

ALS-U Beamline Performance Simulations with Metrology Data Managed through the Bluesky-Tiled Framework

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ABSTRACT

The Advanced Light Source Upgrade (ALS-U) will deliver a diffraction-limited storage ring, which places stringent demands on beamline optics. We present a scripted simulation pipeline that predicts beamline performance from measured mirror figure errors and apply it to the COSMIC-U (7.0.1) and MAESTRO-U (7.0.2) insertion-device beamlines. Ray-tracing models built with `shadow4` in OASYS 2.0 are exported as Python scripts and turned into parameterized builders, which bring the mirror metrology of the ALS X-Ray Optics Laboratory, retrieved by unique identifier from a Bluesky-Tiled server, and the measured influence functions of the adaptive X-ray optics (AXOs) into one pipeline. With ideal optics, energy scans across every grating agree with analytical estimates of the beam size and photon energy resolving power. Before the AXO correction, including the measured figure errors mainly shifts the horizontal focus away from the exit slit, while the resolving power stays above its design target at every energy; grating figure errors are not yet included. Fitting the AXO voltages directly to the beam at each photon energy keeps the horizontal width within 0.6% of ideal on COSMIC-U and slightly below it on MAESTRO-U, with no actuator above 300 V. Including the measured figure errors and the AXO correction, both beamlines are therefore expected to perform close to their design. In general, this approach offers a reproducible way to use as-built optic data in performance predictions during construction, and a starting point for a beamline digital twin.

Keywords: X-ray Optics, Simulation, Metrology, Adaptive Optics, Synchrotron

1. INTRODUCTION

Over the past decade, synchrotron facilities worldwide have begun upgrading to diffraction-limited storage rings (DLSRs), which deliver X-ray beams of far higher brightness and transverse coherence.¹ These gains come with tighter tolerances on the beamline optics. By the Maréchal criterion, a Strehl ratio above 0.8 requires a root-mean-square wavefront error below $\lambda/14$,² which at soft X-ray wavelengths means mirror figure errors at the nanometer level. Meeting these tolerances at newly upgraded DLSRs is widely discussed in the community.^{3,4} As a result, the measured surface of each mirror, and not only its design shape, limits how well performance can be predicted.

The ALS-U project⁵ is an ongoing upgrade of the Advanced Light Source (ALS) at the Lawrence Berkeley National Laboratory (LBNL). Once completed, it will raise the soft X-ray coherent flux by two orders of magnitude over the present ALS.⁶ Several of its insertion-device beamlines share a common optical design:^{4,7} a cooled flat first mirror absorbs most of the power and deflects the beam horizontally, a variable-line-spacing (VLS) plane-grating monochromator (PGM) disperses and focuses the beam vertically, and a final adaptive X-ray optic (AXO) focuses it horizontally. The AXO is a mirror pre-figured to an ellipse, with its shape tunable in operation by an array of piezoelectric actuators to correct errors in the beam. Two flagship beamlines, COSMIC-U

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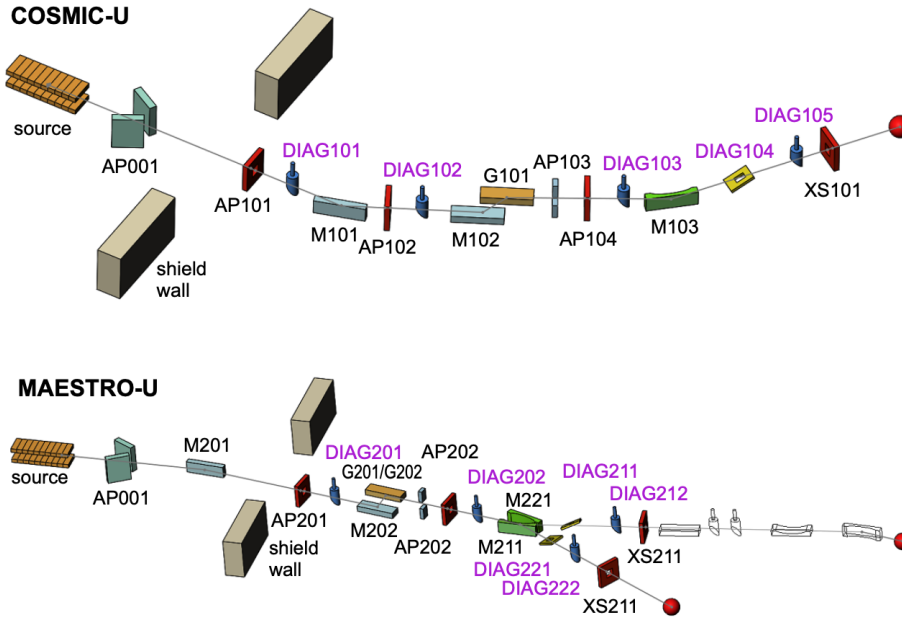


Figure 1. Optical layouts of the COSMIC-U (top) and MAESTRO-U (bottom) insertion-device beamlines. COSMIC-U M103 and MAESTRO-U M221 are the elliptical AXOs that focus the beam horizontally. The microARPES branch of MAESTRO-U (M211 and downstream) is outside the scope of this work. (Courtesy of the ALS-U Project Team.)

