Optics at the Advanced Photon Source: Strategic Needs and Plans

X-ray Science Division, Optics Group

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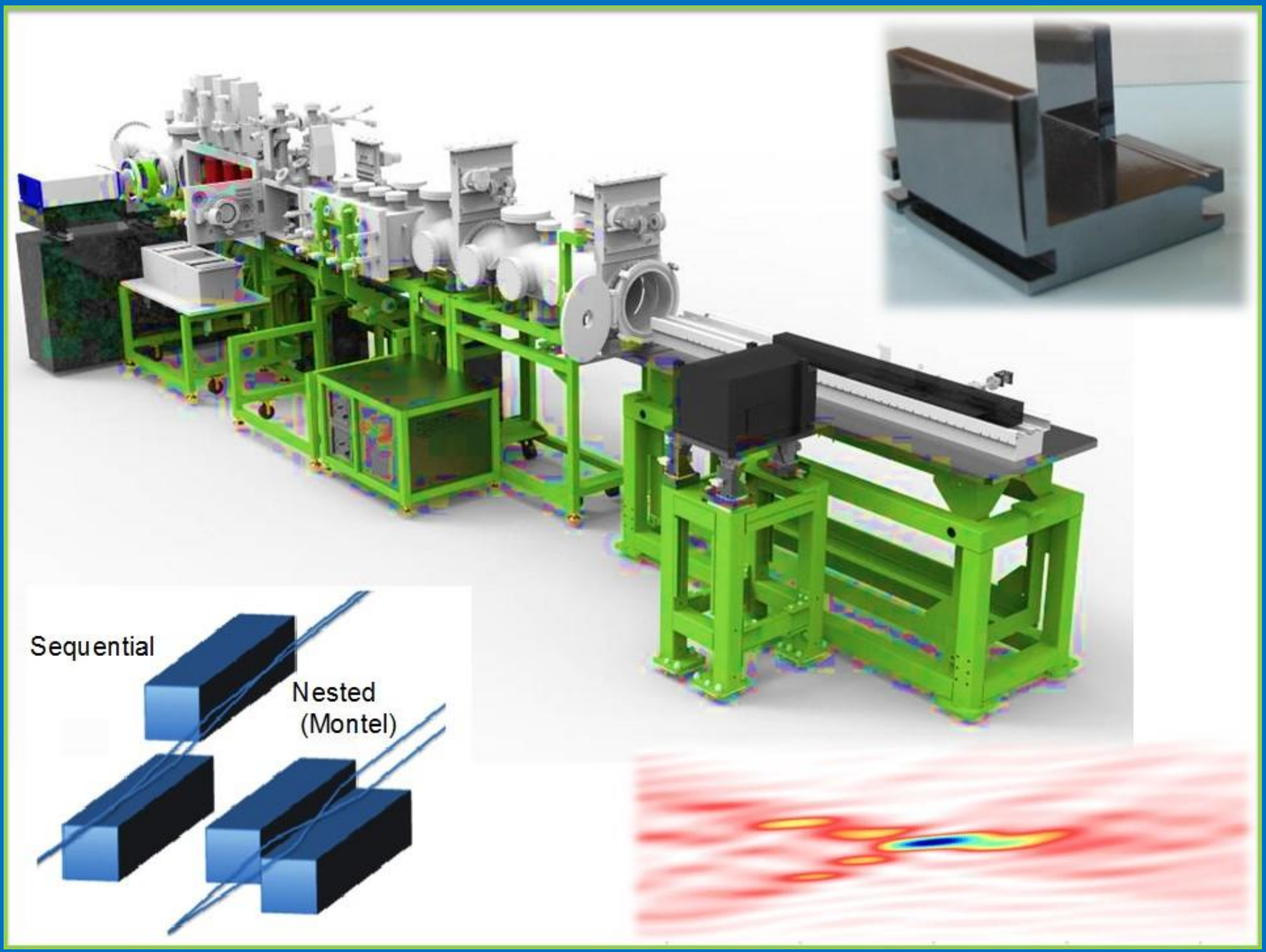

