Advanced Photon Source Five-Year Facility Plan

Enabling frontier science in the national interest

July 30, 2017

Rev. 1

The Advanced Photon Source is a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

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The mission of the U.S. Department of Energy Office of Science-Basic Energy Science's Advanced Photon Source at Argonne National Laboratory is to enable internationally leading research and development by operating an outstanding hard x-ray synchrotron radiation user facility accessible to a broad and diverse spectrum of researchers, and to support the scientific and technical directions of the U.S. Department of Energy, including development of new light source technologies, while maintaining a safe, diverse, and environmentally responsible workplace. .

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1 Executive Summary

The Advanced Photon Source (APS) at Argonne National Laboratory is a U.S. Department of Energy Office of Science-Basic Energy Sciences (DOE-SC-BES) scientific user facility. The core mission of the APS is to serve a multi-faceted scientific community by providing high-energy x-ray science tools and techniques that allow users to address the most important basic and applied research challenges facing our nation, while maintaining a safe, diverse, and environmentally responsible workplace.

The APS has been optimized to provide this nation's highest-brightness hard x-rays (i.e., photon energies above 20 keV). This makes it ideally suited to explore the time-dependent structure, elemental distribution, and chemical, magnetic, and electronic states under *in situ* or *operando* environments for a vast array of forefront problems in materials science and condensed matter physics, chemistry, and the life and environmental sciences.

The APS became operational in 1996, and as mature facility today, the APS must continue to improve beamline performance to take full advantage of its existing source properties, as well as deliver new capabilities required by the large and scientifically diverse APS user community. This includes improving specific beamlines and end stations and continued optimization of the APS beamline portfolio, while maintaining the outstanding reliability and availability of the APS accelerator and storage ring systems. Additionally, research challenges that require vastly brighter hard x-rays or higher coherent flux than the APS currently produces are now within reach because of revolutionary new storage ring lattice designs that dramatically reduce the stored electron beam emittance.

The Photon Sciences Directorate, under the APS-Upgrade Project (APS-U), has prepared a preliminary design for a major upgrade implementing a multi-bend achromat (MBA) magnetic lattice that will increase APS x-ray beam brightness and coherent flux by 100 to 1,000 times over current values. Combining the penetrating power of the hard x-rays produced by the APS with the time structure of the electron bunches in the APS storage ring, this proposed upgrade will make the APS ideally suited to meet the global science and energy challenges of the 21st century, by providing the time-resolved three-dimensional microscopy, imaging, scattering, and spectroscopy methods necessary to revolutionize our understanding of hierarchical architectures and beyond-equilibrium matter, and the critical roles of heterogeneity, interfaces, and disorder.

The current "Advanced Photon Source 5-year Facility Plan" has been revised to incorporate changes since the original Plan was released in March, 2015. This plan also had extensive input and vetting from a broad cross-section of stakeholders including APS users, partners including the collaborative access teams, and the APS Scientific Advisory Committee. During mid-2015, the APS also supported a community process, including a set of six community workshops, to clearly define science targets for the APS-U, culminating in release of the report "Early Science at the Upgraded Advanced Photon Source" in October 2015. Based on these foundations, several milestones toward scope definition of the APS-U were reached, which were necessary for developing a coherent and consistent strategic vision. Following a call in October 2015 for feature beamline proposals for consideration as APS-U project scope, 36 proposals were received and reviewed by the Beamline Review Committee, Scientific Advisory Committee, and the APS/APS-U management. The process culminated in the selection of the suite of eight feature beamlines in July 2016. Subsequently, the proposed physical locations of feature beamlines (the "roadmap") were decided in November 2016. Finally, the process of prioritization of smaller enhancement projects to make all beamlines "APS-U ready" was completed in June 2017. These activities, closely coordinated between APS Upgrade and APS Operations, have provided the framework for this revised "Advanced Photon Source Five-Year Facility Plan."

This Plan charts the path over the next five years for the improvements and R&D that will maintain the APS position as the world-leading hard x-ray synchrotron source while simultaneously preparing for the proposed APS Upgrade. The x-ray science strategy is focused on developing and improving high-energy-, high-brightness-, and high-coherence-driven beamlines and techniques, as well as capitalizing on unique timing and high-speed imaging capabilities. Method and technique developments for x-ray science are described holistically where beamline instrumentation is viewed as a tightly integrated unit, spanning from source to optics to sample to detectors, all held together by effective and smart controls, and seamlessly coupled with analyses and visualization.

Accelerator operations planning must meet the current and future capabilities expected of a world-leading light source while maximizing efficiencies and delivering high beam availability to users. It is currently assumed that the present APS storage ring will stop operation approximately in 2022 and be replaced by a MBA lattice. Thus, this five-year facility document aligns end-of-life plans for accelerator systems to maintain a very high level of APS performance and reliability, with R&D plans that take into account the long-term transition to a MBA lattice source. This is accomplished in three main areas: accelerator reliability, accelerator improvement, and accelerator R&D to advance new concepts and next-generation light sources.

This Plan also describes engineering, maintenance services, and computing infrastructure that directly support and enable world-class performance of the APS accelerator and beamline complex, while ensuring a safe environment for APS users and personnel.

Finally, this plan briefly describes additional activities necessary to address general maintenance and obsolescence issues (mission readiness), improvements for infrastructure and general operations, human capital development, and user processes and scientific access including outreach and training.

2 Introduction

The APS is one of five x-ray light sources that are operated as national user facilities by the DOE-SC (there are four storage rings: the APS, the Advanced Light Source [ALS], the Stanford Synchrotron Radiation Lightsource [SSRL], and the National Synchrotron Light Source II [NSLS II]; and one free-electron laser (FEL): the Linac Coherent Light Source [LCLS]).

Of the four storage rings, the APS operates at the highest electron energy (7 GeV, 100 mA), and has been optimized to be the source of this nation’s highest-brightness hard x-rays (i.e., photon energies above 20 keV). High-brightness hard x-rays can penetrate deeply into materials and can be concentrated efficiently in a small spot. This combination enables *in situ*, real-time studies of internal structures and chemical states in actual environments and under relevant operating conditions.

The APS is also the largest of the DOE light source facilities, both in the size of the facility and its user community. The APS facility comprises an accelerator complex and storage ring, beamlines, and supporting laboratory and office space. There are currently 67 operating x-ray beamlines; of these, 36 are operated directly by the APS (Appendix 1) under operations funding from DOE-SC-BES. The Sector 26 hard x-ray nanoprobe is operated jointly by the APS and the adjacent BES scientific user facility, Argonne’s Center for Nanoscale Materials (CNM). Until May 2016, beamline 8-BM-B was temporarily operated in conjunction with the NSLS-II while that sister facility brought its transmission x-ray microscopy beamline into operation. Beamline 6-BM-A,B is operated jointly by the APS and the National Science Foundation (NSF)-funded Consortium for Materials Properties Research in Earth Sciences. Finally, Sector 23 is operated by the APS as a national facility for structural biology, with funding from the National Institute of General Medical Sciences and National Cancer Institute of the National Institutes of Health.

The beamlines outside of this portfolio of 39 APS beamlines are operated by the collaborative access teams. The APS has by far the largest participation of operational partners at any U.S. light source. These very diverse collaborations of industry and academia operate according to a number of different models, and, to the benefit of the user community, bring in substantial non-BES funding. The APS provides photons and some minimal direct operations support, with recovery of certain costs, in return for each CAT awarding a fraction of its beam time to general users. Normally, this fraction is 25%, with the exception of CAT-operated beamlines that serve as national resources and that award 100% of their time to general users. The specialized nature of beamlines and end-station instrumentation, including detectors and optics at several of the collaborative access teams, also enables complementary facilities that allow the APS community to provide the broadest reach and to build world-leading capabilities in key fields such as high-pressure research, dynamic compression science, and the biological and life sciences.

Access to the APS is obtained via a scientific peer review process, and access is heavily over-subscribed. In fiscal year (FY) 2016, the APS supported 5,521 unique users (on-site and remote/mail-in) from 49 states, Puerto Rico, the District of Columbia, and 33 nations conducting research that spanned the full range of fundamental and applied sciences across fields including materials science, biological and life sciences, geosciences, planetary science, environmental science, engineering, chemistry, and physics. Users of this facility come from academia, industry, and government institutions.

As the APS user program has grown, so has the facility's publication output grown, with 2,110 papers recorded in our publications database in calendar year (CY) 2015 and 2,150 papers in CY 2016, as of this writing. Of those, 1,800 (CY15) and 1,864 (CY16) are peer-reviewed journal articles, with approximately 20% of those in DOE-defined high-impact journals (*Advanced Materials, Angewandte Chemie International Edition, Applied Physics Letters, EMBO Journal, Cell, Environmental Science and Technology, Journal of the American Chemical Society, Nano Letters, Nature Chemical Biology, Nature Chemistry, Nature Geoscience, Nature Materials, Nature Nanotechnology, Nature Photonics, Nature Physics, Nature Structural and Molecular Biology, Nature, Physical Review Letters, Proceedings of the National Academy of Sciences USA*, and *Science*). Macromolecular crystallographers utilizing APS x-ray beams place more protein structures in the Protein Data Bank than do researchers at any other light source in the world.

The APS produced first x-ray light in 1995, and became operational in 1996. Since then, a number of major advances have occurred in accelerator, storage ring, and beamline technologies and techniques. Combined, these advances have dramatically altered the landscape for x-ray science. In particular, research challenges that require vastly brighter hard x-rays or a higher coherent flux than the APS currently produces are now within reach because of new storage ring lattice designs that dramatically reduce the stored electron beam emittance. Therefore, the APS is now developing plans to install a MBA magnetic lattice into the existing storage ring tunnel that will increase x-ray beam brightness and coherent flux by 100 to 1,000 times (for energies above 10 keV) over current values. This upgrade of the storage ring is a cost-effective approach to a "fourth-generation" storage ring as it will reuse much of the existing accelerator and beamline infrastructure.

While the detailed science case and technical design for this proposed upgrade are presented elsewhere, the brightness and coherence increase from the APS Upgrade in the hard x-ray region of the spectrum will revolutionize imaging, microscopy and nanobeam science, high-energy methods, and high-wavenumber scattering techniques. The penetrating x-ray probes produced by the upgraded APS will transform *in situ*, real-time studies of internal structure during synthesis and function in actual environments and under relevant operating conditions, across a hierarchy of length scales from the atomic to the macroscopic. They will also enable time-resolved studies of dynamics over a wide range of time scales from many seconds to less than a nanosecond, allowing relationships between structure and function to be observed. This proposed upgrade will help to maintain the APS world leading position in the hard x-ray community for decades to come.

The APS Upgrade Project received CD-1 approval in February 2016 and CD-3B on October 2016, and has now prepared a preliminary design report that describes the scope of the Project. With a targeted implementation of the APS Upgrade Project years in the future (2023), beamline performance at the APS must continue to increase in order to take full advantage of the existing source in the interim. Additionally, the APS continues to be charged with delivering new capabilities to the user community while meeting the scientific needs embodied in our nation's future challenges and the DOE mission — which are inextricably entwined — as well as provide the highest level of support to APS users. This will include improvements to specific beamlines and end stations, as well as continued optimization of the APS beamline portfolio, while maintaining the excellent reliability and availability of the APS accelerator and storage ring systems.

This "Advanced Photon Source Five-Year Facility Plan" is driven by the above responsibilities. The document comprises an outline of improvements and R&D to be undertaken by APS Operations during the next five years, employing a two-pronged approach: keeping the APS a world-leading hard x-ray synchrotron source while simultaneously preparing for the proposed upgrade.

To achieve this goal, the APS must invest in aging accelerator and beamline infrastructure while developing innovative capabilities and continuing to drive efficient mission execution. By creating a synergy between today's improvements and tomorrow's needs, the APS will enable operational capabilities for the next five years and continue to grow a scalable, forefront science program that will smoothly transition to take advantage of an upgraded accelerator source.

The improvements described herein leverage APS core capabilities, particularly in the areas of *in situ* and *operando* studies. Although this "Advanced Photon Source Five-Year Facility Plan" is primarily focused on the APS-operated, BES-funded beamlines, key developments for other beamlines are included in this plan, because these beamlines function as complementary assets to the BES program at the APS. For example, the large life and environmental sciences communities at the APS also will leverage diverse assets to improve imaging and macromolecular crystallography capabilities.

Objectives described in this plan are comprehensive and have gone through a full facility-wide strategic prioritization process for resource allocation. However, for beamline investments, prioritization is a continuing process based on user needs and trends, and will necessarily involve ongoing, deep engagement with the APS user community and other stakeholders.

It is also important to note that the APS Divisions maintain more detailed plans that are updated annually. See:

https://www1.aps.anl.gov/X-ray-Science-Division/XSD-Strategic-Plans

https://www1.aps.anl.gov/files/download/AES/AES-Strategic-Plan-and-5-Year-Outlook-FY17.pdf

https://www1.aps.anl.gov/Accelerator-Systems-Division/ASD-FY-2017-Projects

3 Facility Goals

The APS has developed the following facility goals in order to fulfill its mission:

1. Operate a world-leading, highly reliable, high-brightness, hard x-ray user facility to enable outstanding science by users and staff; this requires maintaining clear lines of communication with users and partners in order to continually develop and deploy forefront capabilities and the necessary capacity to address scientific need
2. Increase capabilities of the APS by developing and implementing enhanced and/or novel accelerator and x-ray technologies; this includes rebuilding the APS storage ring with a MBA design and high stability to provide the first fourth-generation, hard x-ray storage ring source in the U.S.; developing next-generation undulators; and developing and instrumenting advanced beamlines that fully exploit the new, high-brightness source
3. Enable continued progress in light source technologies and their utilization in order to maintain the world leadership of the suite of U.S. DOE light sources
4. Assure the safety of facility users and staff

5. Maintain a world-class organization that is diverse, inclusive, and focused on innovation, and that provides a rewarding environment for staff and users in order to foster professional growth

The APS will achieve these goals by advancing strategies coupled to investment in the following areas:

1. X-ray operations and improvements, and research and development on x-ray techniques, optics, detectors, and data sciences
2. Accelerator operations and improvements, and research and development on new concepts and next generation light-source technologies
3. Mission readiness
4. Infrastructure, general operations, support, and other miscellaneous improvements
5. Human capital and workforce development

4 National and International Context for Storage Ring Light Sources

4.1 International Storage Rings

Even though more than 70 light sources exist worldwide in more than 25 countries, the global demand for research time still outweighs availability. Several new facilities will become operational or be upgraded over the next decade, including fourth-generation light sources based on next-generation MBA lattices.

The hard x-ray facilities comparable to the APS are the European Synchrotron Radiation Facility (ESRF; 6 GeV, 200mA, $\varepsilon_x = 4$ nm•rad) in France; PETRA III (6 GeV, 100mA, $\varepsilon_x = 1$ nm•rad) in Germany; and SPring-8 (8 GeV, $\varepsilon_x = 3.4$ nm•rad) in Japan. Both ESRF and SPring-8 were built at about the same time (early-to-mid 1990s) as the APS. Both ESRF and SPring-8 are moving toward incorporating low-emittance lattice upgrades. The ESRF upgrade (Extreme Bright Source) is scheduled to be completed by summer of 2020, while SPring-8 is in the early planning stages.

MAX-IV (3 GeV, 500mA, $\varepsilon_x = 0.30$ nm•rad) in Sweden was officially inaugurated in June 2016 and is now in the commissioning phase of the MBA lattice. SIRIUS (3 GeV, 500mA, $\varepsilon_x = 0.28$ nm•rad) in Brazil, also featuring a MBA lattice, is anticipated to come on-line in 2019. It also appears possible that additional facilities in Russia and China will emerge in the next decade.

The APS (with its current accelerator complex) is projected to stay heavily oversubscribed and unable to fully provide the scientific capabilities that are on the horizon and demanded by U.S. users. Furthermore, all 3+ GeV light sources, be they third-generation, enhanced with damping wigglers, or based on MBA lattices offer stiff competition to or even surpass the existing APS for science requiring bright, coherent beams. Therefore, a future upgrade of the APS remains an imperative.

4.2 U.S. Storage Rings

The U.S. has four x-ray storage ring sources operated as national user facilities by the DOE: APS (7 GeV, 100 mA, $\varepsilon_x = 3.1$ nm•rad); ALS (1.9 GeV, 500 mA, $\varepsilon_x = 2$ nm•rad), SSRL (3 GeV, 300-500 mA, $\varepsilon_x = 10$ nm•rad); and the newly-operating NSLS II (3 GeV, 350-400 mA, $\varepsilon_x = 1$ nm•rad). (The sole U.S. x-ray FEL, the LCLS, is being upgraded via the LCLS-II project.)

In addition, the Cornell High Energy Synchrotron Source (5.3 GeV, 200 mA each electrons and positrons, $\varepsilon_x = 145$ nm•rad) is a high-intensity, hard x-ray source supported by the NSF, which provides its users with synchrotron radiation facilities for research in physics, chemistry, biology, and environmental and materials sciences, and in macromolecular crystallographic studies. This light source facility is planning an upgrade that will allow it to move to single-particle operation at x-ray fluxes comparable to today's APS.

Finally, the Center for Advanced Microstructures and Devices (1.3 / 1.5 GeV, 300 / 150mA, $\varepsilon_y = 150$ nm•rad) is a research center funded by the State of Louisiana that provides low-energy synchrotron light for energy, environment, biomedical, and microfabrication research.

While each light source listed above provides a general range of standard x-ray capabilities for users, each of them also specializes in a specific energy range of the electromagnetic spectrum, enabling different types of science. As noted previously, the APS is optimized to be the nation's highest brightness source of hard x-rays in the energy range above 20 keV. The APS also has a very flexible storage ring fill pattern, routinely operating in 24-bunch mode with 153-ns spacing between bunches, 324-bunch mode with 11-ns spacing between bunches, and hybrid fill mode with a separation of 1.5 µs between the superbunch and remaining bunches. These parameters make the APS the leader in broad areas that require unique sample environments or high x-ray energies, including *in situ*, *operando*, and high-pressure studies, as well as timing experiments outside the domain of FELs. This "Advanced Photon Source Five-Year Facility Plan" builds on these world-leading, and often unique capabilities to support a growing user base with expanding research needs.

5 Strategy for X-ray Science

The APS operates a suite of cutting-edge beamlines that address problems across a wide range of disciplines relevant to the needs of the U.S. scientific community. Modern scientific and technological challenges not only require the ability to gain insight about the properties of matter, but to do so with spatial resolution down to a few nanometers, temporal resolutions from nanoseconds to seconds, and under *operando* or extreme conditions. To address this need, the APS long-term strategy includes building a new low-emittance x-ray source, developing beamlines and the ancillary capabilities that exploit this source, and fostering a broad-based and vibrant hard x-ray science community that can provide international leadership in the techniques enabled by this source.

Targeted research and development activities by APS staff lay the foundation for taking full advantage of the upgraded source, as well as delivering new capabilities that make more effective use of the existing facility. A key component of this strategy is leveraging the high-performance computing capabilities both within Argonne and across the DOE complex for accurate and timely analysis of large and complex data-sets. Furthermore, Argonne capabilities in nanofabrication and computing play a central role in the development of hardware and software essential to fully utilizing the APS-U source characteristics, including high-stability/high-precision instrumentation, state-of-the art x-ray optics (e.g., wave-front preserving optics, zone plates, x-ray micro-mirror microelectromechanical systems devices), advanced energy-resolving detectors, and methods in data management and computational x-ray science. APS staff play a quintessential role in this effort by continuing to advance x-ray instrumentation, algorithms and techniques.

Keeping the APS at the forefront of scientific research requires the continued evolution of the beamline portfolio; the hiring, development, and retention of talented scientists, engineers and technical professionals, and the expansion of the depth and breadth of our user community. Investments must be made continually in beamlines, staff, and R&D to continue to improve and expand APS capabilities, and to preserve its leadership positions in hard x-ray sciences. These directions and investments are aligned with four specific priority areas for the APS given below.

5.1 Priorities

5.1.1 Brightness- and Coherence-Driven Beamlines and Techniques

The APS source after the upgrade will provide world-leading beam coherence and brightness. These beam characteristics greatly enhance experiments in the areas of x-ray photon correlation spectroscopy, imaging, and microscopy (including coherent diffractive imaging). The upgraded APS will make possible completely new measurements not feasible today (see, e.g., the "Early Science at the Upgraded APS" document).

Beamline improvements, staffing, and related technical developments that enhance these areas will be given the highest priority. The APS will work to develop, establish, and refine methods and techniques that can take full advantage of the upgraded APS source.

5.1.2 High-Energy Beamlines and Techniques

The APS is unique amongst the present U.S. light sources in providing highly brilliant x-ray beams at high energies (>20 keV) enabling deep penetration into matter, complex sample environments for *in situ* and *operando* experiments, minimizing radiation damage and providing precise structural information. APS staff have exploited this feature to enable a number of world-leading capabilities in materials science, chemistry, extreme conditions, etc. After the upgrade, the APS will have significantly increased degrees of coherence and enhanced flux densities at high energies. This will make it feasible to extend many coherence-based x-ray techniques much further into the high-energy regime, particularly in areas such as imaging, microscopy, x-ray photon correlation spectroscopy, surface diffraction, etc.

5.1.3 Timing and High-Speed Imaging capabilities

The current APS bunch pattern, with ~100-ps FWHM bunches separated by ~ 150 ns (24-bunch mode), is a "stand-out" feature for routine operations mode at a third-generation synchrotron source. To retain the existing and unique APS strength in timing measurements, the upgraded source plans to support a bunch pattern allowing timing and high-speed imaging experiments with ~200-ps bunches FWHM separated by ~75 ns (48-bunch mode). Therefore, the APS will continue to invest in timing and high-speed imaging, particularly where coupled to new approaches that leverage brightness, coherence, and/or high energies.

