelles, thereby providing invaluable information and insight into the influence of fluctuations of elemental concentration and speciation on health and disease. The BNP beam line will complement the Center for Nanoscale Materials (CNM) Nanoprobe beam line currently under construction on Sector 26 because of its exclusive focus on intracellular imaging. Realization of this beam line is envisioned as a collaboration led by NIH, where the APS part will be to develop a suitable undulator, optics, detection and robotics sample manipulator.

2. Beamline construction, upgrades, and optimization

Our immediate highest priority on the experimental floor is the successful completion and delivery to the users of the three beam lines currently under construction. Each brings unique, dedicated capabilities to the APS.

2.1 New instruments coming on line in 2007 - 2008

The hard x-ray nanoprobe, now nearing completion on 26-ID, will be the world's highest resolution hard x-ray microscope for the characterization of nanoscale materials and devices. Its position is unique in that it is both on the x-ray floor of the APS and immediately adjacent to the new CNM, and will be operated jointly by XOR and the CNM when it becomes available to users in 2008. The new instrument will be a gateway for CNM users to the many other nanomaterial science probes around the APS x-ray ring.

Many materials parameters, such as sound velocities, elastic behavior, and local atomic structure and electronic properties, are uniquely accessible through inelastic x-ray scattering (IXS) and resonant inelastic x-ray scattering (RIXS). Today, protein dynamics are being explored using density functional theory modeling constrained by IXS data, and the electronic structures of oxides are investigated in strongly correlated electron systems, in high-T_c superconductors, in colossal magnetoresistive materials, magnetic films and nanostructures. The inelastic x-ray scattering instruments on 30-ID are hosting their first users in 2007, and they, together with the inelastic x-ray scattering instruments already on 3-ID and the possible expansion to 9-ID, will make the APS the best facility in the world for inelastic x-ray and nuclear resonant scattering.

A dedicated high-resolution powder diffractometer on 11-BM will be completed and receive its first users in 2007. This novel instrument exploits the high flux and high energy of the APS bending magnet source, and brings state-of-the-art capability to the powder diffraction user community. This user-friendly high-throughput high-resolution instrument is positioned to initiate leading-edge structural science in fields from condensed matter physics and materials chemistry to pharmaceutical and biological sciences.

2.2 Optimized beam lines

Our scientific strategic plan for the APS calls for simultaneous improvements in beam lines, as well as in x-ray optics, detectors, and scientific software. We have begun significant upgrades, such as that of 1-ID to create a premier facility for high-energy x-ray scattering, the upgrade of 32-ID into a new facility for advanced full-field x-ray imaging, and the upgrade of 12-ID into beam lines optimized for small-angle x-ray scattering, while simultaneously offering more independent operation to a strong end-station facility for surface and interface scattering. Future dedicated beam lines ultimately will include the optimization of all of the beam lines that XOR operates. Several beam line examples are described below, but all are listed in the Table at the end.

X-ray photon correlation spectroscopy (XPCS) measures dynamics in materials not readily accessible to dynamic light scattering. With the installation of an optimized undulator, focusing optics, and fast detectors, XPCS on 8-ID will reach a similar time scale (μs) but a more extended q-range (1 nm^{-1}) than visible light scattering. This opens the door to critical measurements of dynamics in dilute and viscous solutions and suspensions, dynamics at air/liquid interfaces, and rapid dynamics in kinetically changing systems. 8-ID will become a unique XPCS facility in the United States, capable of covering the μs-to-s time range, and complementing the future LCLS which will focus on fs-to-ps dynamics.

A second undulator to be installed on 8-ID will make the x-ray energy independently tunable for a dedicated GISAXS and microdiffraction facility. Enhanced capabilities include an extended range of x-ray energies to study thin-films including high-Z materials. The GISAXS will be capable of high temporal and spatial resolution in both real and reciprocal space.

The wiggler source for three beamlines on 11-ID is being replaced with two undulators for an increase in flux of approximately 5 times at 100 keV to 100 times at 8 keV., and an increased brilliance of approximately a factor of 100 at all energies. Two of the independently operating beam lines (where one of them is focusing) will serve optimized stations for high-energy scattering and the third will serve time-resolved studies and spectoscopy.

X-ray spectroscopy with microprobe spatial resolution plays an important role in synchrotron environmental science and in *in-situ* science more generally. The APS will develop a dedicated spectroscopy microprobe on 20-ID. A canted undulator will be installed, making independent μ-XAFS available on one line and dedicated techniques related to XAFS–x-ray Raman, DAFS and surface-XAFS–simultaneously available on the other.

We propose to build a new facility to provide nanoscale focus white beam and monochromatic Laue diffraction for structural investigation of materials in 3 dimensions. The new experimental platform will enable 3D diffraction investigations with better than 50 nm spatial resolution, and will operate in parallel with the existing μ-focus (~ 0.5 μm) instrument at 34-ID. The development of a dedicated diffraction nanoprobe will enable APS users to be at the forefront in 3D diffraction analysis of engineering materials.