(7.0.1) and MAESTRO-U (7.0.2), follow this design (Figure 1, Table 1). They are the upgrades of the COherent Scattering and MICroscopy (COSMIC) and the Microscopic and Electronic Structure Observatory (MAESTRO) beamlines, respectively. The mirrors modeled here have been delivered and acceptance-tested in the X-Ray Optics Laboratory (XROL) at the ALS,⁸ which measured their surface profiles as well as the response of each actuator of COSMIC-U M103 and MAESTRO-U M221, the two AXOs modeled here.

Predicting whether the beamlines will deliver the specified performance calls for simulations driven by the measured figure errors of their mirrors and the actuator response of their AXOs. Graphical environments such as OASYS and Sirepo are widely used to design such beamlines.^{4,9,10} Exporting the models built in these environments as parameterized Python scripts turns single simulations into systematic studies: the effect of each mirror's figure errors can be followed across the full photon-energy range of every grating, and the ability of the AXO to compensate for these effects can be tested. Scripted models also provide the building blocks for constructing a beamline digital twin, a computational model that is continually refined with data from metrology, alignment measurements, and beam diagnostics as they become available during commissioning and operation. In addition, these scripted models can be called directly by the optimization and machine-learning tools now emerging for beamline automation.^{11–13} To fit naturally into these Python-based workflows, as well as into facility data infrastructure, the measured figure-error data are managed with the Bluesky-Tiled framework,¹⁴ a data management system developed at NSLS-II that retrieves each dataset by a unique identifier (UID) together with its full provenance metadata.

In this work, we build models of COSMIC-U and MAESTRO-U in OASYS 2.0^{9,10} using the ray-tracing code `shadow4`.¹⁵ The models are then exported into a Python-based pipeline that links them with the XROL metrology, including the measured actuator responses of the AXOs. With this pipeline, we perform energy scans across the operating range of every grating and compare the simulated beam size and photon energy resolving power with analytical estimates. We then include the measured figure errors of each mirror, which the builders retrieve by UID from a Bluesky-Tiled server, and show their effects on beam properties at different photon energies. Finally, we correct the horizontal errors with the AXOs, fitting the actuator voltages either to the AXO's own figure error or to the beam of the whole beamline, and show that the whole-beamline correction brings the focused beam back close to its ideal size.

Table 1. Design parameters for the COSMIC-U and MAESTRO-U beamlines. Spot targets are for the horizontal (H) and vertical (V) directions at the exit slit.

Parameter	COSMIC-U	MAESTRO-U
Energy range [eV]	250–2500	60–600
Photon energy resolving power	> 5,000	> 15,000 to > 30,000
Spot target, H×V [μm]	< 10×10	< 25×18
Horizontal focusing optic	M103 (elliptical AXO)	M221 (elliptical AXO)
Undulator period [mm]	38	70
Acceptance [μrad]	210	450

Table 2. Predicted demagnification $1/M$ of the source at the exit slit, for each grating in the vertical (V) plane and for the AXO in the horizontal (H) plane. c_{ff} is the design value of each grating; $1/M = c_{\text{ff}} r/r'$ in the vertical and p/q in the horizontal plane.

	COSMIC-U				MAESTRO-U		
Optic	G101	G102	G103	M103	G201/G202	G203/G204	M221
Plane	V	V	V	H	V	V	H
c_{ff}	1.632	1.577	1.731	—	4.0	2.2	—
$1/M$	5.24	5.06	5.56	4.72	9.44	5.19	3.71

The paper is organized as follows. Section 2 describes the beamline models, the metrology data, and the scripted pipeline. Section 3 applies the pipeline to COSMIC-U and MAESTRO-U in three steps: with ideal optics, including the measured figure errors, and with the AXO correction. Section 4 discusses the next inputs to the pipeline and beam-based correction toward a digital twin, and Section 5 concludes.