5.1.4 Beamline Operations and Development

The APS serves a large number of users across highly diverse scientific fields, who benefit greatly from excellent beamline capabilities and outstanding staff expertise. The APS will continue to optimize and invest in valuable, sought-after programs and facilities, including but not limited to high-throughput approaches, core capabilities, etc. This includes the operation and expansion of support labs that facilitate beamline experiments (e.g., the electrochemistry lab that supports battery related experiments across the APS). The APS must also identify and respond to the current and future requirements of the scientific user community (workshops, meetings, partnerships, etc.) as well as train and develop the user base and disseminate information (workshops, seminars, schools, etc.).

5.2 X-ray Science

The Sections below spell out broad directions for the next five years of x-ray science research related to the areas of materials, chemistry, life sciences, and environmental/geo sciences along with the necessary supporting capabilities required to accomplish these goals. Our strategy ties in with and complements the APS-U early science document, and together with an assessment of user needs, guides the near- and long-term investments required to serve users and maintain leadership in x-ray science. The ultimate goal is to create a suite of state-of-the-art beamlines and ancillary experimental facilities that will fully support the APS user community in its quest to explore the most important problems using high-energy, extremely brilliant x-rays.

5.2.1 X-ray Science for Chemistry

Chemical processes are central to many global energy challenges. A fundamental understanding of chemical transformations and energy flow in complex systems is required to make these processes more efficient and sustainable. At the APS, hard x-rays provide the ability to characterize chemical processes *in situ*, on time and length scales ranging from the atomic to the macroscopic. Correlating chemical structure and function is facilitated by a multimodal approach that combines scattering methods to define atomic positions, spectroscopic methods to identify chemical speciation, and imaging/tomographic modalities to link structure and chemical properties at multiple length scales. The APS operates a number of beamlines that support spectroscopy, scattering, diffraction, and imaging techniques ranging from “tender” to high-energy x-rays, and that are well adapted to the needs of chemical science problems. These beamlines feature the ability to measure spatial resolution that spans distances from directly bonded atom pairs to the mesoscale to the macroscopic scale, and include high-throughput capabilities for rapid screening, standardized reaction vessels for catalysis, and infrastructure for flow and characterization of reactive gases. Electrochemistry is supported by a lab specialized in (but not limited to) battery research. To investigate fundamental energy and charge transfer processes, the ability of an ultrafast excitation to coherently prepare an ensemble of molecules allows one to use x-ray pulses to investigate the dynamics of molecular systems at the atomic-level using pump/probe or pump/probe-probe-probe techniques.

Looking toward the future, the APS Upgrade will provide a 100-fold increase in coherent flux, which will enable a corresponding increase in the intensity of nanofocused x-ray beams and in the ability to study nanometer-size voxels with chemical specificity in complex chemical environments. The APS-U will provide sufficient high-energy brightness to allow micrometer-size focusing without compromising the angular resolution for diffraction and scattering experiments, thereby matching real and reciprocal space resolutions for *operando* experiments in complex sample environments. Hence, the APS-U will enable new opportunities to spatially resolve the foundations for chemistry within complex materials and devices.

5.2.1.1 Energy Transfer and Conversion

Energy transfer and conversion processes in catalysts, solar cells, photosynthesis, mechanical-electric and electric-optical devices, and stimuli-responsive materials typically occur over a wide range of time-scales. For example, solar fuel catalysis, such as light-driven oxidation of water coupled with the reduction of CO_2 to fuels, consists of multiple coordinated reaction steps involving electron/hole trapping, charge separation, and recombination on sub-nanosecond time scales, and bond making/breaking reactions occurring on microsecond-to-millisecond time scales (see Fig. 1.). *In-situ* time-resolved x-ray spectroscopy and scattering methods employing laser-synchronized pulsed x-rays at the APS provide a means to elucidate the charge, energy, and structural reorganization involved in each redox step of such complex processes on time scales down to ~100 ps. These measurements can be performed in pump-probe or pump-probe-probe-probe fashion to access the full range of time scales of interest in the system.

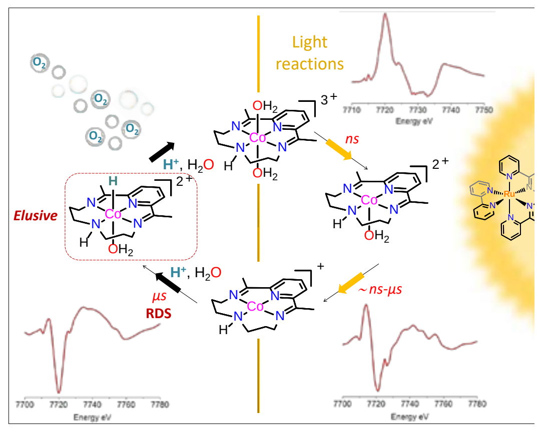


Fig. 1. Pump-probe-probe-probe x-ray spectroscopy of the hydrogen evolution reaction catalyzed by a cobalt complex, capturing multiple transient states simultaneously. J. Am. Chem. Soc. **138**, 10586 (2016).

Looking forward, time-resolved techniques will continue to play a key role in an upgraded APS. The ability to focus the full x-ray beam flux into sub-micron spots will enable time-dependent studies in more complicated energy conversion processes involving heterogeneous materials. Time-resolved coherent scattering is a developing technique for examining the dynamics of structural transitions involved in energy conversion. Realizing these transformative capabilities will require further improvements in the mechanical stability of APS x-ray beamlines, detection schemes, and sample environments for *operando* studies.

5.2.1.2 Energy Storage

Functioning batteries rely on complex mechanisms, occurring simultaneously at multiple length and time scales. These multi-component dynamic systems typically evolve during their lifetimes and undergo pronounced changes in electrochemical performance, phase transformations, and ionic and electronic transport. Often, the mechanisms governing battery performance operate at conditions far removed from thermodynamic stability and involve formation of several metastable phases. Understanding what governs battery performance, including structural and electronic properties that lead to failure, is key to the future design of next-generation rechargeable systems. The suite of x-ray characterization tools available at the APS is essential to advancing the fundamental understanding and the rational optimization of capacity, charge rate, lifetime, and product safety of future energy-storage devices.

The x-ray techniques available at the APS are ideally suited to provide comprehensive insights into complex battery structures at multiple length scales. Bulk techniques such as powder diffraction, pair distribution function, extended x-ray absorption fine structure, and small-angle x-ray scattering are applied routinely to study reaction mechanisms, metastable states, and mesoscale phenomena under *operando* conditions. The dedicated electrochemical laboratory within the APS enables *operando* measurements previously unattainable to general users, e.g., studying electrode degradation mechanisms after extended periods of cycling. For example, the *operando* x-ray diffraction measurements of $LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$ (NCA) materials, pre-cycled at the APS electrochemical laboratory, revealed heterogeneous reaction kinetics that were ultimately attributed to the conductivity loss due to intergranular fracturing as the result of the extended cycling (Fig. 2).

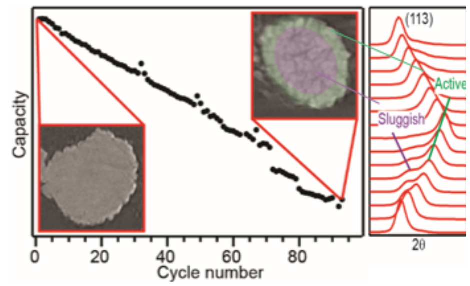


Fig. 2. *Operando* x-ray diffraction revealing how inter-gruanular cracking leads to two populations of battery grains with different reaction kinetics. Nano Lett. **17**, 6 (2017).

Following the electrode's reaction process during prolonged cycling via quantitative *operando* measurements allowed for identification of the dominant capacity fading mechanism in a commercially deployed system [Liu et al., Nano Lett. **17**, 6 (2017)]. High-energy techniques will significantly benefit from the continued development and deployment of super-conducting undulators.

X-ray microscopy techniques are an emerging tool for examining electrode-material performance on a single particle level (spectroscopy- and diffraction-based x-ray imaging). For example, Bragg coherent diffraction imaging recently provided detailed three-dimensional insights into dislocation dynamics in cathode nanoparticles under *operando* conditions [Ulvestad et al., Science **348**, 6241 (2015)]. After the APS Upgrade, the greatly enhanced focusing capabilities and coherence will transform such methods from *tour-de-force* measurements to commonplace. This will, however, require concentrated improvements to the design of *operando* environments such as electro-chemical cells to minimize their effect on the x-ray wavefronts.

5.2.1.3 Catalysis

Catalysts are central to 90% of our nation's chemical manufacturing, which is a major consumer of energy. In addition, catalysts are important for more efficient production of low/non-carbon fuels, better fuel and electrolytic cells, more efficient conversion of renewable resources to fuels, and technologies for the sequestration and utilization of CO_2.

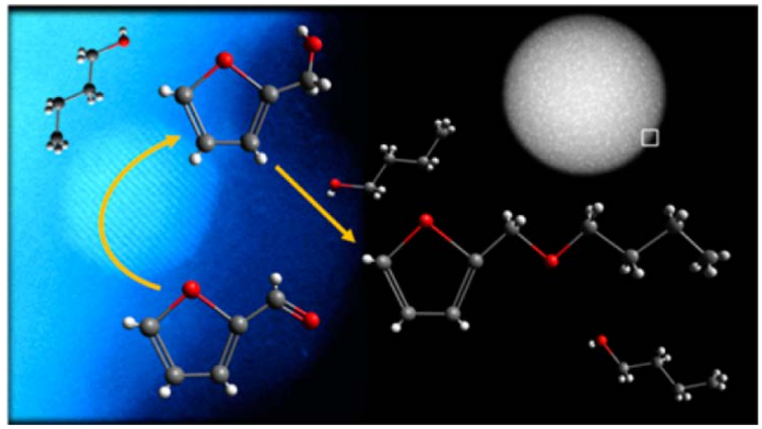


Fig. 3. Pore structure and bi-functional catalyst activity of over layers applied by atomic layer deposition on copper nanoparticles. Nanofocusing in an upgraded APS will enable characterization of individual catalytic particles and their active sites under *in situ* reactive conditions. From Alba-Rubio et al., ACS Catalysis **4**, 1554 (2014).

To optimize the use of catalysts for sustainable energy, two main challenges must be overcome. First, the mechanisms and dynamics of catalytic transformations must be understood. Second, the synthesis of catalytic structures must be designed and controlled (Fig. 3). The past decade has seen substantial advances in the ability of theory, particularly density functional theory, to predict the activity of designer catalytic structures. However, experimental studies under realistic conditions are always central to creating practical catalysts [Yang et al., Science **346**, 1498 (2014)].

X-ray methods are poised to uniquely probe catalytic systems *operando,* validating the computational predictions for new catalytic compounds and solutions to practical problems with existing catalysts. Efficient catalysts are nanoscale and are rendered ineffective by sintering (agglomeration) under operating conditions, which can be harsh (e.g., 10 atm, >700°). Small-angle x-ray scattering is an example of an x-ray technique optimally suited to detect changes in the size and shape of the catalytic nanoparticle or the nanopore in a surrounding capsule, while x-ray spectroscopy yields information on chemical state and nearest-neighbor identities and distances. Combining these techniques with the nanofocusing available from the APS-U will enable a transition from probing large ensemble averages to probing single particles. An example where smaller size resolution is vital is in the over-coating of a catalytic particle by atomic layer deposition to protect the particle from sintering and coking [Lee et al., Energy Environ. Sci. **7**, 1657 (2014)]. Porosity of the coating is produced by heating and is observed by small-angle x-ray scattering. This is a very promising approach for the development of the very robust catalysts necessary for upgrading biomass-derived molecules. The ability to visualize the pore network, and map and quantify the contaminating metals, is very important and requires better size resolution to accomplish.

5.2.1.4 Chemistry in Ordered Systems

Structure determination and structure analysis of new materials is one of the most important tasks for understanding materials properties. The majority of structure determinations are currently carried out with lab-based devices in a physical form and under conditions (e.g., single-crystal at 100K) that are quite different from those used in the industrial and/or commercial settings. While determining new structures may be complicated, powder diffraction, pair distribution function, and small-angle x-ray scattering can be easily used for *in situ* and *operando* structural studies once generalized structural models are known. This application of the high brilliance and high energy of the APS beam enables a better understanding of material structure and microstructure, and perhaps more importantly, their evolution under real, applicable conditions. When more accessible, *in situ* scattering techniques will become widely used after initial structures are determined.

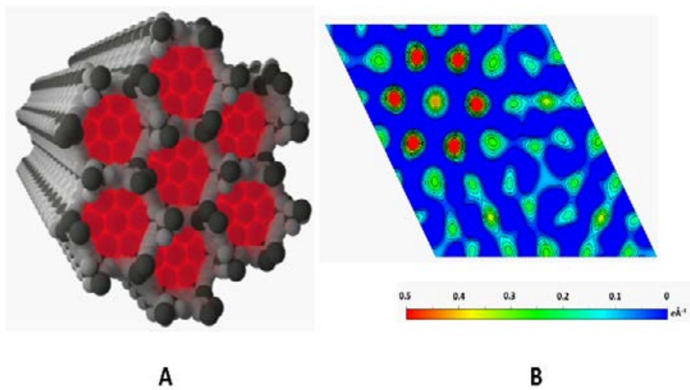


Fig. 4. Neon atoms (A) and Fourier difference map (B) observed experimentally within the pores of NiMOF-74. Wood et al., Chem. Commun., **52**, 10048 (2016).

Examples of chemical functionality induced within spatially organized systems include metal organic frameworks (MOFs). These porous materials, where the porosity and chemical affinity can be controlled by design, can have application for CO_2 sequestration, catalysis, and gas storage and separation. Recent advances in sequential and parametric analysis allows one to utilize the APS beam for *in situ* powder diffraction experiments to track positions and occupancies of hard-to-detect, low-electron-density atoms such as neon in the pores of MOFs (Fig. 4) [Wood et al., Chem. Commun., **52**, 10048 (2016)]. This provides the means to understand and study MOFs used for natural gas storage, which has considerable environmental, economic, and political advantages over petroleum as a source of energy for the transportation sector [Mason et al. Nature, **527**, 357 (2015)].

High x-ray energy and high-angle-resolution scattering instruments available from the APS are crucial to determine superlattices of nanomaterials by design, as these structures have been synthesized with atomic-level precision using DNA linkers [Kim et al. Science **351** 579 (2016)] or rationally designed molecules [Kim et al. Proc. Natl. Acad. Sci. USA **114** 4072 (2017)]. Novel multicomponent superstructures may give rise to unique plasmonic, magnetic, or catalytic properties utilizing both individual and collective properties of the building blocks [Boles et al. Chem. Rev. **116** 11220 (2016)]. Small-angle x-ray scattering provides an *in situ* view of the synthetic process otherwise difficult to visualize with any other tools [Sun et al., Science **356** 303 (2017, and Zhang et al. Nature **542** 328 (2017)]. An upgraded APS will significantly increase the focused flux for these techniques, further leveraged by efforts in super-conducting undulators, high-energy focusing optics, etc. Together, these improvements will make possible the determination of science questions that today cannot be answered.

5.2.2 X-ray Science for Materials

Synthesizing, understanding, and controlling the properties of advanced materials lie at the very heart of modern technologies. The increasingly rapid development of novel materials has been driven by improved synergies between synthesis techniques, theory, and characterization, with the information from each feeding back to the others. Synchrotron radiation plays a key role in this cycle by providing unique characterization tools for probing the structure, topology, electronic configuration, and dynamics of such systems under real operational conditions (Fig. 5) and during synthesis and even nucleation. Synchrotron-based techniques provide information across a wide range of length scales from inter-atomic to several millimeters, and time scales from sub-nanosecond to hours. This enables the direct coupling of the relevant time and length scales to a particular material's functionality.

The APS provides state-of-the-art facilities that accelerate this materials discovery process and the exploration of the complex interactions at the core of modern functional systems. Today, the APS operates a suite of beamlines that encompass the breadth of current x-ray scattering, spectroscopic, and imaging techniques. The new instrumentation developed at the APS for probing materials leverages one or more of the unique core strengths of the facility, particularly the deep penetration of high-energy x-rays. This provides true bulk measurements and capabilities for observing materials *in situ*, that is, in environments relevant to actual operating conditions and at the extremes of pressure, temperature, and other conditions. The extreme brightness of APS x-rays enables high-resolution and multi-modal imaging that can capture heterogeneity in both structure and elemental composition of designer, advanced materials down to the nanometer level. The high-intensity, pulsed APS x-ray beam provides an excellent probe for understanding the dynamics of matter at time scales down to 100 ps.

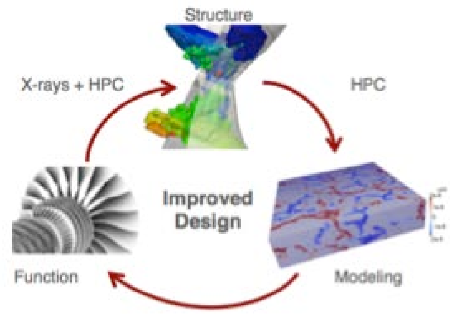


Fig. 5. Rapid development of new advanced materials is driven by x-ray characterization coupled with materials modeling. Courtesy of Robert Suter, Carnegie Mellon University.

The proposed upgrade of the APS storage ring will provide transformative capabilities for nanoprobe imaging and coherence-based techniques, such as x-ray photon correlation spectroscopy (XPCS) and coherent diffractive imaging that probe materials with even greater fidelity.

5.2.2.1 Engineering Materials

The past 15 years have seen remarkable advances in producing engineering materials that are more efficient, safer, and more durable than those previously available. For example, the current generation of airplanes contain 20-50% composite materials in their primary structures. However, the development of newer materials with further functional improvements depends on obtaining experimental data across a wide range of length scales to validate computational models that link performance to materials processing, microstructure, and properties.

The APS has several unique structural characterization tools for probing functional engineering materials, such as high-energy diffraction microscopy (HEDM), nano-Laue, dynamic phase-contrast tomography, and high-speed imaging and diffraction. The datasets that these techniques provide are increasingly being used to stringently test and refine micromechanical models to improve the performance of industrially relevant materials. These capabilities have attracted sophisticated sample environments from partners including (1) a high-precision, in-grip rotation apparatus for *in situ* mechanical loading (Air Force Research Laboratory), (2) a vacuum furnace for *in situ* thermo-mechanical studies of irradiated materials (Argonne Nuclear Engineering Division), and (3) a loading-plus-thermal-gradient system for studying turbine blades (University of Central Florida and DLR, Germany, Fig. 6). Furthermore, new x-ray capabilities for *in situ* time-resolved characterization of additive manufacturing processes have led to insights on how to manufacture such parts with improved physical properties.

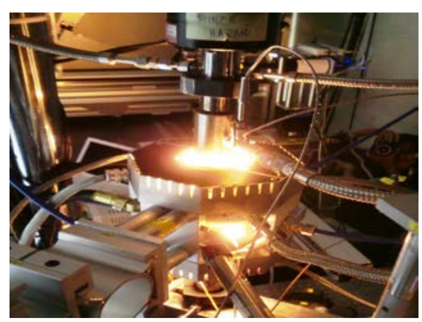


Fig. 6. Innovative load frame and thermal-gradient furnace that mimics the *operando* conditions in turbine engines. Knipe et al., Nat. Comm. **5**, 4559 (2014)

To further enhance these high-energy capabilities, additional developments are needed for high-speed imaging/diffraction to improve spatial and temporal resolution. Improved superconducting undulators, high-energy focusing optics, and new detection schemes will push the spatial resolution and stability of HEDM to 1 µm from the current 5 µm, enabling mapping of the microstructure and strain of intrinsically heterogeneous systems. A new generation of faster high-energy detectors will capture irreversible bulk processes such as additive manufacturing with speeds in the millisecond regime (currently ~0.1s) by leveraging the high x-ray fluxes at these energies. Integrated approaches toward data handling and processing using high-performance computing will be developed to handle the large volume of data generated by these techniques (~10 TB/day). Looking toward the APS Upgrade, the high brightness at high energies of the MBA lattice will extend HEDM and diffraction tomography techniques to increasingly complex materials, with greatly improved resolution.

5.2.2.2 Quantum Materials

Emergent phenomena in quantum materials, from high-temperature superconductivity in strongly correlated electron systems to symmetry-protected metallic surface states in topological insulators, present unique opportunities to transform energy and information technologies. Users of the APS exploit the high brightness, penetrating power, and time structure of APS x-ray beams to probe charge, spin, orbital, and structural orders (together with their dynamics) in these materials. Effort is placed on manipulating and controlling emergent states with external stimuli in bulk- and thin-film samples, as well as with strain and reduced dimensionality at interfaces of artificial heterostructures.

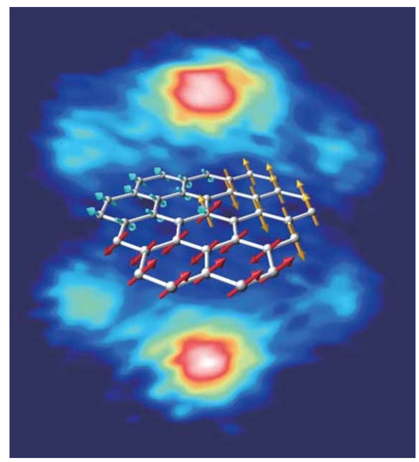


Fig. 7. High-resolution resonant inelastic x-ray scattering probes exotic magnetic excitations in strongly spin-orbit coupled 5d transition metal-oxide, Na_2IrO_3. Chun et al., Nature Phys. **11**, 462 (2015).