Surface and interface scattering offers opportunities for discovery in interfacial chemistry, catalysis, and fundamental materials growth behavior, as well as in important new areas such as nanoscale physics, and materials processing. In addition to the new sector for surface and interface science, 33-ID will support a number of independent and highly specialized growth chambers as well as standard diffractometers to accommodate small, specialized reaction chambers or cells that often require elaborate ancillary gas handling or processing equipment. Capabilities for surface and interface scattering will also be distributed at other end stations to provide complete experimental flexibility. (Please note: some distributed stations, but not all, are explicitly identified in the table.)

3. Detectors, scientific software and optics

For many experiments at the APS, x-ray detectors are not well matched to the capabilities of the source, and we recognize an urgent need for a broad-based detector upgrade and development program. Clearly, improvements in detectors offer the greatest opportunity to improve the data quality and the throughput of x-ray experiments. Participants at a workshop we held on May 11, 2006 looked at the current status of x-ray detectors, proposed a path toward optimal x-ray detectors, and suggested the elements of a serious program to implement of the next generation x-ray detector capabilities. Detector improvements have very high priority at the APS, and will be pursued simultaneously with the highest priority beam line upgrades. Three particular areas of emphasis will be avalanche photodiodes, large solid-angle fluorescence arrays, and pixel array detectors. We will address our detector needs in part through procurement of new detectors from specialized vendors, and in part by development of new detectors and electronics in collaboration with other facilities and with detector manufacturers.

Scientific software for real-time data analysis, modeling and simulation has only been available to users of the APS to a limited extent, even though the data rates at the APS typically far outstrip the users' ability to remain current with their data. In addition, as growth of the user community brings non-x-ray specialists to the facility, it becomes increasingly important that the APS offer robust solutions to data reduction, data analysis, simulation and modeling. Providing these to our users is an important enabler to increase the volume of high-impact APS results. A scientific software workshop was held at the APS August 29, 2006 to address the current status of software, the role of optimal software to improve scientific impact of the APS, and the best means to take the next steps toward improved scientific software. In response, we have formed a Scientific Software section of the Beam line Controls and Data Analysis group, and will host a visiting theorist program to bring scientists to the APS to interact with researchers and experimental data, as well as leave behind scientific software for facility users. These program have very high priority, and will be pursued simultaneously with the highest priority beam line upgrades.

Recent advances in x-ray optics have achieved Kirkpatrick-Baez mirror focusing of hard x rays to less than 40 nm and multilayer-Laue-lens focusing to 20 nm. These accomplishments depended on gaining a more fundamental understanding of optical theory at these length scales, as well as developing technologies such as differential mirror coatings, fabrication of multilayer Laue lenses, and vibration suppression. A workshop to explore optimal optics for the ERL upgrade to the APS will take place April 23, 2007. Recommendations from this workshop are expected to drive the development of x ray optics at the APS to push the limits on spatial resolution and energy resolution.

4. CAT and APS infrastructure

The APS CATs offer an extraordinary portfolio of unique capabilities, and we deeply appreciate the benefit that can be derived from integrating the strategic directions of the

CATs with those of the APS. Several CATs have come forward with important proposals for future development is several areas, such as for high-pressure research at the APS, for time resolved crystallography, for high magnetic field capabilities, for a BioNanoprobe, and for the leveraging of scientific support for biological small-angle scattering, environmental science, and catalysis, to name just a few. We encourage the APS CATs to come forward with more such proposals in the future. The first example we give is the high-pressure dimension at the APS, where this area is an interesting model for partnering opportunities in other areas as well. (This section of our Strategic Plan was last updated in February 2006, and will be updated again shortly.)

4.1 A high pressure center at the APS (HPSynC)

High-pressure (*HP*) experiments reveal new phenomena and are becoming a major dimension of modern science. Pressure drastically alters material properties, thus opening new frontiers in fundamental physics and chemistry, as well as applications to planetary, Earth, biological, and materials sciences. The HP-CAT (Sector 16) and GSE-CARS (Sector 13) at the APS combine many complementary synchrotron radiation (*SR*) diffraction and spectroscopy probes and non-*SR* probes for dedicated high *P-T* studies. However, not every probe is compatible with every other probe that is needed. With moderate modifications, for example, the 3-ID inelastic x-ray scattering beam line was able to add the pressure dimension and produce extraordinary science. Elevating *HP-SR* research to the next level will require an integrated, comprehensive approach at the APS that combines high pressure with structural, electronic, magnetic, and phonon probes that are difficult to realize with isolated programs. We plan new diamond anvil cell development at relevant beam lines to establish the *HP* dimension at APS, and facilities to leverage high-pressure users. The resulting combination will enable us to tackle a range of grand challenges through tuning of the pressure variable. New rules of chemical affinity, reactivity, bonding, and crystal and amorphous structure will be established across the Periodic Table in each pressure regime. Breakthroughs are expected in applications of high pressure to mineralogy, geophysics, geochemistry, bioscience as well as specific areas such as hydrogen storage, stockpile stewardship, and super-hard materials.