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1. Mission

The core mission of the Optics Group is to facilitate the efficient and productive use and operation of APS beamline-based research facilities. In support of this mission, the APS Optics Group:

- Operates and develops instruments and tools to fabricate and characterize x-ray optical elements, such as single-crystal monochromators, mirrors, multilayers, and other specialized optics and substrates;
- Carries out R&D jointly with the APS beamline scientists and user community, often in collaboration with other facilities, to keep the Group at the forefront of x-ray optics;
- Develops and maintains advanced simulation tools for optimizing the design of beamline optics and optical systems; and
- Operates the 1-BM Optics and Detectors Testing Beamline to test and characterize optics for APS beamlines and users.

2. Introduction

The forefront basic and applied research that is the mission of the APS requires high-quality x-ray optics (such as monochromators, mirrors, and focusing optics) to deliver an x-ray beam to the sample, and in many cases to collect the relevant signal from the experiment (such as by using crystal analyzers). As we prepare for the proposed installation of a multi-bend achromat (MBA) lattice to upgrade the APS, we must optimize the APS beamline optics by developing new optics or improving existing optics to fully exploit the new source parameters, which will provide a much smaller radiation source, larger spatial coherence, and a more than 100-fold increase in brightness. The majority of existing APS beamlines still utilize optics that date back to the construction of the facility roughly two decades ago. Optics fabrication technologies have improved considerably since then, and new focusing optics approaches have been developed, so there is considerable room for performance enhancements even with today's source parameters. But as noted in the 2013 DOE workshop report[*], "X-ray Optics for BES Light Source Facilities," the development of ever more powerful x-ray sources in the near future requires a new generation of x-ray optics that will allow us to fully utilize these beams. We present below the Optics Group's R&D capabilities and strategies for meeting both present APS operational needs and the needs of the proposed APS Upgrade (APS-U). One part of our strategy involves working directly with vendors to acquire and characterize the desired optics, such as beamline mirrors, standard monochromators, and other commercially available optics. The other part involves the use of unique in-house fabrication and characterization capabilities to develop one-of-a-kind optics that cannot be acquired from a vendor.

[*] http://science.energy.gov/~/media/bes/pdf/reports/files/BES_XRay_Optics_rpt.pdf

To optimize efficiency, avoid duplication of effort, and save cost, the Optics Group will seek active partnerships with 1) DOE light sources and other institutions; 2) Argonne support groups; and 3) commercial vendors.

3. Beamline optics simulation and optimization

Status: Optics development begins with design and simulation, and in this area the Group has been significantly strengthened within the past two and a half years by strategic staff. Though existing codes based on ray tracing (e.g., SHADOW) and wavefront propagation (e.g., SRW) have been widely used in the past, improvements and new developments were needed. These have already begun to emerge as part of a new code, which uses a hybrid approach combining ray tracing and wavefront propagation. The former addresses the geometrical aspects of the optics and the latter takes into account the diffraction when apertures clip the beam. The main advantage of the ASP Hybrid code, developed in collaboration with the European Synchrotron Radiation Facility, is its speed compared to existing codes. This code is ray-tracing-based and includes diffraction effects from apertures and beamline optics via wavefront propagation. It is able to deal with partial coherence and figure errors in optics and is already serving as a crucial guide for the design of beamline optics required for the APS-U.

Strategic plan: By the end of FY 2016, optics simulations will be under way to support the preliminary design of new APS-U beamlines. The Hybrid code will be enhanced by including fast two-dimensional simulations, better undulator source models, and implementation of new routines for simulation and optimization of new optics.

By the end of FY 2017, all APS beamlines will have been simulated to prepare for the APS-U. Data analysis software for optics characterization will be developed for coherence measurement and wavefront sensing. A simulation package that combines heat load calculation and ray tracing will also be developed. Future R&D within the next five years will include developing packages for propagating Wigner functions or cross-spectral density functions through beamline optics. The above work will be carried out in coordination with other DOE light sources as well as with other synchrotron radiation facilities worldwide.