A number of APS beamlines enable studies of quantum materials with a variety of techniques including fast polarization modulation linear/circular dichroism spectroscopies, resonant/magnetic x-ray scattering, resonant inelastic x-ray scattering (Fig. 7), and high-energy-resolution inelastic scattering [Budai et al., Nature **515**, 535 (2014)].

The APS is collaborating with the Argonne Materials Science and Nanoscience and Technology Divisions in the development of x-ray instrumentation for *in situ* characterization of heterostructures during growth [Lee et al., Nat. Mater. **13**, 879 (2014)] as well as implementation of multimodal probes combining x-ray and thermodynamic/electrical/optical probes of a quantum material's state [Bi et al., Phys. Rev. Lett. **113**, 267202 (2014)]. A unique high-field terahertz pump coupled with nanoscale diffraction has been implemented for studies of field-driven phenomena on ultrafast time scales relevant to information processing. Sample environments allowing concomitant application of magnetic/electric/strain/optical fields at low temperatures are being developed for studies of emergent electronic order using dichroic and resonant scattering techniques. Elucidating the relationship between crystal structure and electronic properties can be studied with *in situ* measurements of interfacial structure during growth of heterostructures in an oxide molecular beam epitaxy chamber at beamline 33-ID and a versatile diffractometer at 12-ID-D accommodating a wide variety of synthesis and processing chambers. The enhanced coherence/brilliance of the upgraded APS will enable use of coherent scattering, nano-diffraction and nano-spectroscopy probes to map nanoscale electronic inhomogeneity characteristic of quantum materials with competing energy scales such as in the vicinity of quantum critical points.

5.2.2.3 Extreme Conditions

Manipulation of matter with extremes of pressure, temperature, and electromagnetic fields provides a route to advancing our understanding of a large array of fundamental problems in condensed matter physics, geosciences, and materials synthesis. The most extreme conditions are typically realized across small, encapsulated volumes, so the high-brightness, penetrating, micron-sized APS x-ray beams are ideally suited for these studies, which include radioactive or irradiated materials and systems under large shock compression.

The APS has been a leader in studying materials properties at high pressure using devices such as diamond anvil cells and large-volume presses. Specifically, the High Pressure CAT is fully dedicated to such studies, while the GeoSoilEnviroCARS-CAT facility provides about 50% of its beam time to these measurements. The recently commissioned Dynamic Compression Sector (35-ID-B,C,D,E) goes beyond the limits of static high-pressure generation to probe structural deformation in real time under shock wave or shock-less compression. State-of-the-art high-pressure programs have also been developed for magnetic dichroism [T. Takayama et al., Phys. Rev. Lett. **114**, 077202 (2015)], resonant and non-resonant magnetic scattering [Wang et al., Nat. Comm. **7**, 13037 (2016)] and nuclear resonance forward scattering [Liu et al., Nat. Comm. **8**, 14377 (2017)] to probe electronic response at extreme pressures in low temperatures and magnetic field environments. Other extreme environments capabilities include high temperature (3500K) levitated nuclear fuel melts probed with high energy x-ray scattering (Fig. 8), scattering in continuous (4.5T) and pulsed (30 T) magnetic fields, and high-pressure inelastic x-ray scattering [Lin et al., Sci. Rep. **4**, 6282 (2014)].

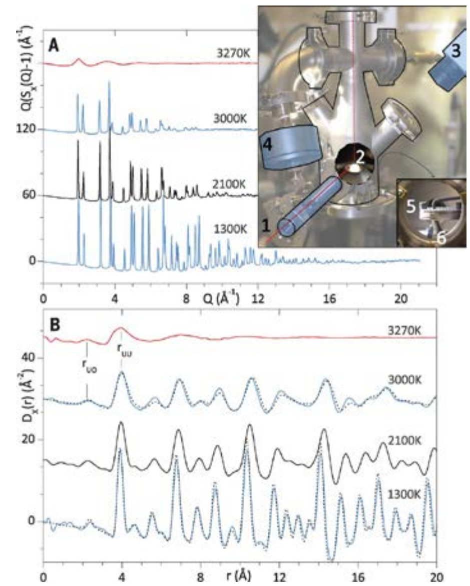


Fig. 8. High energy x-rays were used in combination with aerodynamic levitation to examine the local structure of a nuclear fuel material, UO_2, in solid and molten states to understand the 5.implications for containment of fuels during accidental reactor fuel meltdown. L. B. Skinner *et al.*, *Science* **21**, 346 (2014)

The APS will pursue a coordinated approach to developing instrumentation that expands the range of extreme conditions accessible using hard x-ray techniques. New instruments will provide simultaneous high-pressure, high- and low-temperature, and magnetic field capabilities for x-ray resonant magnetic scattering, resonant inelastic x-ray scattering, and coherent diffraction. A new scheme that utilizes a fast x-ray chopper will be applied to speed up synchrotron Mössbauer measurements (3-ID-B,C,D) to probe hyperfine properties (e.g., magnetic collapse, site occupancy and valence) at high pressure. Common laboratory user facilities for preparation and loading of pressure cells, as well as loading of radioactive samples, will be implemented.

In the long term, the nanoscale beams delivered by the APS-U will enable experiments at even higher pressures and magnetic fields, as well as provide dramatic new capabilities for exploring heterogeneity across materials at extreme pressures using nanoscale spectro-microscopy and coherent scattering methods.

5.2.2.4 Soft Matter

Soft materials play an important role in applications such as food, solar cells, consumer products, and templates for nanolithography for next-generation microelectronics. The function and performance of soft materials is highly correlated to a hierarchy of structural length scales, including atomic, mesoscale, and macroscopic, as well as time scales from milliseconds to hours. The APS offers users several tools, such as small-angle x-ray scattering (SAXS), grazing-incidence x-ray scattering (GIXS) (Fig. 9) and XPCS that access all of these temporal and spatial scales, providing a full picture of how soft matter (self-)assembles and dynamically responds to external conditions.

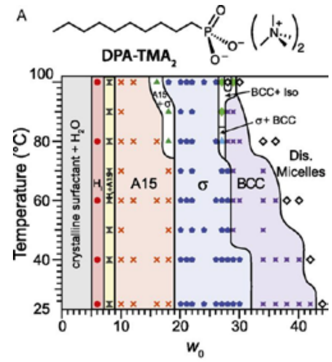


Fig. 9. SAXS used to discover novel ordered phases in surfactants. Kim et al., Proc. Natl. Acad. Sci. **114**, 4072 (2017).

Recent improvements in SAXS measurements have focused on increasing experiment throughput by providing rapid flexible focusing and installing more user-friendly data acquisition and analysis software. Higher-energy GIXS measurements have expanded the range of accessible reciprocal space and advanced studies requiring penetration through various environments such as annealing solvents. Recent advances in XPCS capabilities at the APS have been provided by the deployment of a fast, pixel array detector purchased from X-Spectrum and by improvements in the focusing performance of lenses used to tailor the coherence lengths at the sample position. The combination of these improvements enable XPCS sampling times to span up to 7 decades in time sensitivity. Significant new soft matter capabilities will soon be provided by a dedicated, in-vacuum reflectometer for polarization dependent soft x-ray scattering being developed in collaboration with the Institute of Molecular Engineering at The University of Chicago.

Looking further ahead, the increased coherence at higher energies delivered by the proposed MBA lattice will provide a 4- to-6-order-of-magnitude increase in the time sensitivity for XPCS, revolutionizing the ability to probe the dynamics of systems in attenuating sample environments, such as electrochemical cells with applications to energy storage. The APS-U XPCS beamlines will be designed to take full advantage of the new source properties. The GIXS programs, which are included in the APS-U feature beamlines, are currently housed at 8-ID. They will move to a new location in order to be optimized. Lastly, the resolution of other APS SAXS beamlines will be significantly improved after the APS-U. For example, the sample-to-detector distance of 12-ID-C will be increased threefold to deliver higher reciprocal space resolution and access to smaller wavevector transfers that are necessary for comprehensive studies of hierarchical order.

5.2.3 X-ray Science for Life, Environmental, and Geo Sciences

A grand challenge in life sciences is to understand the structure-function relationship, which connects the structure of proteins and other important molecules to their function within organisms through their role in organelles, cells, organs, and beyond (Fig. 10). This relationship lies at the heart of key questions such as: How do integral membrane proteins perform their very diverse, biologically important functions? How do complex molecular machines perform their tasks? How do drugs interact with their targets? How do pharmacological side effects arise, and how can drugs be improved? Life scientists explore problems at both the fundamental and applied levels, with a major focus on understanding, preventing, and curing disease.

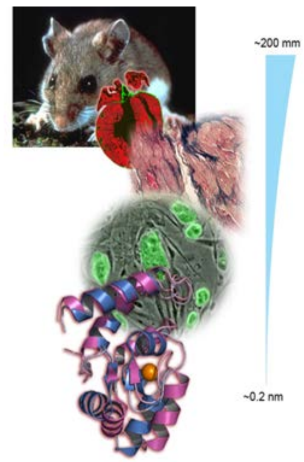


Fig. 10. The Grand Challenge of understanding life is elucidating structure-functions relationships across the entire hierarchy from protein to organism. Figure: Richard Fenner, Advanced Photon Source, Argonne National Laboratory.

The APS provides users with proven capabilities for addressing this relationship. For example, macromolecular crystallography is essential for understanding the structure of the individual components and their complexes at the atomic level. The SAXS/WAXS techniques reveal the behavior of proteins in conditions typical of *in vivo* systems: protein interactions and large scale effects of drug/ligand binding. X-ray fluorescence microscopy explores metalloprotein function, for example when the local chemical/trace metal environment varies. X-ray (micro)-diffraction plays an important role in studies of biomineralization. In addition, a cryo-sample preparation laboratory for soft materials is available to users.

Many of the issues important for biological systems apply also to the environmental sciences. Samples are complex and heterogeneous with multiple length scales. The challenge is to connect atomic-scale processes with field-scale problems. The relevant elements are often highly dilute, and many of the instruments developed for biological systems, e.g., fluorescence microprobes, are equally important for environmental samples.

The biological, environmental, and geo sciences communities at the APS are large and vibrant, accounting for a significant fraction of APS users. Research in these areas is distributed across the APS, taking place on both CAT- and APS-operated beamlines. This research generally falls into four thrust areas that encompass capabilities available at the APS today.

5.2.3.1 Structural Biology

Macromolecular crystallography is the most powerful tool for determining the structure of biological macromolecules with high biomedical importance at the atomic level (Fig. 11), but it requires diffraction-quality crystals. For many Grand Challenge questions, crystals tend to be either small (micron size) or larger, but structurally heterogeneous; both diffract weakly. Recent developments have shown that larger crystals, previously discarded due to poor diffraction, can yield excellent data when only a small and structurally homogeneous portion of the crystal is illuminated with a mini-beam (10-50 µm) or a microbeam (1-10 µm). In addition, data may be collected from crystals that remain within their crystallization device and thus avoid the damaging stresses that occur during cryo-cooling or mounting. It is now even possible to collect data from tiny crystals that grow naturally inside cells — *in cellulo*. Crystals smaller than the range of photoelectron escape may be less prone to radiation damage at higher x-ray energies. These approaches open access to previously inaccessible protein structures such as that of the human β2 adrenergic receptor, a G-coupled protein receptor whose structure and function determination led to the 2012 Nobel

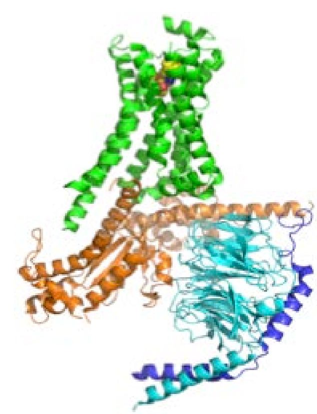


Fig. 11. The ribbon representation of the β_2 adrenergic receptor-Gs protein complex. Integral membrane receptor (green) with an agonist bound (yellow), and the trimeric Gs-protein components (orange, cyan, and purple). Courtesy of Brian Kobilka, Stanford University.

Prize in Chemistry, based in large part on studies at the APS. Nanoliter crystallization technology, serial crystallography, and the use of synchrotron microbeams may revolutionize structural biology.

The current brightness of the APS and the large unit cell parameters of typical protein crystals limit the minimum useful x-ray beam size and therefore crystal size to approximately 5 µm or larger. This is a major bottleneck for structure determination of systems of particular interest to cell biologists. The APS-U will provide a 100-fold increase in brightness and enhance beam stability, which will allow routine structure determination from crystals as small as 0.5 µm. While radiation damage limits the amount of data that can be collected from a single crystal, a complete dataset can be assembled by merging partial data sets from multiple (>10) small crystals. This will overcome not only the problem of growing large crystals, but also avoid the cooling needed to overcome the beam damage problem. Merging procedures will benefit from new tools being developed for serial crystallography at both FEL and synchrotron sources. This will allow the structures of larger protein complexes to be determined routinely and become the next breakthrough area for the treatment of diseases. To meet these challenges, the APS and the collaborative access teams have established collaborations with several groups to implement rapid sample changes via either viscous jet injectors or patterned Si-chips, and a new end station is planned that will provide a high-intensity, 1-µm-beam capability (GM/CA-XSD, 23-ID-D). In addition, new methods of data collection are being explored. Typically, a complete dataset is collected by rotating the crystal in the x-ray beam. However, it is not practical to rotate an individual crystal during such short exposure times, especially if the crystals are in a jet or on a chip; and thus, each image is essentially a "still pattern." With a monochromatic x-ray beam where the energy bandwidth ($\delta E/E \sim 10^{-4}$) is significantly less than the equivalent rocking curve width, each Bragg reflection is only recorded partially, requiring hundreds of thousands of images to build a complete dataset. With a pink-beam ($\delta E/E \sim 10^{-2}$) and static Laue crystallography (BioCARS-CAT, 14-ID-B) most of the Bragg reflections are fully recorded, and the number of images needed to build a complete data set is significantly reduced to only a few thousand images.

Enzymological or biomechanical function derive from dynamical changes in molecular structure. It is therefore crucial to move from a static toward a dynamical picture of biological structure. Picosecond time-resolved Laue crystallography (BioCARS-CAT, 14-ID-B) has resolved structural changes with 100-ps resolution. The increased brightness of the APS-U will allow the study of microcrystals of larger protein complexes. More importantly, microcrystals are better stimulated by the pump laser beam, which both increases the time-dependent diffraction signal and decreases the background.

5.2.3.2 Structure of Biomolecular Complexes in Solution

Since the late 1990s, computational methods for *ab initio* structure determination of non-crystalline bio-molecules emerged [Svergun et al., Rep. Prog. in Phys., **66**, 1735 (2003)]. They allow the visualization of the molecules in solution to be derived from SAXS data. When it is combined with other types of characterization tools such as nuclear magnetic resonance, it may be possible to determine structures at least partly in atomic resolution [Zuo et al., Proc. Natl. Acad. Sci. **107**, 1385 (2010)]. The solution method is particularly powerful in studying the molecular structures of large RNAs and biomolecular complexes in/near physiological conditions because many of them are difficult to crystallize due to intrinsic flexibility. For example, over the past two decades researchers had been unable to

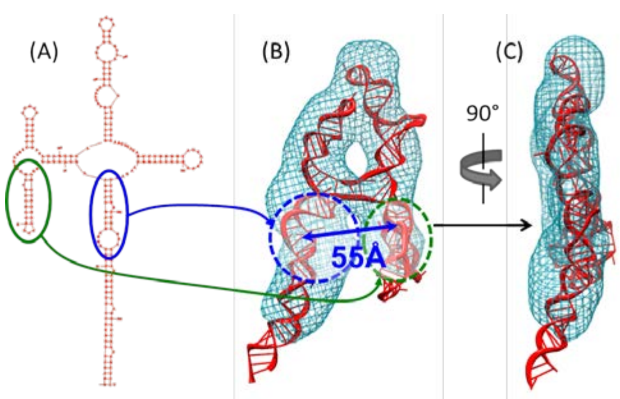


Fig. 12. The secondary structure (A) and two views of the SAXS envelope (cyan in B &C) and derived atomic model (red in B&C) for Rev-protein response element (RRE) in HIV-1 RNA genome [Fang et al., Cell, **155**, 594 (2013)].

crystallize the Rev Response Element (RRE) RNA in the HIV-1 genome, with >230 nucleotides and crucial to HIV viral life cycle, but its structure has first been solved using solution SAXS method (Fig. 12).

The hard x-ray beam provided by the APS is particularly useful for solution SAXS studies of biomolecules, due to its low radiation damage and high penetration power, which significantly improves the signal-to-noise ratio. In order to take advantage of the superb x-ray properties for bio-SAXS, the APS has invested in beamlines and infrastructure such as sample environments that require as little as 10 uL of solution for measurements, utilizing windowless containers, in-line fast protein liquid chromatography (FPLC), and robotic or liquid handling systems for automatic measurements.

High-energy and high-flux x-ray beam makes the APS an ideal place for time-resolved solution SAXS measurements to study not just dynamics but also any structural transition upon various stimuli. Mixing based time-resolved solution SAXS is an important all-atom method to exploit the biomolecular folding landscapes, and to better understand protein mis-folding diseases, such as Alzheimer's disease [Kathuria et al., Biopolymers, **95**, 550 (2011)]. The current temporal resolution of mix-based time-resolved-SAXS is about 100 µs [Kathuria et al., J. Mol Biol., **426**, 1980 (2014)], which covers the mid-to-late stages of biomolecular folding, while the early-stage is expected to appear at ~1 µs. The higher brightness and smaller size of the APS-U x-ray source will allow smaller mixing and flow channels and enable one to extend temporal resolution down to 1-10 us, to exploit the early stage of folding.

A challenge of solution SAXS is to prove the uniqueness and improve the detail of the determined structure. There have been efforts to tackle this issue, for example by simultaneously analyzing data from different light sources or by varying x-ray energy. Using laser techniques to orient molecules along an axis or two, if not three, could be a viable option to reduce the degeneracy, which could be used to leverage the coherence of the APS-U x-ray beam.

5.2.3.3 Structure and Function – Organelles to Cells to Organisms

Transition metals such as zinc, copper, and iron are essential trace nutrients for all forms of life. In humans, their dysregulation can lead to devastating diseases (e.g., Menke's and Wilson's diseases). Numerous neurodegenerative diseases are also believed to have trace-metal associations (e.g., Alzheimer's). Metal homeostasis is also starting to be implicated in reproductive health. In general, transcription factors that regulate gene expression often contain a DNA-binding zinc-finger domain and therefore depend on the availability of zinc, as do many other regulatory proteins. Zinc is also paired with copper in the anti-oxidant protein copper/zinc superoxide dismutase, which has been implied in cellular aging. Its mutant forms have been linked to neurodegenerative diseases such as amyotrophic lateral sclerosis.

Metals are also increasingly used in diagnostic or therapeutic agents for the study or treatment of diseases. Quantitative study of the redistribution of trace elements in response to challenges provides important information about functions and pathways of metalloproteins and allows the cellular targeting of therapeutic approaches to be studied. For example, Cisplatin, with platinum as its active ingredient, is a major chemotherapeutic drug, and numerous metal-based active agents are being actively researched as new drugs (e.g., ruthenium-based drugs). Magnetic resonance contrast-imaging agents are often metal-based. Some are in routine use (e.g., gadolinium-based agents) and others are in the R&D pipeline (e.g., Vanadyl-based compounds). X-ray fluorescence imaging can be used to understand and help model the behavior of new imaging agents at the intracellular level. Similarly, novel nanocomposites combine therapy with diagnosis ("Theranostics") and these are often metal-based.

Trace metals play a major role in plant systems that directly impact human health. All human food is sourced either directly or indirectly from plants, yet in some areas, staple foods lack the required trace metals. Deficiencies lead to numerous diseases and can further exacerbate the effects of toxic trace metal exposure. For example, selenium deficiency is believed to be an underlying factor in arsenicosis (arsenic poisoning resulting from drinking arsenic-rich water over a long period of time) and cancer. Genetically engineering plants to increase nutrient uptake could, for example, ensure that pregnant women in underdeveloped countries get adequate amounts of iron. On the flip side, inhibiting the uptake of toxic metals by food plants could reduce toxicity and, thus, illness.

X-ray fluorescence microscopy offers a unique way to quantitatively image trace metals within whole cells and tissue sections (Fig. 13) with sensitivity about 1,000 times that of electron microprobe analysis. Characterization of precise metal concentrations, their spatial distribution, and chemical speciation in individual cells and cell compartments will provide much needed information to explore the metallome in health and disease, in both mammalian and plant systems. Although transmission electron microscopy offers unparalleled spatial resolution for structural studies of ~100-nm-thin sections and isolated macromolecules, x-ray nanoprobes are able to image whole cells and tissue sections up to many tens of micrometers thick and in three dimensions, thus placing trace metals firmly in their physiological context. The APS already plays a leading role in x-ray fluorescence microscopy studies of trace elements in biological systems. With the increased brightness provided by the APS-U, improved efficiency of nanofocusing optics, and other advances described in the computation and instrumentation part of this facility plan, a roughly 1,000-fold increase in the focused flux is expected. This increase can be used for some combination of improved spatial resolution, trace element sensitivity, increased field of view, and/or improved statistics in quantitative studies involving multiple cells. As an example, the proposed APS Upgrade will enable the acquisition of a dataset such as the zebrafish embryo in Figure 5.1.3.4, to be imaged at 100-nm spatial resolution across the full three-dimensional field of view compared to the current 2-5 µm. In addition, common laboratory user facilities for preparation and loading of pressure cells, as well as loading of radioactive samples, will be implemented.