2. METHODS

Figure 2 outlines the simulation pipeline. The beamline models are built interactively in OASYS 2.0 (Section 2.1) and exported as Python scripts, which we turn into parameterized builders (Section 2.3). The measured figure errors and AXO influence functions from XROL (Section 2.2) are retrieved from a Bluesky-Tiled server by UID. The builders are then called in loops over photon energy, grating, and mirror for the studies in Section 3.

2.1 Beamline models in OASYS 2.0

For both beamlines, we build the models in OASYS 2.0,¹⁰ the recently released version of the graphical environment that assembles different simulation engines into widget-based workflows. For this work, we use the ray-tracing code **shadow4**, which can be driven from Python, so the models assembled in OASYS 2.0 can be exported as standalone Python scripts and integrated into larger workflows (Section 2.3). Figure 3 shows the widget chains of both beamlines.

In OASYS 2.0, changing the photon energy means updating the source size and divergence and recomputing the monochromator with the VLS PGM pre-processor widget (“VLS PGM Coeff Calc” in Figure 3), which gives the grating angles and the positions of the premirror and the grating for the chosen energy. To include the measured figure errors, we convert the XROL data into HDF5 height-error meshes, which a Surface File Reader widget attaches to each mirror in **shadow4**. While this interactive workflow is intuitive for building and checking a model, it becomes harder to use for studies over many photon energies, gratings, or error configurations, where these settings must be entered again for every case.

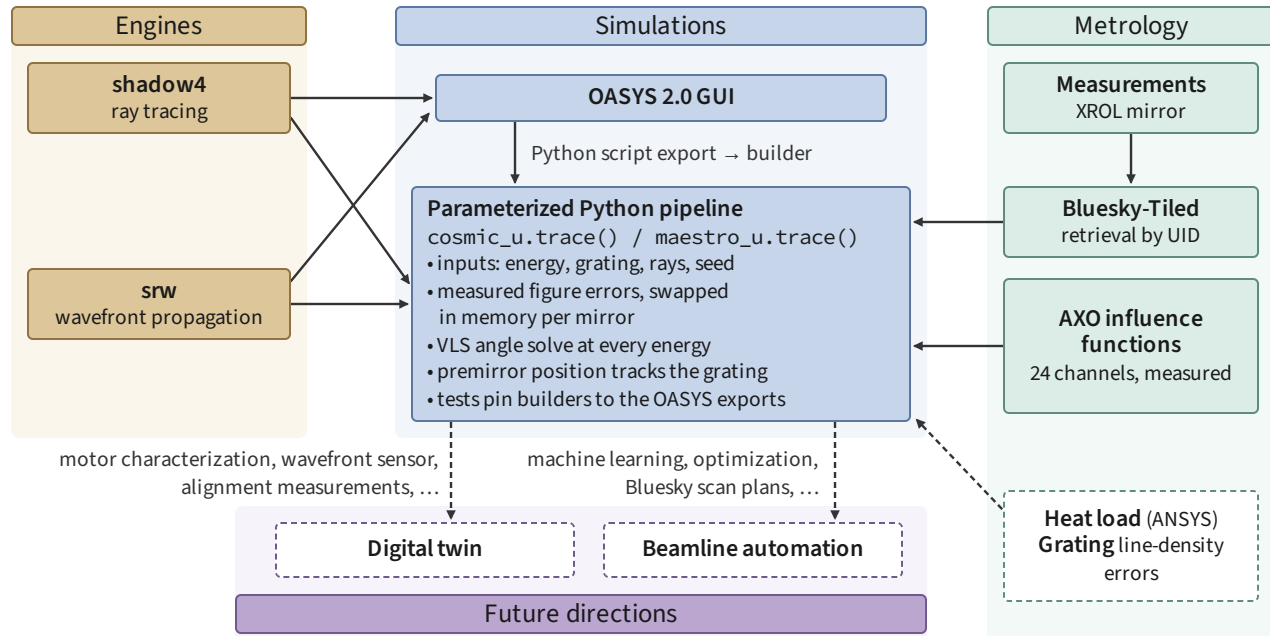


Figure 2. Scripted simulation pipeline. Beamline models built in the OASYS 2.0 GUI with **shadow4** are exported as Python scripts and turned into parameterized builders. The builders take the photon energy, grating, number of rays and seed as arguments, solve the VLS grating angles and the premirror position at every energy, and load the measured figure error of each mirror in memory. The XROL profiles can be retrieved by UID from a Bluesky-Tiled server, and the measured AXO influence functions enter the same pipeline. Dashed boxes mark inputs and directions not yet implemented. The **srw** models are also implemented, but their results are not presented in this work.

