Active and Adaptive X-Ray Optics at Diamond Light Source

Introduction

Reflective mirrors are used on most synchrotron and free electron laser (XFEL) beamlines to transport X-rays from the source to the sample. They are achromatic and provide larger acceptance and less absorption compared to compound refractive lenses. Mirrors whose surface profile can be controllably changed are called “active optics.” This enables users to vary the beam profile or focal position. X-ray beamlines use two categories of active optics: mechanically actuated mirrors, which typically use one or two independent bending motors for cylindrical or elliptical bending [1]; and piezoelectric bimorph deformable mirrors.

Bimorph deformable X-ray mirrors have been used to focus X-rays at synchrotron and XFEL beamlines since early research in the 1990s by Susini et al. [2] and Signorato et al. [3] at the European Synchrotron Radiation Facility (France). Soon afterwards, bimorph mirrors were commercialized by Thales-SESO (France) and deployed at several labs, including the Advanced Photon Source (USA) and Diamond Light Source (UK), called “Diamond” from here on. Research by Diamond’s Optics & Metrology (O&M) group shows that the widely held bad impression of bimorph mirrors as unreliable and excessively complex is outdated and unfounded. With fast, precise metrology techniques developed at Diamond, the difficulties encountered by the early users of bimorph mirrors have been overcome, and Diamond has combined bimorph actuators with specialized substrates for several novel applications. Finally, Diamond’s improvements can help realize the true potential of bimorph mirrors to act as closed-loop, adaptive X-ray optics with real-time correction. Such dynamic optics could match the profile of an X-ray beam to a series of rapidly changing samples of different shapes and sizes, or provide fast, stable wavefront correction.

Evolution of bimorph mirrors

The early “first-generation” bimorph mirrors are shown in Figure 1a. Piezoelectric plates are sandwiched between the reflecting optical substrate and a lower substrate. Conductive electrodes (typically numbering between 8 and 32) are deposited at regular intervals along these piezoelectric plates. A unique voltage can be applied to each electrode through a dedicated electrical wire. This voltage causes localized bending of the optical substrate. Used in combination, multiple electrodes enable both localized control and global bending of the optical surface. These extra degrees of freedom allow the compensation of surface distortions caused by a range of factors, including clamping strain, gravity-induced sag, photon-induced heat bumps, or polishing errors. Bimorph mirrors can also correct higher-order aberrations in the wavefront of the photon beam caused by imperfect optics located upstream or downstream.

 Shortly after commissioning, many first-generation bimorph mirrors were found to suffer from large corrugations on the optical surface. Because the peaks and troughs appeared at the junctions between electrodes, this distortion was named the “junction effect” [4]. However, Diamond was able to repair these early mirrors by having their reflecting surfaces repolished by their manufacturer, Thales-SESO. X-ray measurements in Figure 2 show that the optical quality remained stable after repolishing, even after 4 years of continuous beamline operation. To solve the junction effect problem, second-generation bimorph mirrors were developed by Thales-SESO [5] and characterized at Diamond [6]. Piezoelectric elements are bonded to the side faces of a monolithic substrate, as shown in Figure 1b. Many second-generation bimorph mirrors have been in use at Diamond since 2017, and no junction effect has ever been observed.

Bimorph mirrors have been progressively improved by rectifying problems, including clamping strain from the holder, curvature drifts, and slow and unstable communication with beamline control systems [4]. Diamond’s O&M group solved these problems through a series of industrial collaborations. The first innovation was developing a new low-strain, kinematic opto-mechanical holder in collaboration with Cineo (Italy), and replacing the rigid electrical connectors with flexible wires in collaboration with Thales-SESO [7]. The second was standardizing the use of the HV-ADAPTOS power supply from CAEN & S.R. Tech (Italy) on Diamond’s beamlines. New algorithms onboard the HV-ADAPTOS were developed to provide enhanced user functionality and to correct piezoelectric creep. This reduced the time for stabilization of the reflected X-ray beam from tens of minutes to < 30 s at the Diamond beamline I24 [8]. The third strategy was developing user-friendly au-
Automated optimization scripts for the beamline teams, with training provided by the O&M group [9]. An upcoming improved EPICS driver will enable these scripts to run even more efficiently.

**Diamond’s advances in metrology**

Accurate metrology is essential to guide both the polishing and the opto-mechanical clamping of X-ray mirrors. As at the European XFEL [10], Diamond’s success with bimorph mirrors is underpinned by expertise in metrology.

Diamond has a highly advanced Optics Metrology Lab (OML) that contains a suite of metrology instruments to measure all aspects of surface quality using visible light [11]. This includes the Diamond-NOM slope profiler, which has demonstrably measured slope errors < 50 nrad for curved substrates [12], and a Zygo Fizeau HDX stitching interferometer for rapid measurements (within 30 s) of the height profile over two-dimensional regions [13]. For active optics, ex-situ (off-beamline) characterization of the repeatability and stability of bending prior to beamline installation is invaluable to expose problems and determine the optimal actuator settings to suit the beamline geometry. This approach has often saved significant X-ray commissioning time and effort.