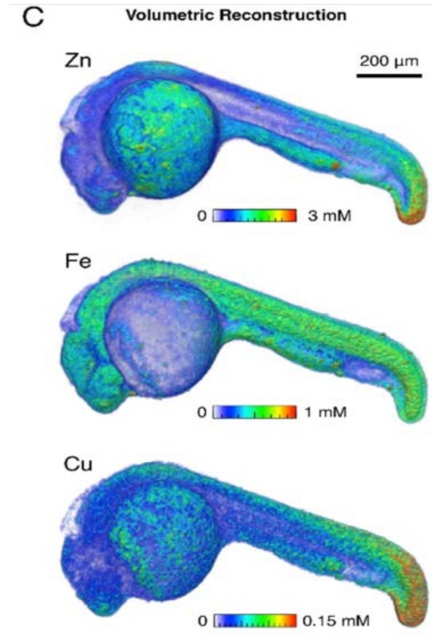


Fig. 13. Fluorescence tomographs of the trace metal distribution in zebrafish a model system. [D. Bourassa et al., Metallomics **6**(9), 1648 (2014)].

5.2.3.4 Environmental Science and Geoscience

Environmental and geoscience systems are inherently complex, heterogeneous, and multi-component. A Grand Challenge is to develop integrated characterization and modeling of such systems at multiple length scales, ranging from atomic (for example, arsenic chemical binding changes as revealed by x-ray spectroscopy, and mineral phases as revealed by diffraction) to mesoscopic and macroscopic (for example, interactions of radioactive materials with sandstones and shale). This knowledge can help optimize the cleanup of wastes from DOE nuclear legacy sites by exploring how subsurface bacteria change the chemistry of their environment and thus affect mineral speciation and precipitation. Understanding the spatial distribution of nuclear wastes is critical to developing effective plans for remediation of contaminated sites.

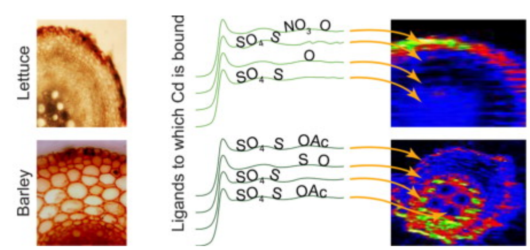


Fig. 14. Spectromicroscopy of Cd contamination in different parts of the plant roots of Barley and Lettuce. [Akhter et al., Env. and Exp. Botany **100**, 10 (2014)].

Spectroscopic methods provide atomic-scale understanding of bonding and valence even for very dilute components, while imaging and scattering techniques extend the characterization from the nanoscale to the bulk (centimeter) scale. A strength of fluorescence detection methods is the ability to detect hazardous elements at very low concentrations. Spectro-microscopy measurements in Fig. 14 show a distinct difference in the uptake of Cd by barley and lettuce. These can be explained by differences revealed in the bonding and transport of the Cd in the plant roots. The APS provides the high flux at high energies (here, E > 27 keV) that make such measurements possible. A crucial strength of high-energy x-ray methods is the ability to study samples *in situ* and at extremes of temperature and pressure.

Geological problems frequently involve complex dynamic systems undergoing physicochemical modifications to their constituent minerals, including fluid phases, under high pressure and high temperature. Better characterization of these systems is needed for better understanding of phenomena such as geological instabilities (mudslides, earthquakes), energy extraction (hydrocarbon and geothermal heat), and ore formation and environmental concerns (CO_2 sequestration and contaminant pathways). Such information is crucial to understanding the fundamental mechanisms that govern such geological systems with *in situ* environmentally controlled experiments. Key pieces of information relate to the three-dimensional distribution of mineral phases and fluids and to dynamic changes in these during fluid infiltration, mineral reactions, and deformation processes. **Fig. 15** shows the pore structure evolution during mineral carbonation of olivine that is obtained from time-resolving microCT (4D microCT). Further *ex situ* nanoCT results of olivine aggregates harvested from 4D microCT suggest the magnesite precipitates in the original olivine grains create transecting channels inside olivine grains, which implies a mechanism for self-sustaining reaction.

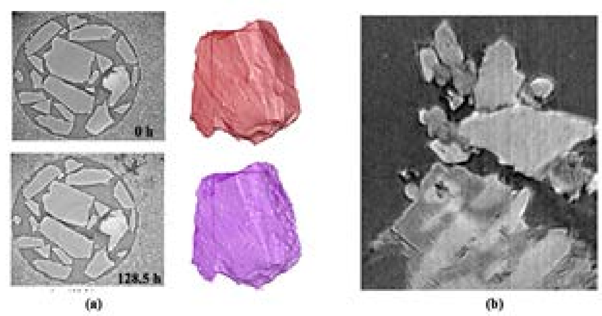


Fig. 15. (a) *In situ* microCT investigation on the pore structure evolution during mineral carbonation of olivine. (b) *Ex situ* nanoCT imaging of the olivine aggregates [W. Zhu et al., Geophys. Res. Lett. **43**, 9535 (2016)].

The APS-U will provide many opportunities for further improvements. Imaging and microprobes will directly benefit from the increased brightness: 10x better resolution or 100x flux for the same spot size, thus yielding lower detection limits, faster scanning, and access to studies at more extreme conditions with smaller beams. In addition to the high spatial and temporal resolutions enabled by the APS MBA source, the high coherence of the beam will also increase the sensitivity in discriminating between different mineral phases. As shown in Fig. 15(b), it is difficult to distinguish olivine from magnesite. With an increase of beam coherence and sensitivity from the upgraded APS source, it is possible to discriminate mineral phases with small density differences, enabling the study of subtle changes that characterize many geological systems.

Another opportunity is the significantly improvement of x-ray absorption near edge structure measurements of environmentally important elements (e.g., Hg and Pb) with high-energy resolution fluorescence detection. This can dramatically improve the resolution of the edge structure with a corresponding improvement in chemical sensitivity. The crystal analyzers needed for such measurements are inherently less sensitive, and currently the spatial resolution for sensitivity to 10-100 ppm levels is limited to ~20 μm. The smaller x-ray beam sizes provided by the APS-U, and continued improvement in analyzer crystals and design, should enable parts per million-level sensitivity down to the sub-micron length scales.

5.3 Method and Technique Developments for X-ray Science

The APS is moving toward a point where beamline instrumentation will be viewed less as an assortment of individual components, but rather as a tightly integrated unit, spanning from source to optics to sample to detectors, held together by effective and smart controls and seamlessly coupled with analyses and visualization. New analysis methods suggest innovative ways of performing experiments with flexibility, speed, and capabilities that were not possible only a decade ago. For example, four-dimensional imaging and video-rate scanning probe microscopy are becoming realities, and will be substantially enhanced by the incorporation of a MBA lattice at the APS. As previously pointed out, the APS-U will dramatically improve coherence- and high-energy-based techniques such as hard x-ray nanoprobes, x-ray photon correlation spectroscopy, coherent diffractive imaging and ptychography, and nanoscale high-energy diffraction and scattering. Advances in x-ray methods are required to optimally use these capabilities after the APS Upgrade. Therefore, we are developing new approaches to x-ray science that take a more holistic view of experiments, starting at the initial experimental model, all the way through experiment setup, control, data acquisition, analysis, and visualization. These include

- Fast, flexible, precise, and "intelligent" data acquisition systems, so that:
  - data acquisition time is only spent on relevant areas of interest
  - can achieve highest spatial resolution, sensitivity (e.g., < 5 nm positional control at 1kHz)
- Streaming acquired data directly into analysis so that data and computationally-intensive tasks required to evaluate and interpret the data can be carried out to enable an interactive optimization of the data acquisition route
- "Intelligent" analysis algorithms that can:
  - provide (preliminary) real-time results to drive measurements
  - determine and correct instrumental imperfections and errors
  - discover "hidden" correlations in complex multimodal, multiscale data

The APS is also developing new instrumentation platforms and infrastructure that are capable of fast data acquisition at the required speed, stability, precision, frame rate, etc. Specific examples include:

- High-speed scanning (< 5 nm, > 1 kHz), on a high-stability platform

Novel optics (wavefront preserving mirrors, nanofocusing optics, and zone-plate optics and microelectromechanical systems)

- optics in collaboration with the Argonne Center for Nanoscale Materials for timing experiments
- Energy-resolving detectors (e.g., based on transition-edge sensors (TES))
- Data handling (acquisition, transfer, reduction) at multiple GB/s per experiment sustained over weeks or with burst rates orders of magnitude faster.

Taken together, this set of thrusts will enable innovative x-ray techniques and scientific approaches that are orders of magnitude faster and more sensitive than those available today. In particular, the upgraded APS, coupled with advances in detectors and x-ray optics, will create a clear opportunity for direct imaging to spatial resolutions of 5 nm and below, and the 1-nm length scale using ptychography, approaching single atom sensitivity. It will also allow unprecedented fidelity in imaging extended three-dimensional volumes. For example, the APS-U will deliver the coherent hard x-ray flux enabling to image samples 1 mm^3 in size at three-dimensional resolutions of 10 nm, corresponding to 10^{15}(!) voxels in less than one day – we will work to develop analysis methods so that reconstruction can happen on the same time scale.

5.3.1 Hard X-ray Nanoprobes

Hard x-ray nanoprobes focus the coherent x-ray beam into a diffraction-limited spot through which the sample is raster-scanned. A variety of detectors provide a custom combination of contrast modes, including absorption, phase contrast, x-ray fluorescence (trace element mapping), and diffraction (structural information including stress and strain). In combination with sample rotation, these contrast modes can also be used in tomographic reconstructions. At the APS, nanoprobes use either zone plates to produce x-ray beams down to 20 nm in size or achromatic Kirkpatrick-Baez mirrors to focus down to 100 nm. Additionally, a multilayer Laue lens-based prototype microscope has demonstrated spatial resolutions better than 30 nm with 17% efficiency at 20 keV.

The proposed APS Upgrade will revolutionize scanning x-ray microscopes. The increased brightness provides a 100-fold increase in focused flux and correspondingly faster data acquisition (and facilitates multimodal inclusion of other brightness/coherence driven techniques such as lens-less imaging). This enables the routine use of tomographic approaches to study extended objects in 3-D at the highest spatial resolution. Combined with advanced data analysis techniques now under development that will further reduce the required x-ray dose per projection, this will enable, for the first time, high-fidelity tomographic datasets with 20-nm spatial resolution and much larger fields of view (millimeters). We will develop methods to zoom in and out for region of interest to reduce the x-ray dose as low as possible and reduce the data amount to the relevant part. Considerable R&D is required to exploit the scientific opportunities an upgraded APS provides.

R&D Work

- Stable, rapid-scanning nanoprobe platforms: a joint need applicable also to coherent diffraction imaging and ptychography.
- Development of focusing optics to achieve high spatial resolution at high efficiency (e.g., 5 nm with diffractive optics, 10 nm with double graded multilayer mirrors)
- Algorithm development for data analysis, e.g., fast imaging and dose reduction using compressed sensing-based techniques
- Routine multi-mode, multi-scale data acquisition
- Detectors with the highest spectroscopic energy resolution (e.g., TES detectors with an energy resolution E <= 1 eV would enable imaging not only elemental content but also chemical state at the native instrument resolution, which could be as low as 5 nm with the APS-U).

5.3.2 High-Speed Imaging and Diffraction

High-speed imaging and diffraction experiments take advantage of the time structure of the APS storage ring to achieve exposure times as fast as 100 ps (single pulse, APS-U: 200 ps) and repetition intervals down to 153 ns (APS-U: 75 ns) to visualize fast processes in thick materials and complex environments. High-speed cameras coupled with x-ray scintillator screens and intensifiers provide full-field imaging capability up to 6.5 MHz at 1-μm resolution in both absorption and phase contrast mode. In addition, it is possible to visualize diffraction signals at comparable time scales, enabling the visualization of fast crystallographic changes in samples. In combination, these techniques attract a broad user community to study a range of transient phenomena in hard and soft condensed matter, such as flow in granular systems, controlled solidification in metals, mixing dynamics in fluids, effects of injector design on fuel spray formation, and electro-catalysis evolution on semiconductor interfaces; particular excitement has been generated in the area of additive manufacturing (see Fig. 16).

The proposed APS-U will further enable high-speed imaging and diffraction techniques. Implementation of Kirkpatrick-Baez mirror-based cone-beam projection will extend the achievable spatial resolution for fast imaging to >100 nm while still preserving the single-pulse time resolution. This new capability will enable hierarchical characterization of dynamic systems and materials. A proposed dual beam operation achieved by canting the two existing undulators will also allow for simultaneous imaging and diffraction characterization.

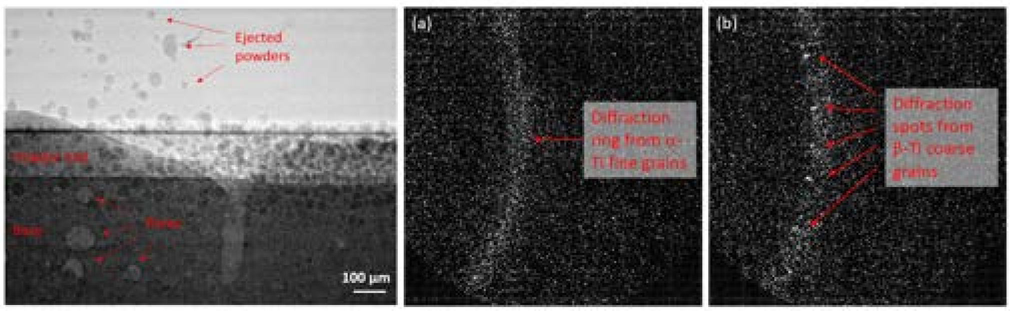


Fig. 16. Dynamic x-ray image of laser additive manufacturing showing the powder ejection and porosity generation (left) and dynamic x-ray diffraction of a Ti-6Al-4V sample at different cooling stages (right). These types of data require the development of advanced algorithms for segmentation and feature labeling.

R&D Work

- Development of advanced data analysis methods for data reduction (segmentation of structural defects, feature labeling, porosity distribution calculation etc.) and for multi-modal data analysis.

5.3.3 X-ray Photon Correlation Spectroscopy

X-ray photon correlation spectroscopy uses coherent x-ray scattering to provide sensitivity to the time dependent spatial arrangement of particles within the coherently illuminated sample volume, yielding a complete picture of the structural dynamics in a sample. This information manifests itself in the x-ray scattering image as bright and dark intensity modulations, called “speckle.” Fluctuations in the structural, chemical, or magnetic order in the material result in fluctuations in the speckle pattern. The time scale on which one can record these fluctuations is presently limited in the small-angle scattering regime to the millisecond range by detector readout rates and at wide angles to the range of seconds by coherent photon flux. The 100-fold increase in source brightness provided by a MBA lattice will provide increased dynamic range and potentially reach simultaneous time and space resolutions of a nanosecond and a nanometer.

The APS offers users the property of relatively bright bunches separated by relatively large pulse separations (~100 ns). While the APS is typical among many third-generation synchrotron sources in having x-ray beams with a transverse coherent fraction of ~10^{-3} and pulse lengths of ~100 ps, the APS Upgrade will have a unique transverse coherent fraction of 0.10 at hard x-rays of 10-keV photon energy. The APS will develop XPCS and time-resolved coherent scattering methods to access a uniquely broad span of time delays encompassing 100s of nanoseconds to 1,000s of seconds. To reach these x-ray photon-limited specifications, considerable R&D in detectors and data analysis/computation is required.

R&D Work:

- High-performance computing workflow development, live big data/HPC processing of detector data streams is required, including compression, sparsification, and correlation computation.

- Detector development: Optimized photon counting detectors will feature high-gain, low-dynamic-range pixel detection, dead-time-less readout, shaping times less than the bunch spacing to prevent pileup, frame spacing of one turn (3.5 µs), and sparse readout. An R&D effort in this direction includes the vertically integrated photon imaging chip detector with on-chip data reduction.

5.3.4 Coherent Diffractive Imaging and Ptychography

Coherent diffractive imaging, a lens-less imaging technique, uses coherent x-ray scattering and iterative-phase retrieval to provide two-dimensional and three-dimensional images with a resolution that is only diffraction and dose limited. Coherent diffractive imaging, a reciprocal-space technique, has demonstrated a world-best resolution of 3 nm using a 1-µm spot size on an isolated object [Takahashi et al., Phys. Rev. B **80**, 054103 (2009)] and with ptychography, e.g., use of overlapping measurements on an extended sample for phase retrieval, and a resolution of 5 nm using a 60-nm spot size in two dimensions [Shapiro et al., Nat. Photonics **8,** 765 (2014)], and 16 nm in three dimensions [Holler et al., Nature **543**, 402 (2017)]. With extended depth of focus, one can envision imaging extended three-dimensional objects with 5-nm voxel sizes. These (present-day) heroic experiments will become routine with the proposed upgraded APS and the planned R&D outlined here.

Coherent diffractive imaging will be transformed by the proposed upgraded APS, where the increased brightness provides a ~200-fold increase in coherent flux. Combined with a recently developed efficient ptychographic reconstruction method that is also ~200 faster [Nashed et al., Opt. Express **22**, 32082 (2014)], this will revolutionize experiments. The APS staff aspires to reach a routinely attainable resolution of 2 nm on an extended sample with ptychographic techniques by investing further in instrumentation, data analysis, and computing capabilities.

Considerable R&D is required to exploit the scientific opportunities an upgraded APS will provide in the area of nanofocusing. The scanning microscopes at the APS use scanning systems that are compatible with per-pixel dwell times of about 1 msec or longer; the scanning nanoprobes typically provide stability at the 10-nm level and below. To make full use of an upgraded APS, per-pixel transit times must be up to a thousand times shorter, and positioning accuracy needs to become ten times smaller. This speed-up in data collection necessitates considerable R&D for improved data analysis and computation and detector data pipelines, which has been started.

R&D Work:

- Develop a rapid-scan nanoprobe platform (jointly with nanoprobes).
- Advanced metrology for precise monitoring of beam, and sample geometries to feed analysis (jointly with nanoprobes).
- Experiment-aware algorithm development for data reduction and analysis: Development of phase retrieval algorithms that are able to handle experimental uncertainties, photon statistics, and beam fluctuations is required.
- Workflow and data pipelines: As data rates increase at least 100-fold due to the increase in brightness with the proposed APS Upgrade and improved detectors, automated, routine high-performance computing-type data processing and related data, network, and computing infrastructure need to be implemented.

5.3.5 Nanoscale High-Energy X-ray Diffraction

The bulk penetration of high-energy synchrotron x-rays, and the easily accessible large reciprocal space, combined with high spatio-temporal resolution, provides unique capabilities for non-destructively measuring the phase, texture, and strain distribution of real-life polycrystalline aggregates under relevant *operando* conditions, such as high pressure, thermo-mechanical loading, or irradiation.

The APS provides users with several leading high-energy structural characterization tools for probing bulk systems. The methods range from high-resolution diffraction probing long-range order to total scattering/pair distribution function sensitive to nearest neighbor ordering, from SAXS providing the shape and size of particles to imaging by phase contrast tomography and high-energy diffraction microscopy. These techniques are frequently used in combination with each other to provide hierarchical information across a broad range of length scales from the same micron-level volume. Understanding the dynamic mesoscale behavior of such systems and how the individual crystalline grains interact, grow, reorient, and redistribute stresses requires further improvements in spatial resolution from the current few-micron spot size. The APS Upgrade will enable just such capabilities since the dramatic increase in brightness can directly translate into significantly smaller high-energy beams with increased flux. However, realizing nanoscale beams will require commensurate improvements in high-energy optics. As the photon energy increases, deploying efficient x-ray focusing optics becomes more challenging due to the increasingly finer features required for fabricated structures, the weaker refractive effect, and smaller incidence angles. Research and development is required to advance flexible high-energy optics capabilities to take full advantage of an APS upgraded with the MBA lattice.

R&D Work:

- Refractive high-energy optics: Develop refractive lenses to provide 0.2- to 1-µm beams for high-energy applications (50-100 keV).
- Reflective high-energy optics: Focusing schemes utilizing multilayer optics in Kirkpatrick-Baez geometry may provide a route toward nanoscale focusing at high x-ray energies; manufacturing such optics will be developed by the X-ray Science Division (XSD) Optics Group in collaboration with APS staff at high-energy beamlines.
- Analysis and management of large data sets: The increased resolution that will be provided by the MBA lattice for techniques such as high-energy diffraction microscopy, coupled with faster detectors for dynamic measurements, will lead to extremely large data sets (>10 TB/day). New integrated approaches toward both data handling and processing that use high-performance computing in near real-time are being pursued, including pilot projects that make use of the leadership-scale computing facilities.

5.4 Enabling Technologies for X-ray Science

Science at the APS relies heavily on beamline and end-station instrumentation: optics for x-ray energy, bandwidth, and coherence selection and focusing; detectors for photon counting, dispersive analysis, and imaging; and experimental equipment for providing a wide range of environmental conditions as well as sample and detector positioning. While preparing for a proposed MBA-upgraded APS, new instrumentation and techniques must be developed to fully exploit the new source parameters and make optimal use of the revolutionary 100-1,000-fold increase in brightness, coherent flux, and detected signal. Many of the planned improvements will impact multiple beamlines; those deemed a priority for R&D investment during the next five years are highlighted in the sections below.

5.4.1 Optics

Achieving the mission of the APS requires high-quality x-ray optics (such as monochromators, mirrors, and focusing optics) to deliver x-ray beams to the samples and, in many cases (e.g., with crystal analyzers) to collect the relevant signal from experiments. Both the APS-U feature beamlines and the existing APS beamlines will require a new generation of x-ray optics that will take full advantage of the ~100-fold increase in brightness, smaller source size, and increased coherence enabled by the APS-U. The XSD Optics

Group coordinates with other XSD Groups, APS beamline scientists, the user community, and other DOE light source facilities and leverages unique APS R&D capabilities to develop the required next-generation optics. Priorities are centered on the key areas of high-performance focusing optics for current and future APS needs and wavefront-preserving optics (novel crystal optics, mirrors, and adaptive optics) and are made possible by the continued development of optics tools and techniques: design, fabrication, optical and at-wavelength characterization and simulation.