4.2 Macromolecular crystallography at the APS

Since 2000, the number of deposits into the Protein Data Bank coming from synchrotron facilities has far outstripped those from home laboratories. Today, the APS is the leading facility in the world for protein structure determination. Building upon this success, plans for the future of biology at the APS call for greatly increased capacity and efficiency through the use of multiple canted undulators, large/very fast detectors, and robotics. In addition, capabilities at the APS will expand in the areas of microbeams, real-time structure solutions, simultaneous measurements with multiple techniques, BSL-3, and new experimental capabilities for time-resolved experiments during structural changes. Regarding the last, a partnership was formed among researchers at NIH, the University of Chicago and the APS to develop a world-class time-resolved x-ray crystallography capability at the BioCARS 14-ID-B beam line. This is now complete, and 14-ID users will be able to obtain a high-quality x-ray diffraction pattern from a “typical” photoexcitable protein crystal with a single 100 ps x-ray pulse.

4.3 Powder diffraction at DND 5-ID

The APS and DND-CAT have developed a partnership in which the 32-ID powder diffractometer and multi-channel analyzer system will be relocated to DND 5-ID. This will enable DND-CAT to offer the powder diffraction community access to a fixed-wavelength, high-resolution, high-throughput powder diffractometer on an ID, while the APS offers access to the dedicated variable-wavelength powder diffractometer located on 11-BM. The highly efficient ID instrument will also serve the industrial and academic partners of DND-CAT where powder diffraction is a major interest.

5. Accelerator upgrades and insertion devices

Over the last several years APS has begun to develop and implement new accelerator instrumentation that would significantly improve the quality of the x-ray source. These developments include an expansion of the variety of undulators and their configurations on APS straight sections. It also includes new designs for the straight sections that could be twice as long as current ones and would be able to accommodate more and longer IDs. Another important development focused on the generation of short, few picosecond x-ray pulses. We can deliver the short x-ray pulse to a single beamline without affecting any other APS sectors. For APS beam line upgrades and new beam line construction, the APS will develop and build unique IDs tailored to beamline science. Examples include short period superconducting undulators for inelastic scattering and high-energy x-ray science and variably polarized undulators for the characterization of magnetic materials. A major program to develop and fabricate new insertion devices is underway that will optimally tailor the source for each of the beam lines at the APS.

APS is currently developing the R&D program toward the revolutionary upgrade of the facility based on the ERL source. That upgrade will bring orders of magnitude increase in brightness of the APS source and open new opportunities in a number of areas of x-ray science.

Future dedicated beam lines operated by the APS

1-BM	Variable energy GISAXS, reflectivity, diffraction	MS, LS
1-ID	High-energy scattering, SAXS, powder diffraction, imaging	MS
2-BM	x-ray tomography	MS, LS
2-ID	2-32 keV STXM, microdiffraction, nanodiffraction	MS, LS, ES
3-ID	IXS, NRIXS	MS, LS, GS
4-ID-C	0.5 - 3 keV magnetic spectroscopy	MS
4-ID-D	2.6 - 45 keV magnetic spectroscopy	MS
7-BM	Ultra-fast imaging	Fluids
7-ID-B	Time-resolved white/pink beam imaging, ps probe	MS, CS
7-ID-C	Time-resolved microbeam scattering	MS
7-ID-D	Laser pump/x-ray probe spectroscopy, ps probe	CS, MS
8-BM	Rapid spectromicroscopy	LS
8-ID-E	GISAXS	Thin films
8-ID-I	XPCS	Liquids, films
9-BM	XAFS/WAXS Catalysis	CS
9-ID-B	RIXS	MS
9-ID-C	Liquid surface scattering	CS
11-BM	Powder diffraction	CS, MS
11-ID-B/C	High-energy powder diffraction, pdf, diffuse scattering	MS, CS
11-ID-D	Laser pump/x-ray probe spectroscopy	CS
12-BM	XAFS, diffuse scattering, diffraction	CS, MS
12-ID-B	SAXS/WAXS	MS, CS
12-ID-C	Time-dependant SAXS, ASAXS, GISAXS	MS, LS, CS
12-ID-D	Surface/interface diffraction	MS
20-BM	XAFS, DAFS	ES, MS, CS
20-ID-B	Micro-XAFS	ES, MS, CS
20-ID-C	DAFS, XRR, surface-XAFS, laser pump-XAFS	ES, MS, CS
26-ID	Hard-x-ray nanoprobe	MS
30-ID	IXS, RIXS	MS
32-ID	Advanced full-field x-ray imaging	MS, LS
33-BM	Diffraction	MS
33-ID	Diffraction, surface/interface scattering	MS
34-ID-C	Coherent diffraction imaging	MS, LS
34-ID-E	3D-x-ray diffraction micro (and nano) scope	MS
New ID	0.2 keV - 2.5 keV ARPES, resonant scattering, diffraction	MS
New ID	Intermediate energy magnetism	MS
New ID	*In-situ* surface and interface science	MS, CS
New ID	Hard-x-ray BioNanoprobe	LS
	High-energy (13 T, 40 T) magnet	MS

Blue lettering indicates proposed Future Beam Lines and capabilities
Red lettering indicates beam line capabilities nearing completion