4. Crystal optics

Status: Nearly every beamline at the APS uses one or more crystal-based x-ray optics. Supporting the APS as the nation's premier hard x-ray facility, crystal optics play a crucial role at the APS in x-ray monochromatization (including under high heat load) and in high-resolution spectrometers and analyzers. The Optics Group has considerable expertise and capabilities in both designing and modeling crystal optics systems and in fabricating crystal optics throughout the entire pathway from silicon boule machining to crystal orienting and cutting with ~0.1° accuracy, super-smooth and strain-free crystal polishing (with RMS roughness ≤2Å), and x-ray topographic characterization. The Group crystal optics team delivers hundreds of crystal-based components to both the APS beamlines and other DOE light source and neutron facilities. These core capabilities and competences, which are unique in the DOE laboratory complex, were established and have been continuously developed since the early 1990s after the commissioning of the APS.

Ongoing R&D efforts include the development of efficient sub-10-meV (as well as sub-1-meV) analyzer systems; bent-crystal monochromators for high efficiency at up to 100 keV; and crystal optics based on exotic materials such as sapphire, quartz, diamond, and others as needed.

Strategic plan: Availability of wavefront-preserving crystal optics is essential for imaging beamlines, as well as for those requiring high resolution and diffraction-limited focusing. To meet the APS MBA needs in this area, our strategy focuses on developing:

- Crystal orienting capability to <0.01 deg.;
- Capabilities for strain-free polishing of crystals to achieve ≤1-Å-rms surface roughness;
- Etching and polishing procedures to fabricate strain-free crystal monochromators and analyzers using new materials beyond silicon, such as germanium, diamond, quartz, sapphire, and lithium niobate;
- Tools for polishing complex crystal optics such as channel-cut crystal monochromators; and
- Dynamical theory calculations and advanced codes incorporating fabricated defects and coherence to simulate real-crystal monochromators.

5. Beamline mirrors

Status: Large grazing-incidence mirrors are essential components of the APS, and are usually delivered by commercial vendors. Many APS beamline mirrors were installed as far back as 20 years ago, when the best mirrors of this type had slope errors of ~5,000 nrad rms and surface roughness of ~0.5 nm rms. Simulations show that the APS MBA lattice upgrade will require mirrors with slope error better than 150 nrad rms over 1 m in length, and roughness ≤0.1 nm rms. A state-of-the-art flat silicon mirror costs as much as $50K to $100K, not including the support and mounting system, and requires at least 6 to 10 months lead time for fabrication, depending on the manufacturer.

Strategic plan: Most of the existing APS mirrors can be improved by stripping off their coatings and deterministically figure-correcting their surfaces (as demonstrated at Diamond Light Source in the UK) so that they meet the future APS MBA lattice source's requirements, thus saving significant cost and time. Therefore, our strategy for mirrors includes two components: 1) refurbish as many existing mirrors as possible using the Modular Deposition System (MDS) described below; and 2) for special mirrors and new mirrors, work closely with vendors to develop procedures that will enable them to fabricate mirrors with the required surface specifications. This collaborative work will be done through simulation and modeling, with validation by optical metrology and at-wavelength metrology and characterization at bending-magnet beamline 1-BM or an insertion device beamline, as required.

6. Thin-film optics

Status: Similar to crystal optics, the thin-film optics fabrication facility and expertise were established in the early 1990s and have been continuously enhanced. Originally, the thin-film facility at the APS was intended for coating of single-layer films on large substrates to produce simple x-ray mirrors. As the field progressed, new equipment and expertise were added to produce simple multilayer mirrors for user applications. With science needs driving the x-ray optics, and x-ray optics enabling new scientific capabilities, it has become clear that the APS must invest in thin-film infrastructure in order to meet mission needs both at the present time and in the era of the future APS. As a result, a new vacuum-processing instrument, the MDS, has been designed by the APS, procured during FY 2015, and delivered in February 2016. The equipment consists of a large, linear substrate translator housed inside a vacuum chamber. This substrate translator incorporates a state-of-the-art, direct-drive, in-vacuum servo system. The machine includes large the vertically planar cathodes, ion beam milling, and *in situ* metrology required for future APS MBA lattice upgrade mission needs. The system has accommodations to allow for mirror figure modification or correction with a combination of ion beam milling, profile coating, and *in situ* metrology.