Optics Group R&D goals for the next 3-5 years include:

- Develop state-of-the-art focusing optics, including diffractive optics and high-precision mirrors. To exploit the MBA lattice, the ptychoprobe will require highly-stable optics capable of focusing the beam to 5 nm. This capability will allow the APS to achieve the highest possible sensitivity to trace elements, and to use ptychography to push the spatial resolution for structural components to its ultimate limit. Three optical elements have been identified to achieve the desired resolution, provided appropriate investment in staff and equipment is available.
    - Multilayer Laue lens, pursued in collaboration with the NSLS II.
    - Advanced zone plates: The APS has been developing stacked zone plate systems to achieve <20 nm at >20 keV, and is pursuing approaches that could lead to 5-nm spatial resolution.
    - Double-graded multilayer focusing mirrors: The Modular Deposition System is designed to develop such optics; we plan to use the system *in situ* metrology and ion beam figuring capabilities to push toward 10-nm spatial resolution.
    - Focusing optics for 40-100-keV x-rays to < 1 µm.
- Develop novel crystal optics for wavefront preservation and for imaging and high-energy resolution.
    - R&D on crystal optics to achieve < 10-meV resolution for resonant inelastic x-ray scattering.
    - Wavefront preserving crystal optics for coherence-based beamlines.
    - Crystal optics for high-energy x-rays, E > 40 keV.
    - Develop high-performance reflective multilayer coatings to increase flux on the experiment.
        - High-performance multi-stripe multilayer monochromators.
        - Engineered bandpass (> 2%) multilayers (maximize flux).
        - Narrow bandpass (< 0.5%) multilayers (increase flux, at improved bandpass).
- Develop adaptive optics and beam wavefront sensing and correction.
    - Develop advanced simulation and characterization tools to support in-house optics design and development, and efficient implementation of APS and APS-U beamlines.

5.4.2 Detectors

While impressive breakthroughs in x-ray sources provide the powerful illumination needed to peer into the nano- to mesoscale world, a stumbling block continues to be the distinct lag in detector development, which delays experimental progress. The mission of the XSD Detectors Group is to deliver cutting-edge detectors to APS beamlines to advance their scientific productivity.

The mission is accomplished in two ways. First, the Detector Group introduces new, cutting-edge commercial detectors to the APS community via the Detector Pool, which provides early access to new detectors that come on the market and thus facilitates their adoption. The Group also provides technical detector advisory services in a variety of ways (e.g., market research, design reviews, etc.) to assist beamlines with detector purchases and best detector practices. Second, the Group develops new, cutting-edge detectors where commercial investment is unlikely. It is engaged in detector R&D projects to meet the future needs of the APS. These projects align with the major scientific thrusts of the APS and the APS-U, taking advantage of the APS source, leveraging strategic partnerships with U.S. domestic detector groups, and taking advantage of unique Argonne facilities.

The detector R&D efforts are focused in three areas: pixel array detectors, high-energy sensors, and emission detection. The approach to the next generation of pixel array detectors is to contribute DAQ Electronics and system-level expertise to collaborations with external detector groups. Currently, this includes the vertically integrated photon imaging chip detector for ultra-fast XPCS with BNL and FNAL. In the future, this may also include the MM-PAD detector with Cornell University. For high-energy sensors, the APS is collaborating closely with the NSLS-II detector group on the Germanium strip detector for high-energy spectroscopic applications, and is contributing system-level design and software expertise. Finally, for emission detection, the group is collaborating closely with the National Institute of Standards and Technology and SLAC National Accelerator Laboratory on transition edge sensors for high energy-resolution emission detection applications, and currently contributing thick x-ray absorber fabrication, TES/SQUID testing, DAQ electronics and software expertise. Recently, the detector group has expanded into application-specific TES sensor fabrication and system-level design.
The APS Detectors Group's 3-5 year goals include:

- Expanded selection of integrating pixel array detector in the Detector Pool
- Deployment of two germanium strip detectors
- Deployment of a megapixel-scale vertically integrated photon imaging chip detector
- Deployment a hard x-ray TES spectrometer
- Identifying new-generation detector R&D projects, e.g., extensions of existing projects or new projects aligned with the major scientific thrusts of the APS.

5.4.3 Scientific Computing

All aspects of APS operation depend on computation, but data acquisition, management, analysis, and computing infrastructure are of particular importance for facility productivity. Demands for increased computing at the APS are driven by the need to satisfy new scientific opportunities, which are created by new measurement techniques, technological advances in detectors, multi-modal data utilization, and advances in data analysis algorithms. The APS and Argonne are particularly well poised to employ advanced computing to maintain a world-leading position in the synchrotron community. The APS has a world-class photon science program with a large and diverse user base, and Argonne is home to world-leading supercomputing infrastructure and computer science expertise in the Computing, Environment, and Life Sciences Directorate (CELS). The APS is the only world-class synchrotron source to be co-located with a leadership-scale computing facility; Argonne has 3 of the 150 fastest computers in the world. This colocation provides an unprecedented opportunity for collaboration, and is in addition to leveraging synergies with other parts of Argonne, across the BES and DOE complex (e.g., the National Energy Research Scientific Computing center, the NSLS II), and with the outside community.

The APS has organized the core groups required to achieve these goals under the X-ray Science Technologies umbrella within the XSD. The XSD Beamline Controls Group is responsible for beamline data acquisition through control and operations systems and software. The XSD Computational X-ray Science Group is mainly responsible for the development of theory, mathematical methods, algorithms, and prototype software, and collaborates with internal and external organizations. The XSD Scientific Software Engineering & Data Management Group is responsible for software engineering for data analysis and data management tools, enabling high-performance computing, and generalizing scientific code. The management and support of information technology resources within the APS is handled by the APS Engineering Support (AES) Division Information Technology and Information Solutions Groups.

Recent and future developments of source, optics, and detectors are leading to ever faster increases in the ability to investigate samples, as outlined above. This leads not only to data rates increasing faster than Moore's law (and significantly increased data volumes), but also increasingly complex data (multi-scale in both spatial and time domains, multi-mode, multi-instrument, multi-dimensional – 4, 5 …). To make full use of the instrument capabilities, and address todays scientific challenges, a new generation of data acquisition, management, visualization and analysis tools is required. Software must be able to interpret data, identify and classify object types within datasets, and enable researchers to ask complex questions on complex data sets across multiple instruments. Software also needs to "drive" the acquisition of data, to answer the scientific question within the radiation dose limits of the sample, as well as to correct for inevitable instrumentation errors and imperfections. Modern software approaches such as data mining and deep learning need to be incorporated through the integration of the developed software with database organization of datasets, to probe and correlate very large datasets potentially acquired over several years, spanning multiple instruments and user groups. As this work is pursued, and instrumentation is upgraded, continued innovation in the area of data acquisition is required, and corresponding software tools must be developed to tackle the increased complexity and variety of the information gathered.

In order to meet these needs, effort in this area prioritizes:

- Modernize APS data acquisition capabilities.
- Prototype experiment control software enabled for adaptive feedback.
- Continue to develop high-performance, computing-enabled software for fast analysis, prioritizing high-energy, high-brightness, and coherent x-rays.
- Further implement facility-wide data management and distribution services.

In practical terms, strategies for increasingly rapid, complex, and flexible data-acquisition represent significant new requirements for custom beamline electronics. For example, on-the-fly ptychotomography requires nanometer monitoring of the spatial location of a rotating object at speed. Tagging acquired data with (X, Y, Θ) requires custom electronics and data-acquisition hardware. A recent field-programmable gate array development (**softGlueZynq**) promises support of this kind in a standard platform that is readily deployable and easily customized for this and many other anticipated requirements. An objective of this development is to learn how to continue to deliver custom beamline electronics as in the past: on demand, with short development, deployment, and modification cycles.

Beamline Control and Operations 5-Year Goals.

- Develop and implement modern, high-level graphical user interfaces.
- Develop general-purpose automation tools, including improved remote access and mail-in capabilities.
- Develop modern diffractometer control and data acquisition software (e.g., implement Bluesky) for both routine operations and to provide real-time feedback and adaptive control.
- Intelligent data acquisition: real-time feedback and adaptive experiment control
  - Develop high-speed signal handling that integrates motion, acquisition, and detector controls to expand beyond current capabilities.
  - Integrate data acquisition with online data analysis tools and high-performance computing software for fast analysis.
  - Develop a generic mechanism to provide real-time feedback to adjust experiment parameters (e.g., using Bluesky in collaboration with NSLS II).
  - Provide easily configurable, hardware-based acquisition and feedback solutions using field programmable arrays/softGlue.

Algorithms and Data Analysis 5-Year Goals:

- Research and develop new algorithms for multi-modal data analysis methodologies needed by the APS-U and future beamlines, in collaboration with the Argonne Mathematics and Computer Science Division and Lawrence Berkeley National Laboratory- Center for Advanced Mathematics for Energy Research Applications.
- Create and deploy a robust set of high-performance computing-enabled software tools utilizing the next-generation Xeon Phi processors that address critical needs in coherence, imaging, high-energy, and multi-modal techniques in collaboration with the Argonne Mathematics and Computer Science Division and the Argonne Leadership Computing Facility.
- Integration of general-purpose data streaming, feedback, adaptive control, and verification tools with beamline control software, high-performance computing data analysis software, and data management resources.
- Continue to advance the APS world-class and widely-adopted software packages such as TomoPy and GSAS-II.

Data Management and Distribution 5-Year Goals:

- Continue to develop and refine the APS Data Management System collaboratively with the Globus Services team to enable the automation of data transfer from acquisition systems to distribution and archival systems. In addition, the APS will further develop data analysis workflow tools for the automation of complex and sophisticated data analysis methodologies.
- In order for facility users to fully employ and effectively disseminate their data, full data lifecycle management (from acquisition through publication) is needed. The APS will integrate workflow tools with outside data search and registry services for data lifecycle management (e.g., the Materials Data Facility and the National Institute of Standards and Technology Materials Data Repository). This entails the integration of experiment control software at beamlines with data management tools, the assignment of permissions to data, adding data to catalogs, and integration with user and publication databases. The APS will explore this jointly with the NSLS II.
- Mechanisms for cross-beamline and cross-facility exchange of instrument metadata will be implemented, with initial attention to priority techniques for the APS-U and the NSLS II.

Computing and Network Infrastructure 5-Year Goals:

Routinely utilize high-performance computing resources for big data problems such as high-energy diffraction microscopy (e.g., National Energy Research Scientific Computing Center [NERSC], Argonne Leadership Computing Facility, Laboratory Computing Resource Center, etc.).

- Develop methods (e.g., virtualization and containers) and strategies for on-demand utilization of leadership facilities that have minimal impact on the core missions of those facilities, but allow the APS real-time use for moderate-scale and large-scale computing problems. Deploy collaboratively with the Argonne Leadership Computing Facility, NERSC, Laboratory Computing Resource Center, etc.
- Assess, maintain and expand the capacity of network connections to computing resources at Argonne as needed, and increase APS core network bandwidth to terabit capacity as required by the feature and enhanced beamlines in the APS-U.

5.4.4 Beamline Instrumentation

In order to study real materials under real conditions in real time, experiments must happen under actual working conditions, including pressure, temperature, fields, and environment (e.g., fluids). This task becomes particularly challenging in nanofocusing applications where complex sample environments must be combined with positional stability, minimal vibrations, and short working distances. With the proposed APS upgrade to a MBA lattice, instruments must also be able to achieve unprecedented rapid-scan times to fully exploit beam brightness in nanoprobe experiments.

To preserve the expected high brightness of the upgraded APS beams, the stability of beamline components and optics must be improved. Full utilization of the APS-U enhanced coherence will require development of optics and windows that do not distort the wavefront; several approaches are being explored using windowless-to-air, perfectly crystalline, and amorphous materials.

Beamline instrumentation goals for the next 3-5 years include:

- Develop low-vibration, rapid-scanning, nano-positioning-capable end stations to exploit the upgraded source. A promising approach is the Velociprobe, an ultra-high-resolution ptychographic hard x-ray nanoprobe currently undergoing commissioning at 2-ID-D.
- Develop designs for high-stability beamline components and optics, e.g., for monochromators, mirrors, and slit assemblies to preserve the upgraded beam brightness. Leverage designs developed for APS-U beamlines and implement them at non-APS-U beamlines as appropriate.

6 Accelerator Operations and Improvements

6.1 Introduction

The APS accelerator complex is the backbone of the APS scientific program. It includes a 7-GeV, 1.1-km storage ring operating with a 100-mA electron beam; a full energy booster synchrotron; a 400-MeV particle accumulator ring; a 400-MeV pulsed linac; and an S-band radio frequency (rf) thermionic electron gun. The APS has the largest installed 352-MHz CW rf power system in the U.S. and the second largest installed pulsed S-band rf power system. The APS uses over 1,500 power supplies to power various magnets, supports over 50 insertion devices, and utilizes numerous precision diagnostic devices to maintain beam quality.

Maintaining the high reliability of APS accelerator operations presents significant challenges. The accelerator systems continually undergo improvements directed at meeting new needs of scientific experiments. As already mentioned, the APS is in the midst of developing a technical design for a new storage ring using a MBA lattice. Replacing the existing storage ring with a new ring is foreseen early in the next decade and will result in a dramatic, two-to-three order of magnitude increase of the x-ray brightness. Careful provisions have been made in the Accelerator Systems Division (ASD) strategic plan to align current accelerator improvements and upgrades with the needs of a new ring, thus balancing requirements of current and future APS operations. The strategic plan is based on reaching three primary goals:

- Continue to operate the APS with excellent availability and beam quality
- Prepare the APS accelerator systems and staff for the APS Upgrade
- Pursue research in accelerator science and technology to benefit x-ray science

6.2 Accelerator Reliability

The APS accelerator complex has been in operation for more than two decades. One of the challenges facing ASD is maintaining reliable operation of the complex while preparing for the APS Upgrade. Replacement of obsolete components, end-of-the-lifetime equipment, and consumable parts while maintaining high beam availability is a permanent mission requiring significant resources. The goal of APS staff and management is to ensure that this is done in the most cost-effective and efficient manner. Through dedication to this mission, the APS has become one of the world leaders in accelerator reliability with beam availability above 98%. This involves an on-going interaction of technical staff and management to assess risks to reliable operation and to prioritize activities targeting high-risk issues.

For example, in the area of safety interlocks, the plan is to replace obsolete and life-expired access control interlock system components as well as front-end equipment protection system components. Because of the age and unique nature of many APS systems, spare parts may be difficult to obtain, with long procurement lead times, so maintaining a healthy stock of spares is part of the APS strategy for minimizing machine downtime.

6.3 Accelerator Improvements

6.3.1 Magnetic Devices

The Magnetic Devices Group within the ASD is responsible for all APS magnetic systems, including over 45 insertion devices (IDs) in the APS and is the world leader in superconducting undulator (SCU) development. The ASD continues improving the undulator performance, meeting challenges for the APS and light sources in general. Future work is focused on development of three-way-position revolver undulators, improving construction efficacy of hybrid IDs to meet technical and construction goals for the APS and the APS-U, development of automated ID magnetic tuning procedures, and development of a novel ID mechanical system that would allow faster gap change and better control of “strongback” deformations.

In a preparation to a mass production of hybrid IDs for the APS-U, special attention will be given to development of U.S. industrial partners to handle the majority of ID assemblies outside of the APS. The ASD will continue to improve the planar SCUs and will build a 3.5-m-long SCU with the extended “good field region” using NbTi wire and a thin vacuum chamber. A significant leap in superconducting undulator development will take place and will include the completion of NbTi SCU technology development and transfer of that technology to an industrial partner for SCU fabrication outside of the APS. The ASD will begin using the Nb_3Sn wire and a high-temperature superconductor in a new generation of SCUs, and will continue reducing the fabrication cost.

The ASD will also work on development of special IDs for “fast” polarization control, both SCUs and electromagnetic, on development of IDs with a small period and small gap, and on development of the SCU module suitable for FELs. Benchmarking of the magnetic modeling of SCUs will continue as well as development of the magnet measurements techniques for a short-period, small-gap undulators and SCUs.

Fig. 17. SCU18-2 in Sector 6 of the APS ring (left); the high-temperature superconducting magnet in the impregnation mold (right).

6.3.2 Radiofrequency Systems

The RF Group within the ASD maintains and improves the rf system reliability and lifetime for all of the APS accelerator systems, addressing aging, obsolescence, and performance issues that will allow the existing hardware to provide reliable performance up to the APS-U dark period and beyond. Specific attention is given to identifying and replacing weak and aging components and to proactive maintenance for 352-MHz storage ring rf systems. Replacing the outdated low-level rf components with a modern digital system that utilizes a common platform for the APS 9.77-MHz, 117-MHz, and 352-MHz rf systems is the other goal. The 352-MHz rf test stand is used on a routine basis to condition and test new “green” tuners, couplers, and dampers in order to maintain a stock of conditioned and verified spare parts for the 352-MHz rf cavities. The test stand will also be used to evaluate new and spare klystrons by allowing full-power operation into a 1-MW rf test load. Other development projects include the design of new rf cavity tuner drive motor control electronics and development of a new 352-MHz, 300-kW input coupler to provide increased power handling capability for the booster and storage ring rf cavities. To insure an adequate supply of 352-MHz klystrons into the future, effort is under way to secure a second vendor for these essential devices.

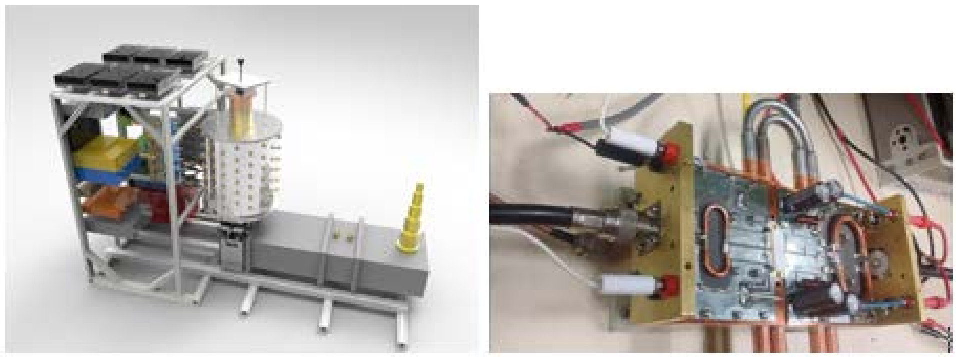


Fig. 18. Left shows a conceptual layout of a Solid-State rf source at 352 MHz. Individual sources at a few kW each feed a combiner cavity that couples power to a waveguide. The right image shows a single 2 kW amplifier developed in the ASD rf Group.

Solid-state technology is being investigated as an alternative to klystron vacuum tubes. Solid-state technology at 352 MHz holds promise to provide higher efficiency, longer lifetime, and lower maintenance costs than traditional klystron power amplifiers. A project centered on development of a small-scale prototype of a 350-MHz, 200-kW CW rf system based on lateral diffused metal oxide semiconductor transistor devices and a resonant output combining cavity is under way. Development of a solid-state, high-voltage mod-anode regulator system is planned to eliminate reliance on the obsolete and unavailable tetrode vacuum tubes presently used for this purpose. A Laboratory Directed Research and Development proposal funded by Argonne has made substantial progress toward a conceptual design for such as system. Shown in Fig. 18 is a concept for development of a test stand in the linac extension area for conditioning of linac structures before installation into the linac. A new thermionic rf electron gun is under development in cooperation with an industrial partner; the existing injector test stand will be used for its testing and tuning before including it into facility operation. Other R&D topics include medium-T_c superconducting cavities based on a thin-film MgB_2, Nb_3Sn and others, photonic band-gap structures, superconducting microwave undulator, THz and sub-THz accelerating cavities, and metallic and dielectric-loaded structures for a wakefield acceleration.

6.3.3 Power Supplies

One of the critical functions of the Power Supplies Group within the ASD is in the area of power supply systems. The ASD will continue to identity and replace weak and aging power supply hardware before it impacts the operations, namely, continue the proactive maintenance, continue thermal imaging program to identify any overheating parts and electrical connections and repair them before an actual failure, and thoroughly test all the power supplies including stress tests during the machine start-up before each user run to ensure reliability of power supplies for the operations. The ASD will continue to closely monitor the conditions of the power supply equipment during operations and schedule repair and replacement during machine interventions for equipment that has signs of elevated temperatures, voltage ripples, and/or communication issues. Examples are rising temperatures of the aluminum electrolytic capacitors in power converters, and communication issues with power supply controllers caused by increased voltage ripples from the low-level control power supplies. Obsolescence of a large number of components is a long-standing issue. Next in line for the ASD is replacing the programmable logic controllers, the GESPAC PS controllers, and digital signal processing controller. Many commercial power supplies in the injectors, particularly in the linac, are close to 30 years old. The plan is to replace the power supplies that are not supported by vendors. New commercial power supplies will not be 100% compatible with the original ones and in-house solutions will be developed, in particular for many kicker power supply systems.

6.3.4 Beam Diagnostics

The ASD Diagnostics Group maintains and upgrades existing storage ring and injector diagnostics systems addressing aging, obsolescence, and performance issues that allow the existing hardware to provide reliable performance up to the APS Upgrade dark period and beyond. More specifically, booster beam position monitors (BPMs) have been migrated to a field programmable gate array-based system, particle accumulator ring BPMs with Libera SPARC electronics have been upgraded as have obsolete BPMs and current monitors in the linac, transport lines, linac extension area. Bunch cleaning was installed in the booster, and obsolete current monitors and flags for beam profile measurements were replaced.