Ex-situ testing is complemented by a range of in-situ, X-ray metrology techniques developed at Diamond’s bending-magnet versatile optics Test Beamline B16 [14], and performed on beamlines throughout Diamond. In-situ testing measures mirrors under real operational conditions, including vacuum forces and photon-induced heat loads. The pencil-beam method [15] has been applied at Diamond beamlines with a repeatability of 80 nrad and is in good agreement with ex-situ measurements in the OML [16]. A Foucault knife-edge method is regularly used to measure profiles of X-ray focal spots with widths below 1 µm. Several novel, in-situ metrology techniques are also being developed at Diamond. A super-polished bimorph mirror was optimized for focusing in only two iterations, and its final slope error reduced to below 200 nrad rms, using a grating interferometer to measure the wavefront error in the reflected beam at the coherence branch of the Diamond beamline I13 [17]. The phase and absorption gratings and the detector were all conveniently located downstream of the focus. Each measurement of the wavefront error required only a single image of the Moiré fringes produced by the two gratings, which was recorded with an exposure time of 0.5 s. Another novel metrology method, X-ray speckle tracking, was also tested using this mirror at B16 [18]. A speckle pattern is generated by a diffuser placed in the X-ray beam reflected from the mirror. As the diffuser is translated in the beam, the variation of the speckle pattern is captured and the wavefront error derived from it. By this means, the slope error on the bimorph mirror was reduced from 2.3 to 0.2 µrad rms.

**Novel combinations of bimorphs with special substrates at Diamond**

Super-polished bimorph mirror

Diamond has designed, tested, and installed bimorph mirrors with specially processed substrates to give unique X-ray reflecting properties. The first is a super-polished bimorph mirror shown in Figure 3 [19].

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**Figure 1:** (a) End view of a first-generation bimorph mirror. (b) Second-generation bimorph mirror, with piezo ceramics bonded to the side faces of the substrate to solve the junction effect.

**Figure 2:** Slope error of a first-generation, vertically focusing bimorph mirror on Diamond’s I22 beamline, just after repolishing and nearly four years afterwards. This demonstrates that the junction effect can be removed by repolishing and that it does not reoccur.
The 150-mm-long silica substrate of this mirror was polished by JTEC (Japan), using the elastic emission machining (EEM) technique [20]. It was pre-figured to a tangential ellipse with a source-to-mirror distance $p = 41.5$ m, a mirror-to-image distance $q = 0.4$ m, and a grazing incidence angle $\theta = 3$ mrad. Thales-SESO then bonded the piezoceramic bars to the substrate to create a bimorph with eight electrodes. The finished mirror was characterized on the Diamond-NOM, and the optimal voltages found to shape its surface to two very different ellipses, $E_1 \ (p = 46.5$ m, $q = 0.4$ m, $\theta = 3$ mrad) and $E_2 \ (p = 46.5$ m, $q = 0.33$ m, $\theta = 2.5$ mrad). In both cases, the residual height error was below 1 nm rms. For the first ellipse, the residual slope error was $\sim 150$ nrad rms. This mirror was then tested with X-rays at B16. Optimization was performed using both the pencil-beam method and X-ray speckle. In all cases, optimization was achieved by determining the bimorph mirror’s response to a voltage increment applied to each electrode (“piezo response function”) and then using the interaction matrix method to calculate the best voltages to achieve the given shape [15, 16]. The mirror successfully defocused the width of the beam from $<1$ µm to 50 µm with acceptable striations, as measured by a PCO4000 CCD camera and a 5-µm-thick Eu:LuAG scintillator. A 20× objective gave an effective pixel size of 0.45 µm (Figure 4 left, showing defocusing up to 26 µm). The mirror also achieved a focal spot of FWHM 0.77 µm for $E_1$, and 0.52 µm for $E_2$ (Figure 4 center and right), which matched with theory. These measurements were taken with knife-edge scans using a 200-µm-diameter gold wire. The X-ray energy was selected at 8 keV by the B16 Si (111) double-crystal monochromator. This makes the

Figure 3: (a) Measurement geometry for the super-polished bimorph mirror on the Diamond Test Beamline B16. (b) Photograph of the super-polished bimorph mirror. (c) Typical image of a speckle pattern.
super-polished bimorph mirror promising for shaping X-ray beams to highly desired, non-Gaussian profiles, in particular a uniform-intensity “flat top” of chosen width. Multiple parabolic arcs have been added to the surface of the super-polished bimorph mirror using the piezos to achieve defocused beams on B16 with reduced structures [21].