Strategic plan: R&D on figure correction and *in situ* metrology is currently under way with strategic Laboratory Directed Research and Development funding. Provisions for a dynamically actuated aperture will be used to explore methods for three-dimensional multilayer deposition intended to enable the use of new optical geometries and to allow for higher efficiency and mirror figure correction. Such new optics will enable frontier science, utilizing new methods of inelastic x-ray scattering and small angle x-ray scattering. This area was explicitly called out in the 2013 DOE x-ray optics workshop report as one of the Grand Challenges. In fact, the new MDS can be put to use in exploring three of these Grand Challenges and providing experimental verification for the fourth.

7. Nanofocusing optics

Pushing x-ray microscopy into the nanoscale is crucial for understanding complex hierarchical devices on length scales approaching the atomic dimension. Nanoprobe experiments (including coherent-diffraction variants such as ptychography) require a high degree of spatial coherence to achieve a focal spot size that is limited by diffraction from the optics. The 100-fold brightness improvement expected from the APS-U translates directly into increased coherent flux for these experiments. This transformative change allows one to achieve higher spatial resolution, scan larger areas, and image more representative sets of specimens. There are still APS beamlines that either lack adequate focusing optics or are in need of further optimization to take full advantage of the current APS properties. Furthermore, the planned APS MBA lattice upgrade is expected to deliver beams with a much smaller emittance and a 100- to 1000-fold increase in coherent flux at high x-ray energies in the multi-10-keV range compared to the current APS, thus underscoring the need to further pursue the development of high-energy x-ray focusing optics. R&D in this area includes focusing capabilities of multilayer optics, multilayer Laue lenses (MLLs), and total reflection mirrors; improvement of refractive optics such as sawtooth lenses and compound refractive lenses for sub-micron focusing; improvement of bent crystal optics for focusing; etc. Our three primary areas of strategic development in nanofocusing optics are discussed below.

7.1. Fresnel zone plates

Status: Fresnel zone plates remain the optics of choice for many x-ray microscopes because of their compactness, simple normal-incidence alignment, and large imaging field. Traditionally, they have required compromises on either resolution (determined by the narrowest fabricated zone width) or efficiency (determined by the thickness of the zone material) because of limitations on achievable nanofabrication aspect ratios. However, recent developments have widened the horizon for Fresnel zone plates for hard x-ray nanofocusing by improving high-aspect-ratio nanofabrication methods and intermediate-field zone plate stacking. In alignment with the APS-U and future operations needs, the primary goal for Fresnel zone plate development is 20-nm focusing at 25-keV x-ray energy and 20% focusing efficiency by 2018.

Drawing upon Argonne strengths in nanolithography and atomic layer deposition, a team effort has begun on developing zone plates using both direct photoresist writes and gold electroplating, and the zone-doubling process developed at the Paul Scherrer Institute. This collaborative effort has resulted in a demonstration with multiple zone plate layers written on a single substrate and having 60:1 aspect ratios, employing the metal-assisted chemical etching process that has been utilized in recent zone plate fabrication experiments at the SLAC National Accelerator Laboratory. For high-efficiency focusing at high energy, zone plates will be stacked in the near and intermediate fields to achieve the desired zone thickness. It has long been known that multiple zone plates can be stacked together in the near field to enhance hard x-ray focusing efficiency. More recently, it was shown that multiple zone plates can be stacked in larger numbers at more practical distances from each other, provided that each zone plate design is tailored for its position. A cross-divisional team from the Optics, Microscopy, and Imaging groups in the APS X-ray Science Division (XSD) and the APS Engineering Support Division has demonstrated the stacking of six zone plates with 80-nm outer zone width to achieve 28% efficiency at 27 keV.