The R&D activities are centered on the verification and testing in Sectors 27 and 28 of the APS storage ring prototype orbit feedback system consisting of new BPM electronics, grazing incidence x-ray BPMs, and a DSP-FPGA-based orbit feedback controller, as illustrated in Fig. 19. Results are extremely promising with demonstration of closed-loop orbit feedback at 22 kHz (the highest of any light source) and a new unified algorithm that combines slow and fast correctors. When R&D is complete, the prototype system will be delivered in FY18 to operations and interfaced with the existing real time feedback system running at 1.5 kHz.

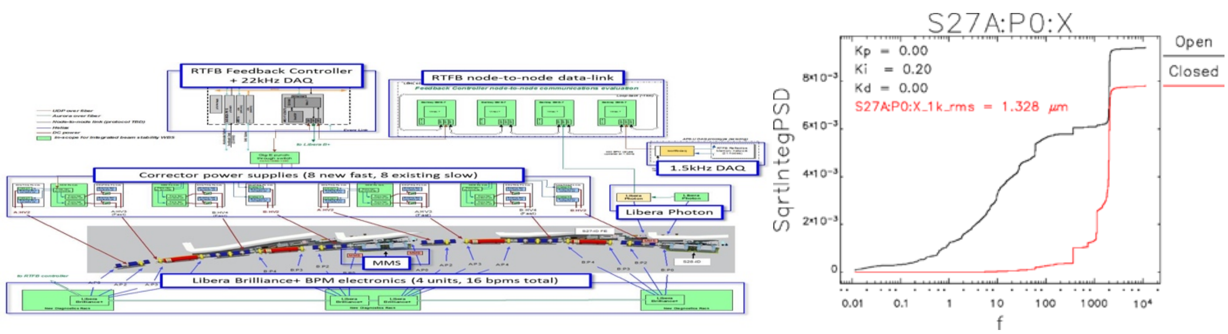


Fig. 19. Layout of the prototype orbit feedback system in Sectors 27 and 28 (left) showing the major components. Right shows the integrated beam motion at the upstream Sector 27 ID rf bpm that meets the horizontal RMS specifications of 1300 nm in the band 0.01 to 1000 Hz. Results of initial testing show the vertical RMS specification is also met over the same band (400 nm).

6.3.5 Accelerator Operations and Physics

The Accelerator Operations and Physics Group within the ASD is responsible for managing reliable operation of the APS accelerator complex, and is the main source of accelerator physics theory and simulation to understand and improve the APS electron beams. A strong emphasis of the Group is thorough automation of machine operation and analysis, since these are key to high reliability. For example, The Group is improving real-time detection and monitoring of malfunctioning power supplies and BPM electronics to further enhance orbit stability by allowing the malfunctioning devices to be quickly removed from the orbit feedback system and facilitate repairs. Other automation improvements include beam dump analysis, injection optimization, and lattice and filling pattern switching. The Group is improving the bunch-by-bunch feedback system targeting operation with a reduced chromaticity in order to improve beam lifetime, in particular in a non-top-up, 324-bunch filling pattern where variation on the synchrotron radiation intensity with the decreasing current affects pointing stability in the users' beamlines.

The ASD is a world-leader in modeling storage ring light sources with the continued development of the *elegant* code and a related suite of tools. The Accelerator Operations and Physics Group continues improving and enhancing high-performance computing accelerator simulations and continues making these state-of-the-art codes available to the entire accelerator community, benefiting many accelerator projects beyond the APS Upgrade. Specific plans include increasing of parallelization in simulation codes and SDDS tools, further development of a graphics processing unit-based version of *elegant*, and continued benchmarking of single-particle and collective effects.

6.4 Accelerator R&D to Advance New Concepts and Next-Generation Light Sources

The APS has an earned reputation for staying on the cutting edge of accelerator science and technology beneficial for Argonne and the other DOE light source facilities. A suite of accelerator R&D programs focused on a versatile, cost effective, and energy efficient future light source ensures that the U.S. and the APS continue to maintain this competitive edge.

The APS core strategy is to perform high-impact accelerator research by concentrating on several areas that maximize key APS strengths: sophisticated, high-fidelity simulation; development of advanced insertion devices; and innovative ideas for improved accelerator performance. While the main path forward focuses on a MBA lattice, opportunities also exist to explore whether the APS can supplement that with additional capabilities for use by specific user groups and for activities beyond the APS Upgrade.

Another component of the ASD strategic plan is innovative accelerator research and development advancing cutting edge accelerator science and technology in the area of synchrotron light sources and other accelerator research areas beneficial for the greater accelerator community. The ASD will continue researching the advanced concepts in free-electron lasers, often jointly with the XSD, The University of Chicago, and groups from SLAC National Accelerator Laboratory, and other institutions. More specifically, the ASD will continue investigating alternate out-coupling schemes to increase x-ray free-electron laser flux and brightness, collaborate with The University of Chicago to fully characterize x-ray free-electron laser stability requirements, and continue working with the XSD to assess diamond resiliency in high-power-density x-ray environments. The ASD also seeks to take maximum advantage of existing infrastructure to preform R&D at the cutting edge of accelerator physics and will fully develop linac interleaving operations to allow a non-mission critical exploitation of the APS injector linac for long-term accelerator R&D in the linac extension area. Specific examples are development of the compact accelerator based on a dual-beam wakefield accelerator technology, development of new wakefield-based diagnostics and instrumentation, and advancing the concept of a tapering, enhanced, stimulated super-radiant amplification among other new accelerator technologies.

7 APS Engineering Support

7.1 Introduction

The AES Division provides engineering, maintenance services, and computing infrastructure in direct support of enabling world-class performance of the APS accelerator and beamline complex, while ensuring a safe environment exists for APS users and personnel.

The support provided by the AES Division includes the following:

- Leading-edge information technology and computer infrastructure through support of networks, servers, data storage, and desktop computers.
- An accelerator controls system that maintains the high reliability of the APS accelerator facilities and plays a leading role in advancing accelerator control system technology.

- Mechanical and operations support services for the accelerator facilities that help the APS achieve its goals for high reliability, high availability, and long mean-time between failures.
- Engineering design and drafting services in support of highly reliable accelerator facilities.
- Precision survey and alignment services essential for the positioning and alignment of the accelerator components.
- Responsibility for work on all radiation shielding safety systems.
- Maintaining a reliable safety interlock system for personnel access control and equipment protection of the APS accelerators to ensure a safe working environment.
- Significant coordination with the Facilities Division in the Infrastructure Services Directorate for APS conventional construction and facility maintenance projects to provide effective and efficient site services.

7.2 Guiding Principles

In the Argonne Hard X-ray Sciences Prime Focus Area developed by the APS, it is noted that the facility is an essential international resource for advancing mankind's science and engineering knowledge across a large number of fields. The APS is also essential to maintaining international leadership in these fields by advancing the forefront of hard x-ray science. The APS is a core capability at Argonne — APS capabilities are a critical enabling component of Argonne's broad R&D programs, and serve an extraordinarily diverse and large user community.

The AES Division is a direct enabler in ensuring the accelerator complex design and facility is safe, operable, and available at a level that permits users to conduct research to enable major scientific breakthroughs.

The goals for FY2017 and beyond required by the AES Division mission are:

- Provide world-class engineering, design, maintenance services, and computing infrastructure in the most efficient manner to enable outstanding user science.
- Provide modern software and hardware systems to sustain excellence in operations and take full advantage of scientific aspirations.
- Enable the realization of the proposed APS Upgrade state-of-the-art designs and future operation through efficient transfer of resources and oversight of performance with the Project.
- Attract, develop, and retain human capital to enable the AES Division mission. Maintain a vibrant, challenging, open, diverse, and inclusive work environment where innovation, excellence, and perseverance flourish.
-

The strategy to achieve the AES Division vision is to concentrate on:

- People: The AES Division staff is key to providing the expertise in system and component design and maintenance for the accelerator complex, including beamline support. Retention of staff is vital due to the facility complexity, demands of the APS Upgrade Project, and unique design criteria and requirements, which are difficult to draw a comparison to in most commercial environments, with few exceptions. Knowledge transfer is crucial as early-career staff are hired to develop system ownership as late-career staff move to retirement. Opportunities must be provided to employees to pursue next-generation designs, as well as R&D efforts, whether on the APS Upgrade, Lsboratory directed research and development projects, strategic partnership projects, or other funding mechanisms.
- The AES Division will make full use of Argonne human resources best practices, including Talent Reviews as well as the performance appraisal process steps to reinforce workforce planning. Critical skills matrices have been developed for the Division to anticipate skill gaps that could form with attrition and plan for training, job rotations, or mentoring to fill these gaps before they materialize.

- Processes: The AES Division must rely on safe, diligent, and thorough processes in the course of daily operations. Convoluted, redundant, and wasteful steps are eliminated, replaced by lean processes that represent a unified APS facility approach, rather than Divisional mandates. Policies and procedures must follow suit in order that a documentation standard is maintained.
- The AES Division is currently undertaking a host of efforts related to APS facility and process improvements. A white paper has been issued proposing enhancements to the design review process as well as the number and type of safety committees in practice. A document management system is well under way, based on best practices gleaned from prior working groups and other DOE laboratories. Lastly, enhancements are being made to the shutdown planning process in order to bolster the fidelity already in place for preparation ahead of the three annual shutdowns.
- Technology: Many AES Division Groups have an implied mandate to modernize legacy hardware and software systems due to obsolescence or driven by increased operating requirements, such as those of the APS-U Project design. Engineering, design, survey, control, diagnostic, and monitoring tools should challenge state-of-the-art principles in support of ongoing operations.
- The AES Division has already implemented state-of-the-art rendering tools for three-dimensional models, instituting a burgeoning reverse engineering capability that has generated substantial demand once publicized, and has started the supply of three-dimensional printing not only for modeling but for use in beamline component installation, drastically reducing conventional production durations. In R&D, the Mechanical Engineering and Design Group has a project under way for acoustic levitation on 2- and 3-axis sample holders as well as developing advanced COMSOL multiphysics simulation predictive capability for next-generation synchrotron light source compact vacuum chambers.

7.3 Implementation

Detailed Group-by-Group summaries that outline how the AES Division will invest in efforts, projects, and people to provide required support to the APS is described in the “APS Engineering Support (AES) Division Strategic and Five-Year Development Plan.” The Group reports outline their respective staff’s mission, operational responsibilities, projects for addressing end-of-life hardware or software concerns, obsolescence issues, infrastructure development needs, R&D undertakings, and direct support of strategic partnership projects like the LCLS-II. Anticipated staffing levels by fiscal year are summarized at the conclusion of each Group report. This plan is a working document and is updated on an annual basis or as needed. It is utilized to guide planning and decision making by the AES Division and the Photon Sciences Directorate management.

AES Division mission readiness involves providing design, maintenance, and operations support for the APS. As the facility nears its 23rd year of operation, this has become increasingly complex for the AES Division. Additionally, the APS Upgrade Project will utilize many existing systems and infrastructure from the current APS facility, so it is in the APS best interest to consistently review, prioritize, and carry out work related to replacement or upgrading components that are obsolete or at their end of life, to ensure long-term mission readiness.

The AES Division makes heavy use of the core APS processes for identifying, prioritizing, proposing, approving, and implementing projects that address the APS facility in primarily four categories: spares and replacement of end-of-life equipment, obsolete hardware, infrastructure development, and hardware improvements or upgrades. Each AES Division Group is tasked with identifying projects in each of the categories above, the estimated resource and materials costs, and risk register ratings captured for consequences of completing or postponing a project and probabilities of these consequences to materialize. Project needs are forecasted out for five years as captured in the AES Division strategic plan.

Projects with significant scope and cost, or far-reaching impact take advantage of a centralized APS process. A board of APS senior management, inclusive of the APS-U, reviews new project requests, rankings, and status of work in progress and then proposes the path forward to the APS Associate Laboratory Director based on the APS strategic plan. Projects at the Divisional level as well as this Directorate review are captured in the same database with reports and a Web interface to view resource and material demands of each project, even if it entails a multi-year implementation effort. Project progress and closeout is tracked in the same database. Upon approval (or postponement/rejection) of proposed projects, summarized minutes and results from this senior management meeting are distributed to appropriate decision makers for transparency and coordination among Divisions.

One example of this type of project with Directorate coordination has been the aforementioned document management system. This project is charged with providing a common interface, network, naming, or identification convention and linked portals to marry together a number of formal and informal databases currently used for document archival and retrieval. This project is nearing 75% completion as of the time of this writing and will fundamentally change how documents are organized, archived, and retrieved within the APS, providing a common framework between APS Operations and the APS-U.

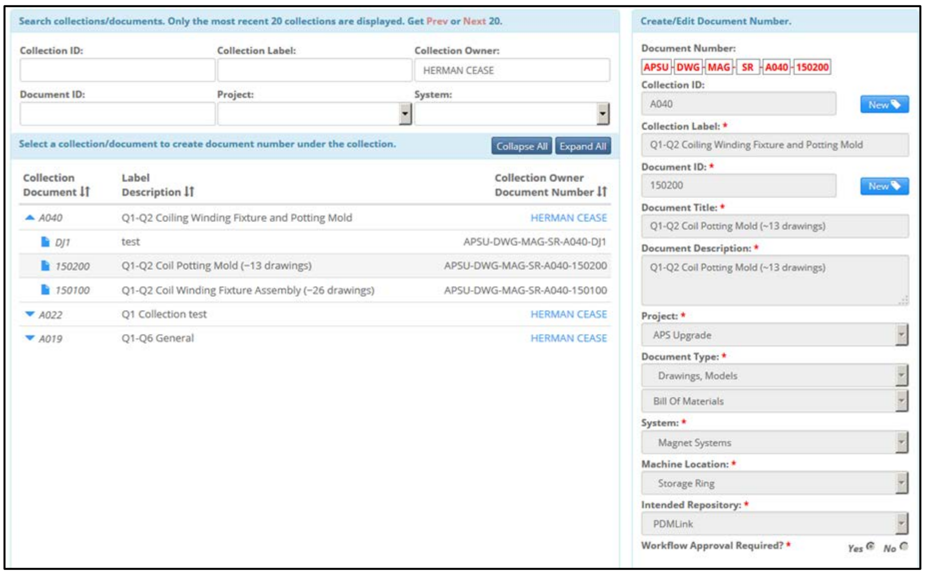


Fig. 20. Document management system simple interface, linking multiple repositories in use at the APS.

Mission readiness also entails consistent interface with projects outside of Argonne and the APS, in support of strategic partnership projects such as LCLS-II. This was highly evident for the AES Division Mechanical Engineering and Design Group in FY16 with the shipment of the horizontal gap vertically polarizing undulator and the continuing work in support of soft and hard x-ray vacuum chambers.

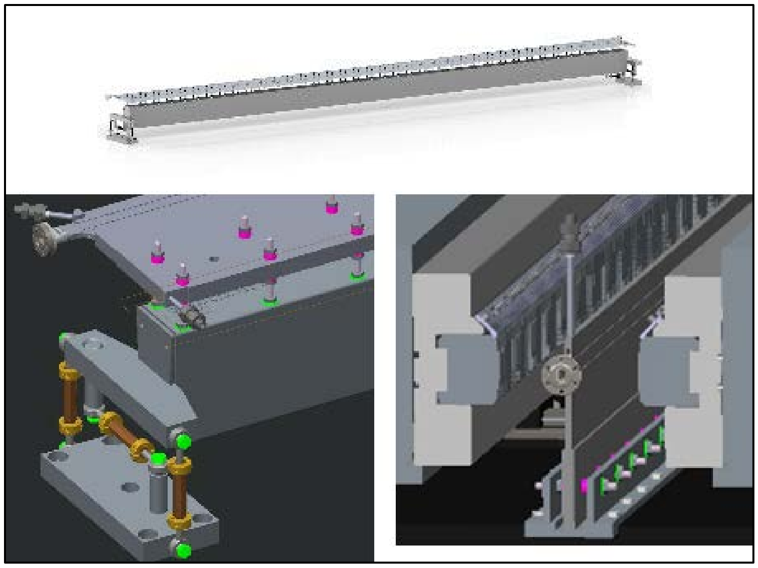


Fig. 21. Vacuum chamber models in support of LCLS-II.

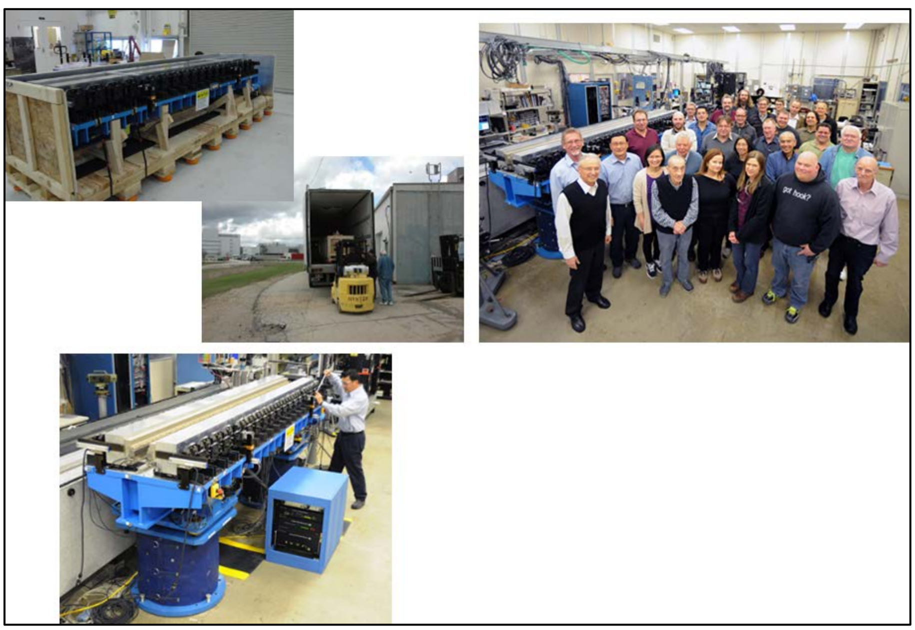


Fig. 22. Horizontal gap vertically polarizing undulator preparation and shipment to LCLS-II.

Within the APS, mission readiness for the AES Division includes anticipation of future facility demands for ongoing operations as well as looking ahead to needs for the APS Upgrade Project. One example of this anticipation was the work largely completed in FY16 for establishing the technical basis as well as the process steps to remove nearly 58,000 lbs. of waste metal from the APS accelerator complex.

This was a significant achievement in heavy coordination and cooperation with many Argonne central services as well as with the DOE Argonne Site Office and headquarters. The establishment of this process laid a foundation for future removal of components and equipment for the APS-U, through continual refinement of this process, now performed at each subsequent shutdown period for ongoing APS operations.

Fig. 23. Material sorted (left) in the 800 Area at Argonne for eventual offsite disposal, after removal from Sealand containers (right) and from the APS accelerator tunnels.

8 Mission Readiness

Mission readiness as defined for the APS facility is the development of projects that anticipate and mitigate risks associated with beamline and accelerator equipment reliability, end-of-life failure, and obsolescence. This approach is applied to all work that will not be included in the scope of the proposed APS Upgrade Project, but that is required for the long-term, reliable operation of the APS.

Mission readiness-related projects for the APS accelerator complex and related technical systems are largely captured in the internal "Accelerator Systems Division Four-Year Development Plan and APS Engineering Support Division Strategic and Five-Year Development Plan." A similar plan has been developed for beamlines and the balance of the facility. Details of mission readiness for beamlines and associated support technical infrastructure (optics, detectors, beamline instrumentation, etc.) is captured by the internal XSD "Beamline Development Projects Document," which details maintenance and obsolescence issues for beamlines and optics support over a 5-year time frame. This document includes both the maintenance and obsolescence projects, and the strategic upgrades and improvements in order to be ready for the upgraded facility.

In order to effectively allocate APS funds (both effort and non-effort) for mission readiness projects, mission readiness categories were incorporated into the APS Integrated Management System.

The Preliminary Design Report for the APS Upgrade was completed in June 2017. As the technical scope of the Upgrade becomes better defined, respective responsibilities, either Operations or Upgrade, for replacing or improving technical systems will follow suit. The two sides of the house will work closely to ensure that the upgraded APS will continue to operate with the reliability of a world-leading facility for the next 25+ years.

9 Infrastructure, General Operations, Support, and Improvements

9.1 (Cost-) Effective Operations

The APS continually pursues top-down and bottom-up mechanisms for assessing the efficiency of APS operations, not only to provide the optimum in user support and mission achievement, but to maximize, to the fullest extent, the investment by U.S. taxpayers.

The APS senior management assessed the APS organizational structure and, following detailed stakeholder discussion and benchmarking against other facilities, developed a structure that is intended to achieve greatly improved accountability, ownership, efficiency, and communications. The principal result of this was the shifting of beamline technology functions from the AES Division to the XSD, and realignment of user program office and user work planning directly to the APS Director's office.

Finance and human resource functions in the AES Division, the ASD, and the XSD were realigned in 2016 so they report to the APS Business Manager rather than the individual divisions. The human resource functions were streamlined so all divisions are served by an APS-level team where each team member has a specialty but can perform all functions. Benefits of the new model include improved workflow, specialized assistance, more backup options, consistent communication within APS regarding human resource topics, and consistent application of human resource and related policies. Argonne moved to a new financial software system in March of 2017, and APS finance functions will be reviewed as the new Argonne-level systems stabilizes, for efficiency and opportunities. The finance team meets weekly to make assure consistent communication within APS regarding financial topics and that the team provides backup to each other as needed.