2.2 Metrology data

XROL measures the tangential slope of each mirror over its full measured length, and integrating it gives a one-dimensional height profile. To characterize the flat mirrors (COSMIC-U M101 and M102, MAESTRO-U M201 and M202), we fit a straight line to the measured slope over the length listed in Table 3 and integrate the residual into height, which removes piston, tilt, and curvature. The residual height error is shown in Figure 4 (top) and listed in Table 3, along with the radius of curvature R from this fit. In the simulations, the full measured profiles (curvature included) enter as errors of these mirrors, and for simplicity each profile is treated as uniform in the sagittal direction, forming a two-dimensional mesh. It should be noted that, although COSMIC-U M102 and MAESTRO-U M202 exceed their height-error specifications over this length, our simulations show that the beam illuminates less than half of either mirror over the whole operating range (Section 2.3), and over the illuminated region alone their rms height errors are within specification.

The last mirror of each beamline, COSMIC-U M103 and MAESTRO-U M221, is an AXO, an elliptically pre-figured mirror with 24 piezoelectric actuators. Figure 4 (bottom) shows their figure errors, obtained by subtracting from the measured profile an ideal ellipse that focuses the beam as designed, with the design source and image distances; the grazing angle of this ellipse and an overall tilt are fitted to the measured shape. Table 3 lists their rms values.

Although these errors, 8.82 nm rms on COSMIC-U M103 and 34.6 nm rms on MAESTRO-U M221, are far above the specifications, they lie well within the correction range of the actuators. A voltage applied to an actuator bends the mirror locally. Assuming a linear response, the corrected surface is the measured surface plus a linear combination of the influence functions of the actuators, the height change per volt of each one (Figure 5), with the voltages as coefficients. Beyond its own figure error, the AXO can also compensate the horizontal errors that the beam accumulates from the mirrors upstream, as shown in Section 3.

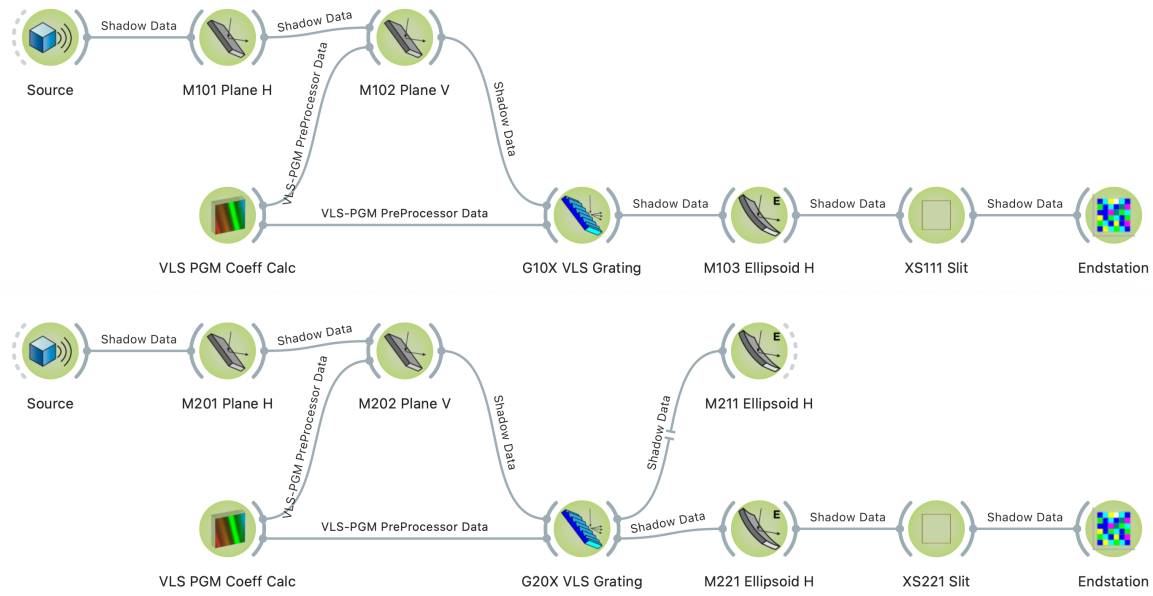


Figure 3. OASYS 2.0 **shadow4** widget chains. **Top:** COSMIC-U, where the grating G10X stands for G101–G103. **Bottom:** MAESTRO-U, where G20X stands for G201–G204; the microARPES branch (the “M211 Ellipsoid H” widget) is outside the scope of this work.