Strategic plan: Development of both near- and far-field stacking techniques will proceed in parallel with zone plate fabrication development to try to improve the focus spot size and efficiency simultaneously. Taken together, these new developments in high-aspect-ratio zone plate fabrication and zone plate stacking promise high-resolution, high-efficiency nanofocusing. By the end of 2016, the fabrication process for zone plates with 20:1-aspect-ratio zones down to 16 nm in width will be developed to meet the APS-U goal. Also, sets of zone plates with 40- and 20-nm zone widths will be stacked to test the stacking-apparatus capabilities and to guide engineering improvements to achieve 20-nm focus. The Optics Group will continue to improve the capabilities at APS beamlines by incorporating the zone plates that are developed.

7.2. Kirkpatrick-Baez mirrors

Status: Mirrors used for nanofocusing can provide higher efficiency than diffractive optics if the same numerical aperture is used, and they can be achromatic for spectroscopy if one uses simple specular reflectivity. Two-dimensional focusing with a Kirkpatrick-Baez (K-B) mirror pair can be accomplished either by bending a properly shaped flat optic into an elliptical form or by pre-figuring a mirror with a fixed elliptical surface (the latter approach is used for stable nanofocusing applications). The APS has a long history of producing profile-coated mirrors for submicron- and nanofocusing applications. These mirrors are fabricated by depositing a profiled platinum thin film through a figured mask on either a flat or a spherical substrate to generate an elliptical shape. This method provides a quick and cost-effective way to produce fixed-geometry K-B mirrors to match custom beamline configurations at the APS.

A new profile-coating system for mirrors less than 150-mm long has been commissioned at the APS, replacing a system with lower performance. This new deposition system has already been used to fabricate K-B mirrors for sub-micrometer focusing. The best prototype profile-coated K-B mirrors produced so far at the APS have a focus of approximately 75–85 nm, and 200-nm to 1-µm focus for routine use. The Optics Group worked with the APS Engineering Support Division to incorporate these into an in-house-designed mounting system, and then pre-aligned and characterized the full mirror assembly at beamline 1-BM prior to delivery for experiments at 8-BM. This integrated system approach marks a significant advance over past practices, where profile-coated mirrors were delivered to APS beamline scientists as single components.

Strategic plan: At present, the main limiting factors in profile-coated K-B mirror technology are metrology and the deposition system. *In situ* metrology will be incorporated in the new MDS for *in situ* monitoring of mirrors during ion milling and profile coating, but an *ex situ* metrology tool will be required both to use as a backup system and to evaluate future advanced beamline mirrors procured from vendors. The new MDS will enable the exploration of new coating materials that might have better long-term stability than the metal coatings now used for in-air mirror systems.

7.3. Multilayer Laue lenses

Status: Multilayer Laue lenses offer a path toward sub-10-nm focusing, especially for fixed-energy experiments. While these optics were conceived and first demonstrated at the APS, the National Synchrotron Light Source-II project at Brookhaven National Laboratory (BNL) has chosen to concentrate on their development. Focusing below 15 nm in the hard x-ray regime has already been demonstrated, and an MLL that doubled the largest aperture width ever achieved, to 102 µm, was measured to have efficiencies of more than 13% at 12 keV at beamline 1-BM. However, R&D effort is required to produce sub-5-nm focusing and functional optics for day-to-day operation. This effort includes research on new bi-layer material combinations to increase efficiency, optimum deposition parameters, and conditions to reduce built-in stress, etc.

Strategic plan: The new APS MDS will have capabilities complementary to those at BNL for MLL development (such as better control of partial gas pressures for thick-film stress control and 1-A substrate biasing capability), enabling the APS Optics Group to continue to contribute to MLL R&D in collaboration with BNL.

8. High-heat-load and thermo-mechanical stability

Status: Liquid-nitrogen-cooled silicon has remained the monochromator cooling method/material of choice at the APS since the facility's commissioning in the early 1990s, and is expected to remain so for the APS-U. The reason is that the thermal expansion coefficient becomes zero at about ~124 K and the thermal conductivity improves by about an order of magnitude compared to room temperature. Many different cooling schemes are being used or tried, including internal cooling channels, side cooling, and hockey-puck geometry. Because of their ease of maintenance, water-cooled diamond monochromators are also used, particularly in beamlines where the narrower bandwidth of diamond compared to silicon is either desired or not an issue. Since the APS began operations, much has been learned about silicon monochromator cooling efficiency, and mounting stability and design. Side cooling has proven to be the most effective approach for mitigating heat load on silicon monochromators.