Effective July 1, 2015, the XSD had been managed through three sections, each headed by an Associate Division Director with full line-management responsibility and accountability: two Beamline Operations Sections and a Beamline Technologies Section, which includes the Optics, Detectors, Beamline Controls, Scientific Software Engineering and Data Management, Computational X-ray Science, and Beamline Instrumentation Groups. However, in order to provide more coherent management oversight, the two Beamline Operations Sections have further been consolidated into a single Section as of the first quarter of FY17; this will be evaluated for sustainability given the number of beamlines operated by the XSD.

The APS improves delivery of core support services through specialized technical groups working in harmony with customers in the APS accelerator and beamline organizations, and with centralized Argonne mission support services. To insure that support services are at once responsive to customer needs and carried out in the most cost-effective manner, the APS employs a work breakdown structure for operations to track effort and integrate this into the APS Integrated Management System. In addition, the APS created a Resource Evaluation Group to help plan and execute projects.

9.2 Data Management and Distribution Facilities

The APS has been working closely with the Globus Services team and the Argonne Leadership Computing Facility to implement and deploy data management tools that integrate with beamline data workflows and large data storage systems. These tools help automate the transfer of data between acquisition devices, computing resources, and data storage systems. Ownership and access permissions are maintained based on an experiment's user group. A metadata catalog allows beamline staff to populate experiment conditions and information for access via a Web portal. Users can download data at their home institutions using Globus Online. Short-term data storage is available within the APS; larger storage systems for longer-term storage are hosted by the Argonne Leadership Computing Facility (Fig. 24). These resources are now available at a number of XSD beamlines: 1-ID-B,C,E, 2-BM-A.B, 2-ID-E, 7-BM-B, 7-ID-B,C,D, 8-ID-E, 11-ID-B and -C, 23-ID-B and -D, 26-ID-C, 32-ID-B,C, 33-ID-D and -E, and 34-ID-C and -E. In the coming years, these tools will be deployed at other APS beamlines. Based on feedback, these resources will be improved with new features and capabilities.

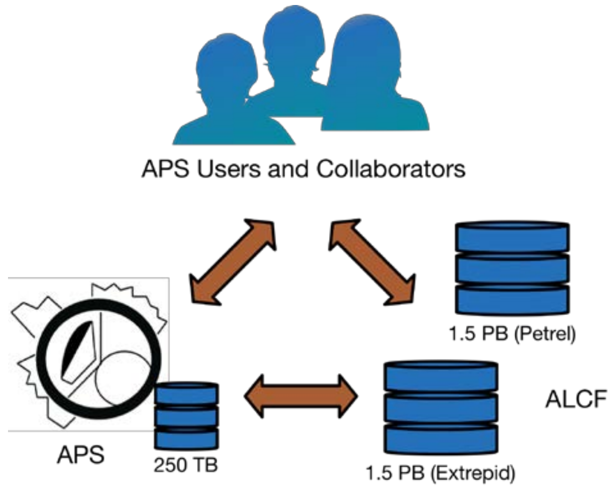


Fig. 24. Data storage options available at the APS. A 250-TB data storage system located at the APS serves short-term needs. The Petrel system housed in the Theory and Computing Sciences building is managed by the Argonne Leadership Computing Facility and provides 1.5 PB of storage. The Extrepid system housed in a Leadership Computing Facility computing center in Argonne Building 369 provides an additional 1.5 PB of storage space for the APS. Data management tools are currently deployed at many APS beamlines that automate the transfer, organization, and distribution of data on these storage systems. APS users and collaborators can access data on any of these systems using Globus Online.

9.3 Network Infrastructure

The networking infrastructure at Argonne and the APS must remain world-class by being designed and engineered to provide sufficient capacity for analysis, storage, and transfer of big data to meet the scientific needs of the future. Additional networking objectives include maintainability, adaptability, accommodation of future growth, and cost-effectiveness.

The APS runs an extensive set of computer networks that provide beamlines and experimenters with a reliable and secure environment in which to operate. A wireless guest network is provided for visitors that allows them to access the internet and certain APS facilities such as printers via their own computers. Beamline networks provide an appropriate level of security to ensure that only authorized users can access the equipment.

Network connections to beamlines have been engineered with capacities to match beamline needs and capabilities. The APS has secure mechanisms to allow beamline staff or users remote access to beamline facilities when required. Beamline control systems are built on a common set of tools based on the Experimental Physics Industrial Control System tool kit and the SynApps package of beamline control applications. This provides a flexible, adaptable control system environment that accommodates changes in experimental set-ups and the integration of user-supplied equipment. The beamline computing environment has been engineered to be robust and reliable. Design of these systems takes into account the fact that there has been a growing interest from several collaborative access teams to transfer network and computer administration to APS.

Single points of failure have been avoided whenever possible. Distributed beamline servers provide a wide range of network services to users, including Internet access, printing, authentication, and other distributed data services. There is an ongoing program to keep APS beamline computing technology current and to anticipate future needs of the beamline user community. Close collaboration between the APS and Argonne's major computing facilities along with Lab infrastructure support is key to the success of this program.

9.4 The Argonne Leadership Computing Facility

The APS will continue to work with the Argonne Leadership Computing Facility to deliver leadership-scale computing resources for use by the APS. The facility and the APS will collaborate to host large data storage systems needed in the future, including tape backup systems, for the continually increasing amounts of APS experiment data. The APS and Argonne Leadership Computing Facility will continue to expand networking bandwidth between the two facilities as demand increases. With the addition of the power and flexibility of the next-generation super-computer, Aurora, the computing facility will be in a position to host on-demand computing jobs from the APS, and provide scalable levels of computing power on the time scale needed for APS experiments.

9.5 The Laboratory Computing Resource Center

APS scientists, Laboratory Computing Resource Center staff, and Argonne Mathematics and Computer Science Division computer scientists are working to adapt the Laboratory Computing Resource Center's computation resources to provide improved performance for the real-time, on-demand computing required for most APS experiments. Work is under way to modify the Laboratory Computing Resource Center computing architecture to host virtual machines using the OpenStack virtualization infrastructure. The use of this remote resource affords the APS many benefits: Virtualized environments allow the APS to install, configure, and update its data analysis and reduction software easily and without interference to other users on the system; its scalability allows the APS to provision more computing resources when larger data sets are collected; and the underlying hardware is supported and maintained by professional, high-performance computing engineers, relieving APS staff of this burden.

9.6 The National Energy Research Scientific Computing Center

The National Energy Research Scientific Computing Center is the primary scientific computing facility for the DOE-SC, providing computational resources and expertise for basic scientific research (http://www.nersc.gov). The APS is currently prototyping the use of the NERSC for beam-time data analysis. Computational scientists at the APS are working with NERSC staff to evaluate the use of high-energy diffraction microscopy grain-finding software on NERSC real-time queues. Scientists at the APS, NERSC, and Lawrence Berkeley National Laboratory are currently working to adapt the SPOT/SPADE suite of tools to automate the processing and distribution of tomography datasets from the APS.

9.7 Helium Recovery System

Liquid helium is one of the essential cryogens in the search for new states of matter by enabling access to low temperatures for samples and for cooling superconducting magnets, which are necessary for applying large magnetic fields to a sample. During the past few years, the increased cost and demand for liquid helium has jeopardized the APS ability to operate instruments and conduct experiments that require liquid helium.

The APS, together with the Argonne Center for Nanoscale Materials, is installing an Argonne-wide helium recovery system to capture large quantities of helium currently lost during such operations as cooling of superconducting magnets and sample cryostats. This system is located in the Argonne 200 Area near Argonne Tandem Linear Accelerator System operations and the future Materials Design Laboratory.

Satellite collection locations are scheduled for installation in FY17 in the 400 Area, where the Center for Nanoscale Materials and the APS are located. Together, this system will capture ~100,000 L of helium annually, which would otherwise be lost to the atmosphere. This project will significantly reduce risks associated with both price and availability of helium. A 3-fold increase in the price of liquid helium over the last decade has been observed, in addition to a 2-fold increase in user demand for instruments that utilize significant quantities of the gas. Currently, in APS Sectors 4 and 6, consumption of liquid helium is approximately 20,000 L annually. The target date for the installation of the complete system is December 2017.

9.8 The Actinide Facility

The Argonne Actinide Facility in the Argonne Chemical Sciences and Engineering Division works in partnership with the APS to enable x-ray measurements on radioactive materials. The Actinide Facility supports experiments using radioactive materials and assists users in proper containment practices so that spectroscopy, diffraction, and scattering measurements can be carried out safely at the APS. Radioactive samples are loaded into appropriate sample-chamber containment devices at the Actinide Facility under controlled conditions, and then the sample chambers are transported to the APS for measurements, after which chambers are transported back to the Actinide Facility for unloading.

9.9 Automatic Beam Steering

After a year of intense development, an innovative automatic beam steering pilot program was inaugurated in the 2016-1 user run (Fig. 25). The significance of this program is that users can now independently steer the beam in order to optimize beam alignment with sample for specific experiments without relaying requests to the main control room. The goal to extend the program to all beamlines in 2016 was achieved successfully.

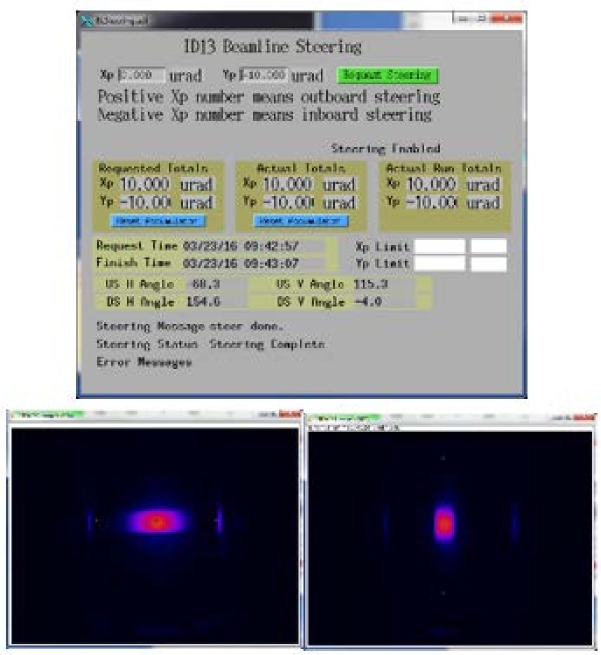


Fig. 25: User interface screen (top). Examples showing 10-µrad steering outboard (bottom left) and 10-µrad steering down (bottom right). Courtesy of Peter Eng, The University of Chicago, GeoSoilEnviroCARS-CAT.

10 Human Capital and Workforce Development

Argonne has a rich history in research and development because it has drawn many of the best and brightest minds in their respective practice areas and/or discipline to join the Laboratory community. To ensure that the APS remains at the scientific forefront, management is recruiting, retaining, and developing an outstandingly qualified, high-quality, innovative work force in a dedicated, diverse, and inclusive work environment. The APS is committed to the highest standards in recruiting, hiring, mentoring, and domain-specific professional development opportunities.

Through the stewardship of its Human Resources Manager, dedicated from Argonne's central Human Resources Services organization, the APS utilizes various human resources activities to perform talent reviews/strategy to support managers with identifying staff opportunities career growth and professional development. The APS also uses this activity to develop and maintain succession plans for strategic functions within the organization.

The APS prides itself on a workforce that includes a diverse collection of outstanding scientists, professionals, and support personnel dedicated to scientific discovery and to finding solutions to intractable problems of national and international importance. The APS is utilizing its own Diversity and Inclusion Working Group to assist the organization in fostering diversity in its workforce practices and environment, including execution of an annual diversity and inclusion action plan with specific goals and metrics.

The key for the future of any organization lies in its dedication to the development of skills and competences of its people in a diverse and inclusive work environment.

11 User Processes and Scientific Access

As noted in the introduction, the APS supports more users than any other DOE facility. The user program at the APS includes an integrated, comprehensive suite of outreach, administrative, support, and educational activities to facilitate quick and easy access to the beamlines and to fill the pipeline of future users and x-ray staff. Below are highlighted elements of the user program and delineated enhancements planned for the next five years that will provide even better services to APS users.

11.1 Outreach to Users

The APS fosters and promotes scientific communication and collaboration through the organization and support of a diverse array of conferences, workshops, schools, and short courses, as well as hands-on training opportunities encompassing the use of x-ray techniques, software, and data collection systems designed to familiarize APS users with the ever-evolving technology at the APS and to expand the user base.

- In-house and online lectures that explain the technical parameters of the proposed APS Upgrade assist resident users, particularly CAT resident users, to best align their plans for near- and long-term detectors and optics purchases to maximize the benefits they will derive from the improved source.
- Conferences and workshops focused on diffraction-limited light sources, techniques, and science areas in the sweet spot addressed by a MBA source expose current and future users to the capabilities and scientific opportunities of the proposed APS Upgrade. Input from these activities and from other mechanisms is being used to align the selection of upgraded beamlines and accelerator source parameters with user needs and the most transformative science opportunities.
- Conference support for users continues to evolve with the implementation of tools such as RegOnline registration software to improve the registration, access, and payment processes for users.
- A Web-based tool developed in-house is shared with resident CAT users to help them choose the optimal undulator system in preparation for the improved source of an upgraded APS.

- With input from our sponsor, users, and staff, the APS Website was refreshed to align with DOE and Argonne Websites in terms of design. This has also afforded an opportunity to evaluate the site in terms of functionality and service. The modern Web development platform Drupal was implemented to reduce the amount of effort required for maintaining the site.
- The User Program Office continues to work with the DOE-SC, the NSF, and the Society for Science at User Research Facilities to provide a consolidated voice for those engaged in supporting and/or interested in research conducted by users of America's national user facilities. This is accomplished via professional communities and research networks, and by promoting awareness about the benefits and significance of user facility research.

In addition, outreach to CAT funding agencies and organizations will help the collaborative access teams sustain their operations and implement capital improvements to their facilities.

11.2 User Support/Access

The APS provides both administrative and scientific-access support for users. User-related systems are being expanded, streamlined, and integrated resulting in better service for users, better data collection for future planning, and cost savings.

- The APS user database system now feeds directly to Argonne's Workday Human Resources system, which is an integral part of Argonne's site access system and other critical systems.
- The User Program Office developed and continues to refine a user portal that provides a customized platform for users to find all administrative details about their user record and their scientific program (e.g., proposals, training, site access, etc.) with the APS.
- A set of tools was developed to identify scientific hosts on each Experiment Safety Assessment Form. Automated e-mails provide this data to hosts, users, and Argonne's Foreign Visits and Assignments Office.
- Additional automation between the registration, Argonne foreign national visitor, and the Argonne site access systems is being discussed.
- "APS/User News" and email correspondence are utilized to increase user awareness of the toolkit offered in the User Portal, which includes a link to each user's individual data via the registration system as well as links to systems for online user training, proposal submission, experiment safety approval forms, and end-of-experiment form.
- The online APS Beam Time Access System is continually updated to meet the changing needs of the user community and expanded APS research capabilities. Improvements to the system will include modifications to better serve the needs of beamline and panel reviewers in supporting their effort to ensure the quality of proposals being awarded beam time.
- Industrial user requests for access are handled through a special proposal process designed to streamline requests for beam time. The APS is aggressively developing new approaches and outreach programs, such as offering a new guest research agreement to cover the typical one-time measurement access mode.
- Review and update of email communications to users generated by the various APS systems is on-going. The APS implemented an automated e-mail renewal process for users. Automated notifications reminding users to re-register are sent at 60- and 30-day intervals prior to site access expiration, followed by a final notification if a user fails to re-register. This was previously managed manually.
- As a major enhancement to the APS emergency preparedness system, cell phone numbers are now collected during registration and are automatically fed to the Argonne Mira 3 emergency notification system, which contacts users via text and phone calls in the event of an emergency. Emergency contact (e.g., family member) information is also gathered.

- More than 560 legacy legal agreements were terminated and new master user agreements have been implemented.

11.3 User Training

Most required user training is now available on the Web and can be taken by users online before arrival at the APS, saving time and money. The online training course options have been expanded to include access to radiation worker training, a course formerly only available on-site. Individual user training expiration dates are included in the Experiment Safety Assessment Form to ensure that users participating in hands-on work are up-to-date with all required training. The APS plans to eliminate the use of "mirrored" training and solely use the Argonne training system. Another objective, in conjunction with the Office of Science and the Society for Science at User Research Facilities, is to investigate "reciprocity" with other national user facilities for training in common core areas such as cyber security. These and other innovations continue to improve the user experience at the APS.

11.4 Proposal Review Process

A credible and transparent user proposal review process is critical to a successful user program. The APS Proposal Review Panels (PRPs) are composed to provide the best possible peer review for beam time proposals, whether organized by technique- or science-driven expertise. The APS uses 14 PRPs to evaluate general user proposals. The number and make-up of the PRPs have evolved, and will continue to evolve in order to best support the changing scientific landscape at the APS. The PRP categories and panel membership are being expanded to address new areas of research at the APS, such as shock physics, which will see a boom in users with the opening of the Dynamic Compression Sector beamline at Sector 35.

- A real-time score assignment tracking tool has been newly developed by the User Program Office in conjunction with the Information Solutions Group. This tool will be implemented to allow PRP members to track the distribution of scores by panel and by individual beamline in real time when rating proposals.

Teleconferencing has been integrated as an option for PRP reviewers in order to save time and travel expenses.

11.5 Training the Future Science Generation

APS staff members have been strong and active advocates for training graduate students to more effectively and efficiently use U.S. national x-ray facilities. The APS is continually looking for new avenues to expand networking and education programs, such as the National School on Neutron and X-ray Scattering, developed by the APS.

For the last 15 years, the APS has co-hosted the NXS (originally with the former Intense Pulsed Neutron Source at Argonne, but now in partnership with the Spallation Neutron Source at Oak Ridge National Laboratory). This program has educated approximately 1,000 graduate students. Some of the former students are now sending their own students to this summer program. School organizers are expanding the curriculum to train potential users of the next generation of high-brightness sources, such as the proposed APS Upgrade.

More than 40% of the experiments at the APS involve participation by undergraduate or graduate students who are generally part of a larger, university-based research team led by an experienced researcher. This hands-on experience helps students learn to formulate new scientific ideas, prepare successful research proposals, plan and conduct experiments, and analyze and interpret data.

Postdoctoral scholars, often as principal investigators, participate in an additional 22% of APS experiments. It is anticipated that there will be an increase in the number of students using the APS as the capabilities at the facility expand. A strong postdoctoral program at the APS stimulates partnerships with various universities. APS staff members bring postdocs to the facility and seek opportunities to foster x-ray science programs at external institutions.

The APS staff and resident users at the CAT sectors continue to participate in Argonne's growing Exemplary Student Research program (organized by the Argonne Educational Programs effort) for high school students. Teams of students work closely with an APS beamline staff member to learn about careers in x-ray science and conduct experiments. The APS continues to look for ways to expand this program by leveraging users who have outreach components of their funding.

11.6 Five-Year Plan

The APS User Program Office will focus on updating the platforms and processes that support the registration and site access systems. The registration process for first-time users is approximately 20 years old and will be moved to a new platform using modern technology. To simplify the registration process for returning users, the User Program Office plans to develop a renewal form that auto fills key information (e.g., name, date and place of birth, completed education levels) already extant in our database. Only specified fields will require updates (e.g., institutional affiliation, additional educational degrees received, and emergency contact information). This will streamline the registration process for both the user and the User Program Office staff.

Additional work is planned to fully integrate the APS User Database with Argonne's Workday, the Foreign Assignment/Visit Online Report System, and gate pass systems to ensure consistency, improve communications with users, and automate several processes that are currently done by hand.

The User Program Office will continue to work with the Office of Science and the Society for Science at User Research Facilities to pilot a training reciprocity system that could be used across the DOE complex. This would eliminate the need for users who use multiple facilities from having to repeat training.

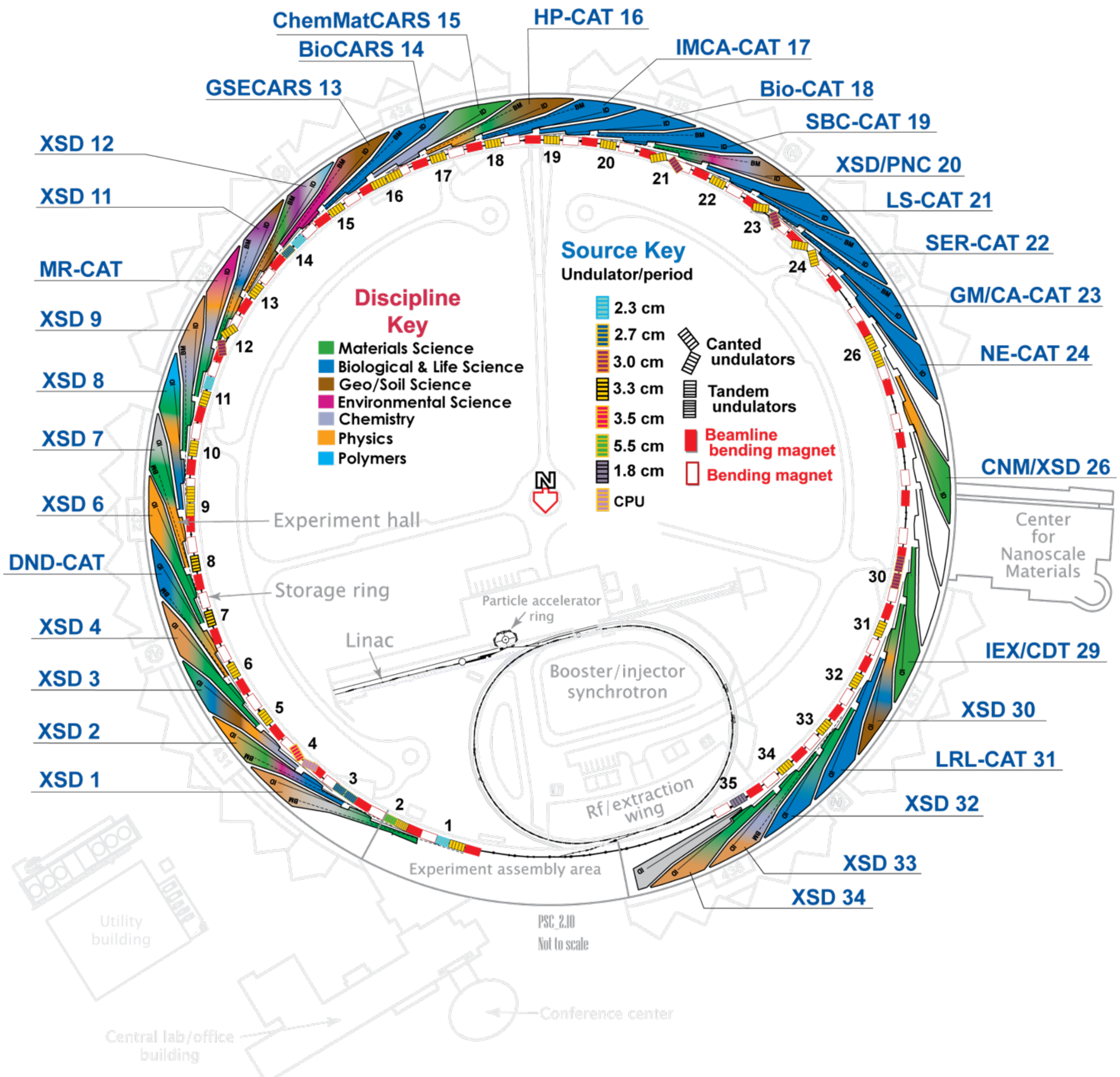
There are two user data repository systems currently in use by the User Program Office (the user database and data warehouse). These interfaces will be merged and streamlined, simplifying their data feeds to other user-related systems and improving the efficacy of data retrieval.