Multilayer-coated bimorph mirror

Diamond’s X-ray pair distribution function beamline I15-1 needed an efficient optical element with a large aperture to vertically focus its wiggler beam to a spot size of 20 µm at X-ray energies of 40–80 keV and with a variable focal distance over a range of nearly 1 m. Because no such optic was commercially available, a novel design was developed to produce the world’s first 1-m-long, multilayer-coated bimorph mirror that operates up to nearly 80 keV (Figure 5) [22]. Its manufacture was coordinated by Cinel, in collaboration with Diamond. The substrate was polished by Thales-SESO to the required ellipse $(p = 31.8$ m, $q = 4.0$ m, $\theta = 4.2$ mrad) with a tangential slope error below 1 µrad rms. A micro-roughness below 2 Å rms was needed to ensure high multilayer reflectivity. Rigaku Innovative Technologies (USA) coated the active area with three parallel, 10-mm-wide, laterally graded multilayer stripes: Ni/B₄C for 40.0 keV, W/B₄C for 65.4 keV, and Pt/B₄C for 76.6 keV. After coating, Thales-SESO glued the piezoelectric actuators to the sides of the substrate and deposited 16 electrodes to create a versatile second-generation bimorph. Diamond-NOM scans confirmed the polishing quality and piezo functionality. In-situ pencil-beam scans optimized the voltages for focusing at three different distances (3.8 m, 4.26 m, and 4.72 m) downstream of the mirror. At each position, knife-edge scans of the focal spots yielded a FWHM of ~ 13 µm for all three energies. The peak reflectivity exceeded 70% and the error of the multilayer d-spacing was acceptably low (< 1%). The mirror met all of the design specifications and has been successfully used since 2015 for user experiments on the I15-1 beamline.

Dynamic, adaptive bimorph mirrors

Bimorph mirrors show their true worth when flexibility of focal length and beam shape is required. Traditionally, bimorph mirrors at synchrotrons and XFELs have been operated quasi-statically in open loop. Such mirrors typically operate at a fixed curvature for many hours, days, or even months, with only small, intermittent corrections.

Now, great changes are afoot. As synchrotrons and XFELs are upgraded around the world to produce brighter X-ray beams, there is a
growing demand for quick and frequent sample changes. Many beamlines, particularly those dedicated to macro-molecular crystallography, now routinely measure hundreds, and sometimes thousands, of samples per day. Such beamlines wish to rapidly manipulate the size and shape of the X-ray beam to suit the dimensions of each sample, or to illuminate different-sized regions of larger samples.

Bimorph mirrors are better suited than mechanically bent mirrors for rapid, controllable changes because the piezoelectric effect operates almost instantaneously, without generating heat or mechanical wear. However, even with improved holders and creep compensation [7, 8], each transition from an initial curvature to a final shape must be uniquely compensated. To solve these issues, Diamond is developing high-speed “adaptive” X-ray optics to operate in closed loop with real-time correction based on fast metrology feedback. Absolute displacement feedback of the optical surface is provided by embedded ZPS™ interferometric sensors from Zygo (USA) (Figure 6), as also demonstrated at NSLS-II [23]. Up to 64 sensors can be operated simultaneously at > 200 kHz. ZPS sensors have been tested on the Diamond-NOM [24] on a second-generation bimorph mirror with 600 mm length and 16 electrodes [7]. Software on the HV-ADAPTOS was upgraded to automatically calculate and apply the voltages necessary to correct the surface to the required profile at 1 Hz. The Diamond-NOM and the ZPS sensors agreed well in their measurements of the mirror’s height profile. The ZPS sensors could demonstrably resolve changes in the mirror’s sagitta (depth of center) as small as 500 picometers. The ZPS sensors were able to record the mirror’s figure as it changed between a fourth-order polynomial, a Gaussian curve, and a Lorentzian curve every 10 s. This demonstrates not only the real-time capabilities of the ZPS sensors, but also the superior adaptability of bimorph mirrors. X-ray demonstrations at B16 of closed-loop, adaptive optic performance are being submitted for publication [25]. In future, closed-loop control could be achieved using direct feedback from the X-ray beam. Feedback at tens or hundreds of Hz to compensate vibrations and drifts caused by other optics and motion stages on the beamline would enhance the beam’s stability.

Summary

An extensive R&D program at Diamond over the past decade has led to the enhanced usage of bimorph mirrors on several beamlines. The past problems with first-generation bimorphs are mentioned because of the unjustified, yet still widely held, belief that bimorph mirrors are not reliable for synchrotron and XFEL beamlines. Diamond has resolved many of the initial issues: by repolishing, by upgrading the opto-mechanics and the HV power supplies, and by the adoption of second-generation bimorph technology. Since then, Diamond has applied these lessons to create novel active X-ray optics, combining bimorph technology with specially prepared substrates to achieve unparalleled X-ray shaping capabilities. One such optic, the super-polished bimorph mirror, achieved sub-micron focusing of an X-ray beam and was able to expand the X-ray beam at the focal point by a factor of over 50. A long multilayer-coated bimorph mirror achieved X-ray focusing of a large wiggler source of high photon energy (up to 76.6 keV) at distances controllable over a range of nearly 1 m. All such advances have gone hand-in-hand with corresponding advances in metrology and many close collaborations. Now, the rapid, real-time control of X-ray beam shapes by fast, stable “adaptive” bimorph mirrors at Diamond appears within reach thanks to the ZPS displacement sensors, which are capable of measuring mirror surface errors with sub-nanometer resolution at kHz frequencies. The successful tests of these sensors are an indispensable step toward closed-loop operation, which will enable X-ray beam shaping and wavefront correction within seconds. Furthermore, non-specialist beamline users can achieve the advantages of bimorph mirrors without expert assistance.

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