Strategic plan: The APS MBA upgrade will likely increase the power load on the first optics in the beamline. The power density increase for a single undulator will be less than a factor of two and a standard liquid-nitrogen-cooled monochromator could work. But R&D will be required to meet the needs of the most extreme cases, such as when two undulators are used in series. More specifically, realizing the full potential of the APS MBA source may require high-heat-load monochromator assemblies that provide minimal thermo-mechanical distortions along with outstanding opto-mechanical stability. Simulation studies and testing may be required to determine the optimum cooling geometries needed to minimize the impact of thermal distortions on the transmitted wavefront; that is, to preserve brilliance and do so while maintaining angular stability at better than 50 nrad.

Indirect cooling of high-heat-load monochromators is highly advantageous compared to direct cooling because of its simple design, reduced maintenance, and low flow-induced vibration. However, it is generally achieved through an indium foil clamped between the optics surface to be cooled and a copper cooling manifold. As a result, the cooling efficiency depends heavily on the conformance of the interface material (i.e., the indium foil) and the clamping force. We plan to investigate new cooling schemes and geometries in collaboration with relevant light sources in the U.S. and abroad and with manufacturers.

9. Coherence-preserving mirrors and windows

Status: The MBA lattice upgrade of the APS will deliver x-ray beams with a much higher degree of coherence, and those coherence properties must be preserved as much as possible while the beam is manipulated using x-ray optics. The current and future capabilities at the APS for producing nanofocusing mirrors with profiled deposition, or correcting figure errors with a combination of *in situ* metrology and either ion-beam figuring or differential deposition, are directly applicable to exploration of coherence-preserving mirrors, since many of the surface finish and figure requirements are similar.

Finite-element studies show that, when exposed to the APS MBA beams, water-cooled mirrors will be significantly distorted if they are used as the first beamline optics. This in turn will dramatically alter the source and beam wavefront properties. With two undulators in series, the power load will double, rendering water cooling totally inefficient. Here, to preserve the source brilliance, liquid-nitrogen cooling may be necessary.

Beryllium windows have been reported to act as an additional effective source, with the consequence that a portion of the radiation has a sharply reduced coherence length after passing through a window far downstream of an undulator. The net effect was reported to produce a sharp intensity peak in the center of coherent diffraction images of nanocrystals. Other deleterious exit-window effects have been found in topographic studies. A sizable body of work has been done at SPring-8 (Japan) on both beryllium and diamond windows, including characterization using shearing interferometry. PETRA III (Germany) has also employed diamond exit windows. Differential pumping has been implemented as an effective means to replace some of the Be windows at several beamlines. A number of beamlines at the APS have successfully implemented differential pumping to reduce the prevalence of Be windows.

Strategic plan: A supply of acceptable mirrors, window materials, and multilayer substrates will be ensured through close collaboration with vendors. Samples produced by different vendors will be studied to select optimum window materials, and mirror and multilayer-substrate polishing methods. Related coherence measurement and beam wavefront characterization work will be performed at beamline 1-BM or, if necessary, at an insertion device beamline. This work will be conducted by a postdoctoral appointee to be hired during 2016. R&D and testing must be conducted on cryo-cooled mirrors to determine the cooling geometry that best preserves beam integrity.

Diamond as an optical element—for use as windows, substrates for fabrication of x-ray optics, reflecting surfaces, or otherwise—will have an increasing impact on light source facilities worldwide. The Optics Group will continue to monitor the current status of polycrystalline and single-crystal diamond growth and fabrication techniques in order to best serve the APS community.

10. Adaptive and beam-shaping optics

Status: Even the best reflective optics available today have some residual slope and form errors, which affect their nanofocusing properties, and some scientific applications are best served by mirrors that have variable focal lengths or produce designed beam profiles that are tailored to specific experiments' needs. The Osaka/SPring-8 team has demonstrated that an adaptive mirror can be used to correct aberrations of focusing, graded, multilayer optics to obtain a sub-10-nm focal spot. The team also demonstrated that deformable mirror technology is suitable for building K-B zoom optics to provide coherent x-rays with controllable beam size for applications such as coherent diffraction imaging and microscopy.