12 Input and Review Mechanisms for the APS 5-Year Facility Plan

The "Advanced Photon Source Five-Year Facility Plan" is a baseline guide for large-scale operations spending, user support, and infrastructure/equipment improvements. The inaugural document was completed in March 31, 2015, and this is the revised original document. Subsequently, the plan will be reviewed annually and revised on a rolling basis. Updates will also be made as needed to accommodate significant changes in funding, shifts in the priorities of DOE, or new research avenues and opportunities.

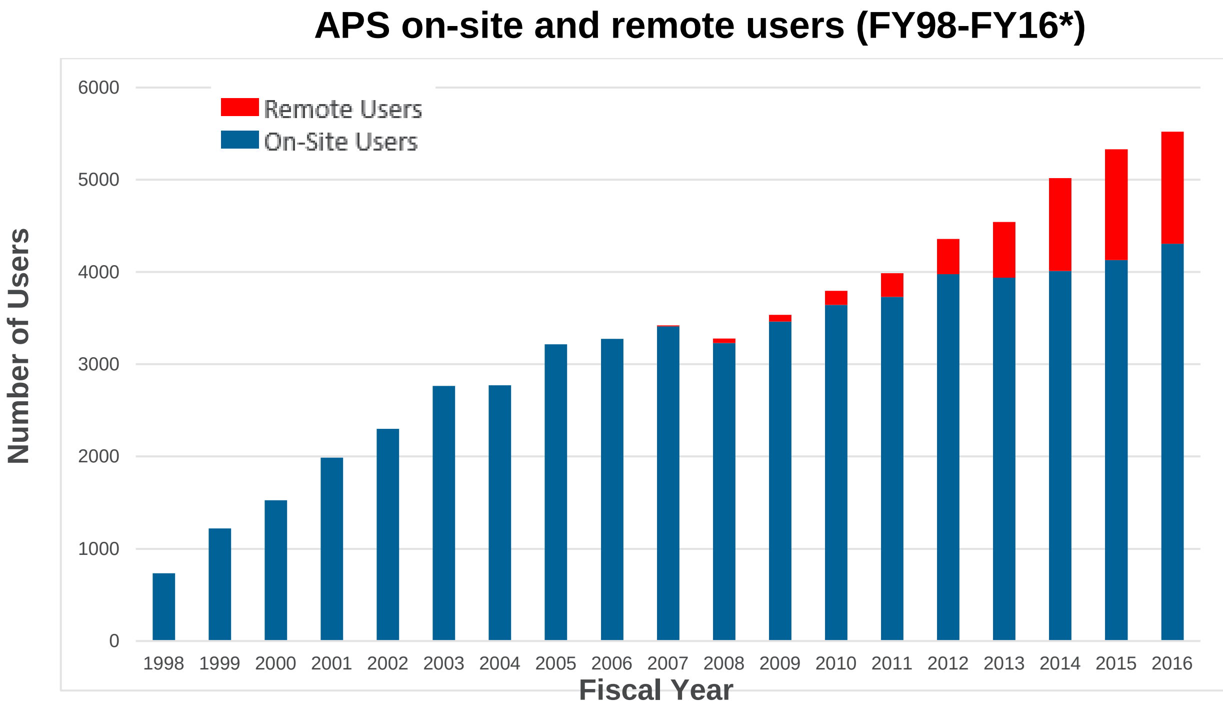
Input to this plan was obtained through many channels, including discussions with and/or review by DOE sponsors, the APS user community, sister facilities, resident users, APS staff, Argonne leadership, and the broader scientific community. Review was obtained by direct request for input to this specific document. Discussions (both specific to the document and on a broader basis) occur at regular meetings and reviews (e.g., APS Scientific Advisory Committee, APS User Organization, APS Partner User Council, DOE reviews of APS Operations and the proposed APS Upgrade Project, and the University of Chicago, LLC, Board of Governors reviews of the APS), regular international meetings and workshops of the synchrotron and general scientific community, and special workshops to consider future strategic plans for the APS and similar facilities.

Appendix 1: Beamlines at the APS

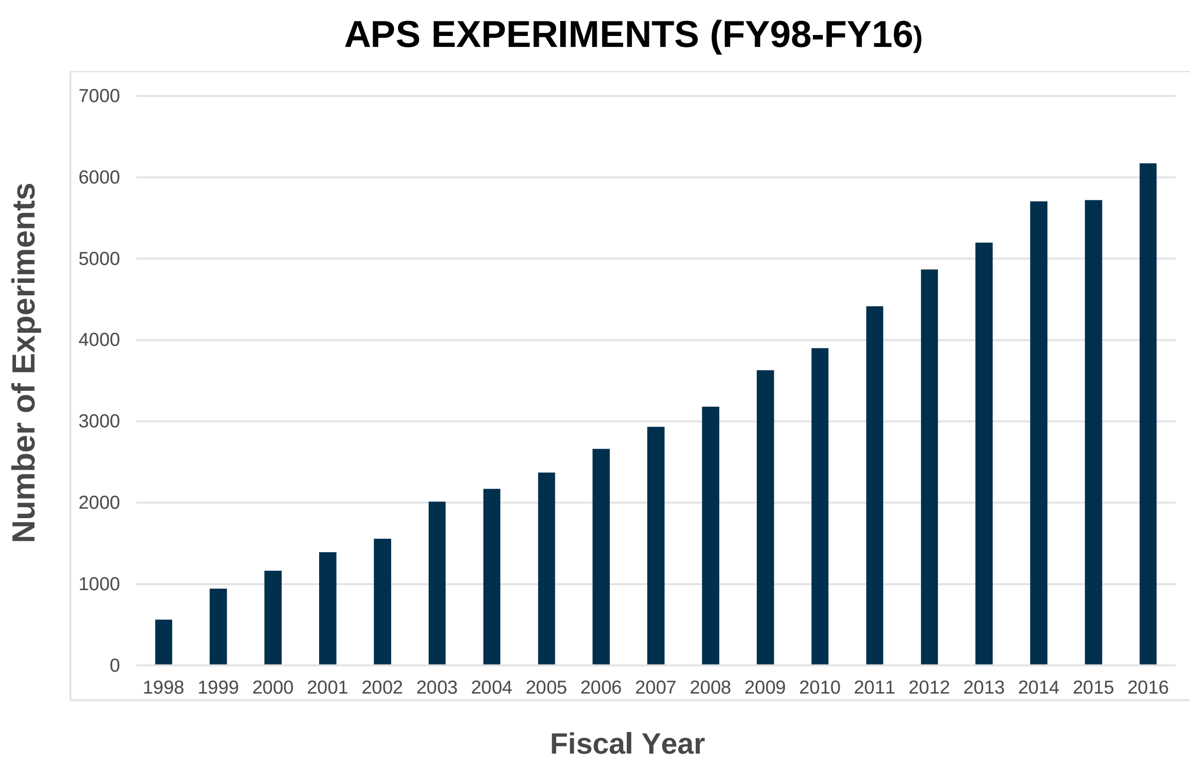


Map of APS beamlines. There are 67 simultaneously operating beamlines at the APS divided into 46 insertion device and 21 bending magnet (BM) beamlines. The XSD is currently responsible for a total of 39 beamlines, which includes 25 ID and 11 BM beamlines funded by DOE-BES, and 2 ID and 1 BM beamlines funded by the National Institutes of Health through GM/CA-XSD. In addition, the APS is a minor partner in three additional beamlines: the Dynamic Compression Sector (35-ID), BioCARS-CAT (14-ID), and the Nanoprobe (26-ID). The rest of the beamlines are operated by the collaborative access teams.

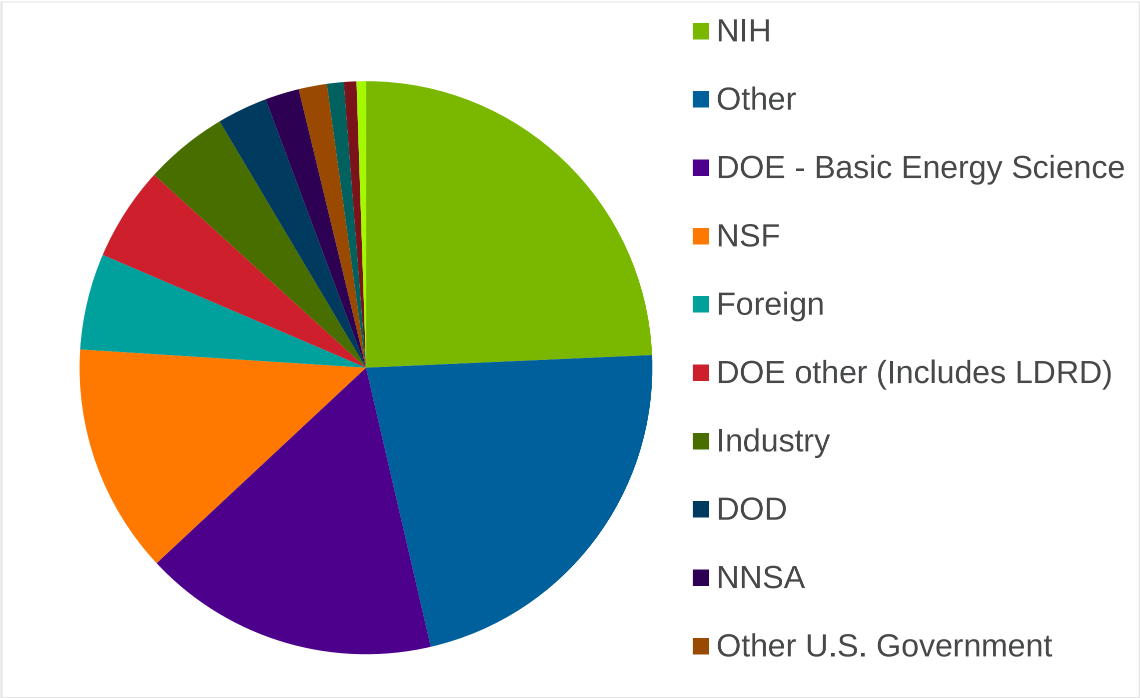
Appendix 2: User Data



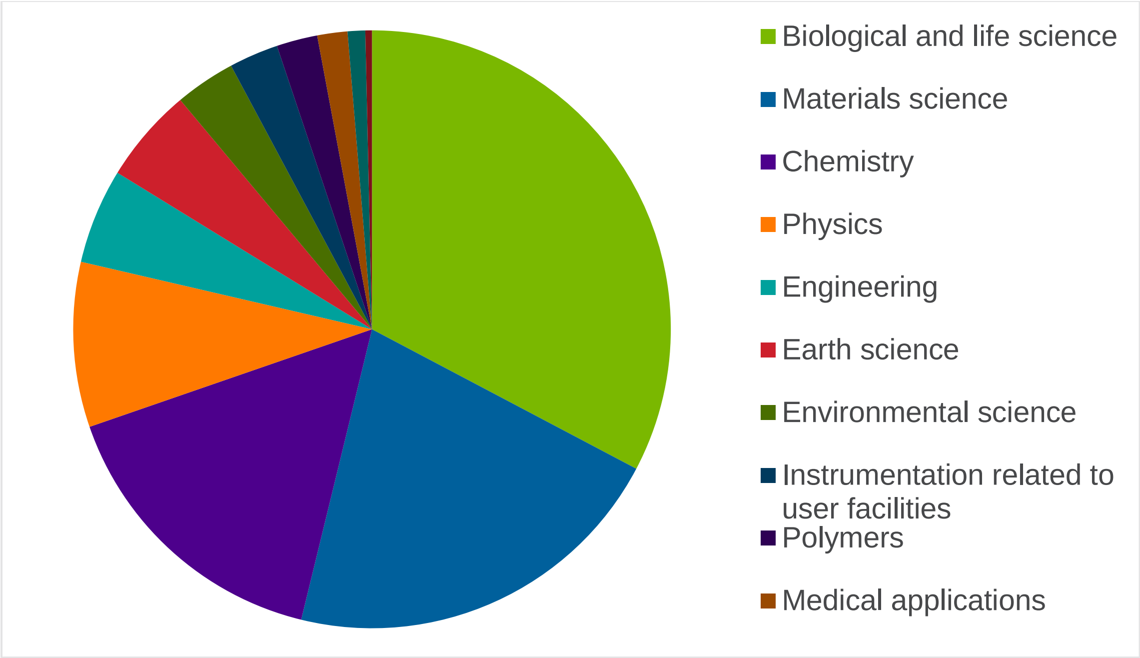
*Prior to FY14, mail-in users were not included in the Remote category



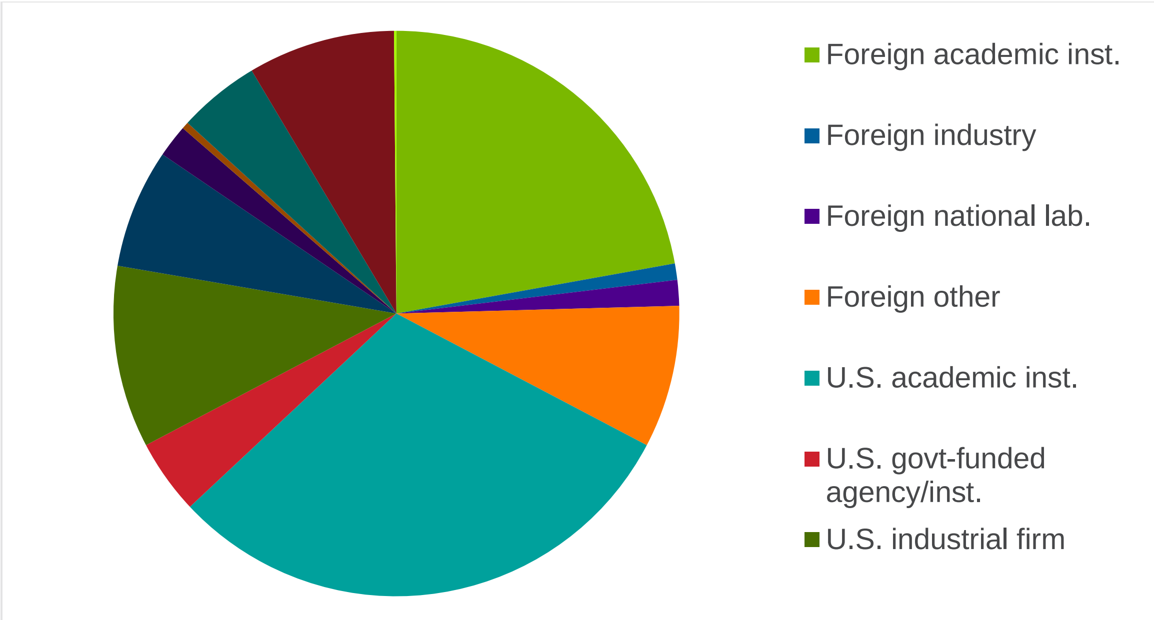
APS USERS BY SOURCE OF SUPPORT (FY16)



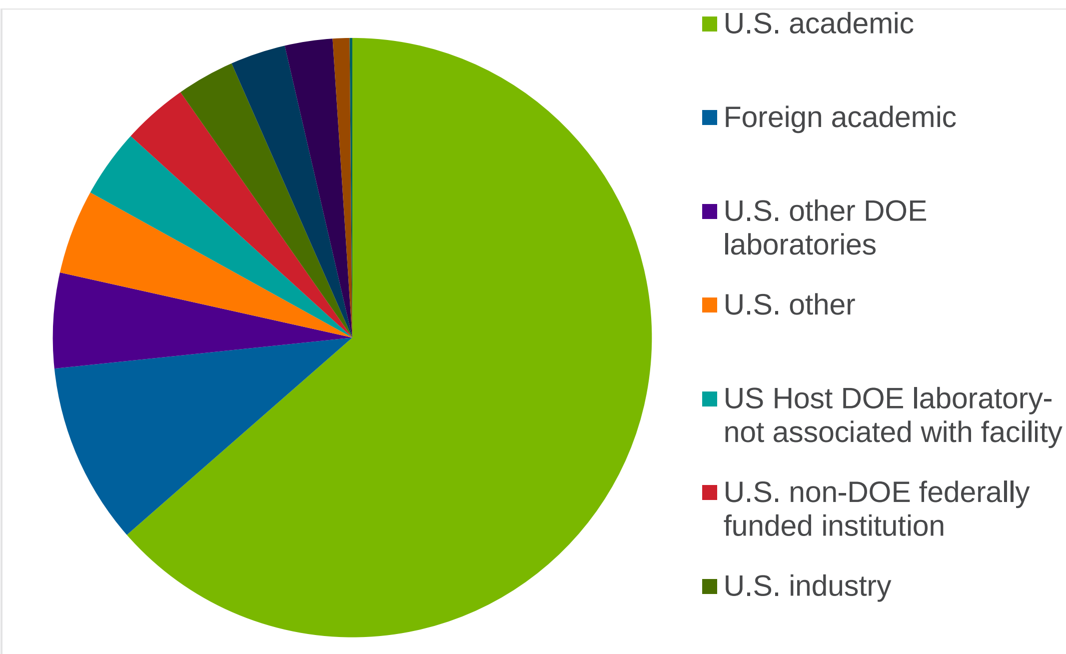
APS USERS BY EXPERIMENT SUBJECT (FY16)



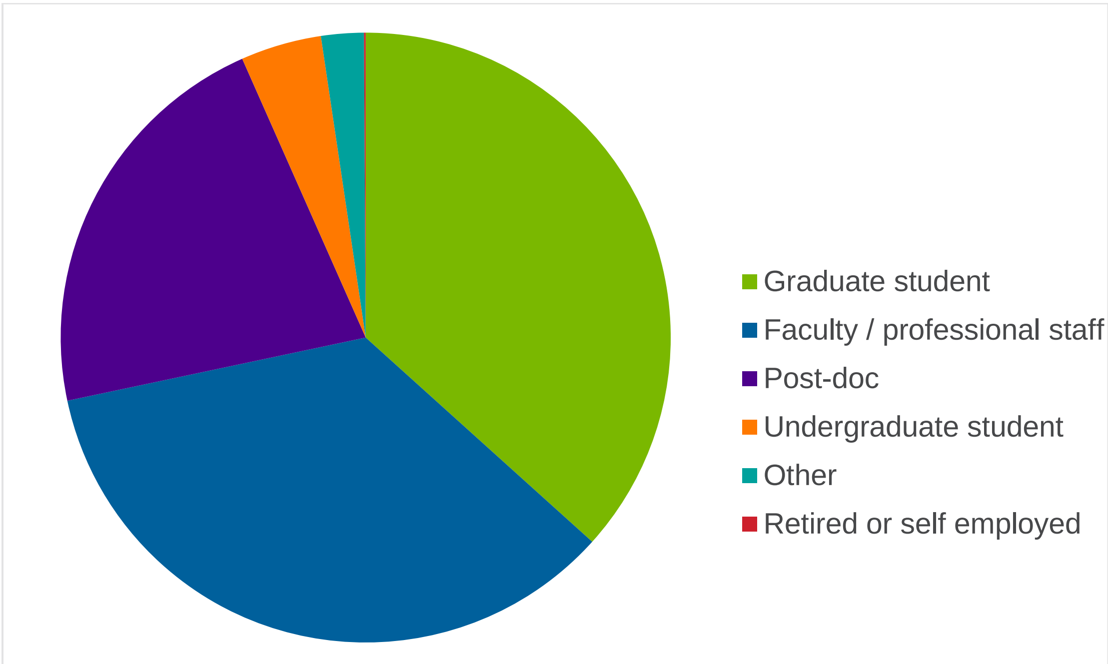
APS USER INSTITUTIONS BY INSTITUTION TYPE (FY16)



APS USERS BY EMPLOYER (FY16)



APS USERS BY EMPLOYMENT LEVEL (FY16)



APS USERS BY USER TYPE (FY16)