Strategic plan: While the APS Optics Group does not have in-house expertise in producing adaptive x-ray mirror systems, it is exploring collaborations with other institutions and industry to test and make available adaptive optics for specific future needs at the APS.

11. Optical and at-wavelength metrology

Status: From the beginning of operations, the APS has had a metrology laboratory that houses an array of commercial and custom-made metrology instruments to measure mirrors, both to verify that the manufacturers have reached contract specifications in terms of surface roughness, slope, and shape errors, and to predict the performance of beamlines as built. The metrology lab includes a stitching interferometer for measurements of figure over sub-0.01-mm to 100-mm-length lateral scales, a laser Fizeau interferometer for surface figure measurement of optics up 150 mm in diameter at normal incidence angle, and a new long-trace profilometer (LTP) that offers sub-50-nrad slope measurement accuracy on mirrors up to 1.5-m long. While the LTP is quite new, other metrology instruments are in need of replacement.

At-wavelength testing of optics is carried out at beamline 1-BM. A portable grating interferometer has been built for beam coherence and wavefront measurements. The system was commissioned during early FY 2016. It will be primarily used at 1-BM, but could be deployed at other APS beamlines. Rocking-curve topography leading to high-resolution strain mapping has also been implemented at 1-BM for the characterization of high-quality single crystals.

Currently, beamline 1-BM contains five Be windows, each 0.25-mm thick, which severely affect the interpretation of beam wavefront aberrations and coherence as well as high-resolution topography measurement data. Replacement of the double window in the 1-BM-A experiment hutch with a differential pumping setup, as done, for example, at beamlines 12-BM and 20-BM, is under way and should be completed in 2016. The remaining three windows cannot be replaced with differential pumping because they need to open onto experiment space in the 1-BM-B and 1-BM-C hutches.

Strategic plan: Simulations showed that the APS MBA lattice upgrade will require nano-focusing mirrors with slope error better than 50 nrad rms, and figure error <1 nm rms. Our strategy is continued development of metrology tools and methods to verify the quality of mirrors with such unprecedented surface parameters. To this end our future plans include the following:

- Improving optical metrology tools by upgrading obsolete tools and developing new sensors;
- Developing *in situ* metrology and new coherence measurement techniques;
- Improving the remaining three windows in beamline 1-BM by polishing, or possibly replacing them with diamond windows; and
- Using an insertion device beamline for testing optics for the APS-U that require an x-ray beam with a smaller horizontal emittance, larger coherent flux, or larger power load than the beam that can be obtained from 1-BM.

12. Optics systems approach and beamline integration

As part of achieving readiness for the APS-U, the performance of the suite of X-ray Science Division beamlines is being evaluated by measuring key parameters including flux, beam size, vibration, and coherence. The data collected, together with beamline simulations, are essential for future optimization and improvement. The measurements carried out on 14 APS beamlines have shown that the performance of most beamlines is affected not only by the quality of the optics, but also by the vibration and instability of the opto-mechanics, and in some cases by high heat load. Therefore, it has become clear that it is necessary to take into account the performance of the entire optics assemblies in the design, implementation, and integration of beamline optics. More specifically, the APS MBA upgrade has the potential for increasing the power load on the first monochromator optic. Therefore, realizing the full potential of the APS MBA will require optical assemblies with exceptional vibrational stability along with lower thermo-mechanical distortions and drift.

To meet this challenge, as recommended in the APS Optics Advisory Committee's first report,[†] we must consider a systems approach involving optics design and fabrication, cooling manifold design, assembly, and testing. This approach will require additional support staff as well as close coordination and partnerships with the beamline scientists and resident users, the relevant APS support groups, and the optics industry.

[†] The APS Optics Advisory Committee was established in January 2015. Its first meeting was held at the APS on March 16, 2015.