2.3 Scripted simulation pipeline

Each exported Python script is a fixed sequence of calls that reproduces one configuration of the OASYS 2.0 model. We copy it once into a builder function, in which the quantities that a study varies become arguments: the photon energy, the grating, which mirrors carry figure errors and which profiles they use, the position of the observation plane along the beam, and the number of rays and random seed. Everything else is kept as exported, and automated tests check that each builder reproduces the original export when given the same inputs.

For this work, the builders retrieve the measured figure errors from a Bluesky-Tiled server by their UUIDs. At XROL, measured profiles are currently stored as files and shared through cloud storage, so we wrote them to the Tiled server ourselves as a proof of concept. Bluesky-based acquisition is being developed and tested at XROL;

Table 3. Mirror specifications and measured figure errors for COSMIC-U and MAESTRO-U. Length is the tangential length over which the profile is evaluated (the measured length less its edges, or the clear aperture); orientation denotes the deflection plane. Specified height-error tolerances are defined over the CA to satisfy the Maréchal criterion. Measured values are the rms residual height errors of the mirror surface profiles measured at XROL over that length (Section 2.2).

Optic	Shape/type	Length [mm]	Orientation	Height error rms [nm]		R [km]
				Spec.	Measured	
COSMIC-U (7.0.1)						
M101	flat/cryo	141	Horizontal	0.8	0.11	40
M102	flat	295	Vertical	1.1	1.87	263
M103	elliptical, AXO	238	Horizontal	1.3	8.82	—
MAESTRO-U (7.0.2)						
M201	flat/cryo	111	Horizontal	1.88	0.09	31
M202	flat	272	Vertical	1.88	2.44	212
M221	elliptical, AXO	238	Horizontal	1.0	34.6	—

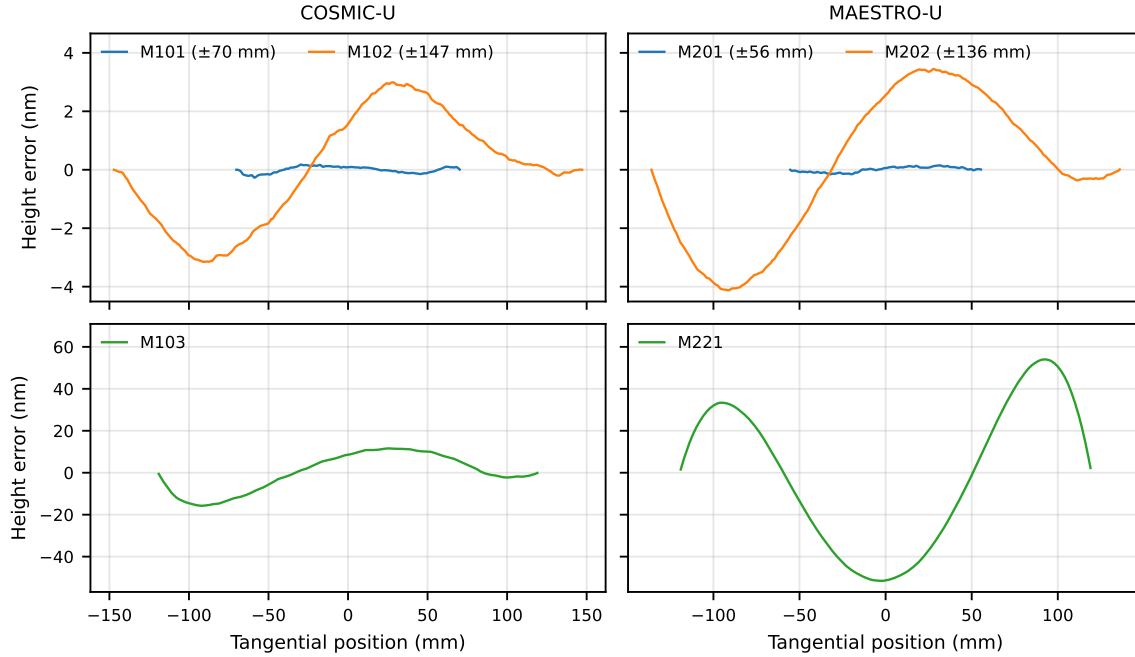


Figure 4. Tangential height-error profiles measured at XROL. **Left:** COSMIC-U. **Right:** MAESTRO-U. **Top:** flat mirrors, over the length in Table 3, shown after removing a best-fit line from the measured slope and integrating to height. The simulations use the full profile. **Bottom:** AXO mirrors, over ± 119 mm, as residuals from the ellipse fitted at their installation angle, before the actuator correction. Each row shares one vertical scale.

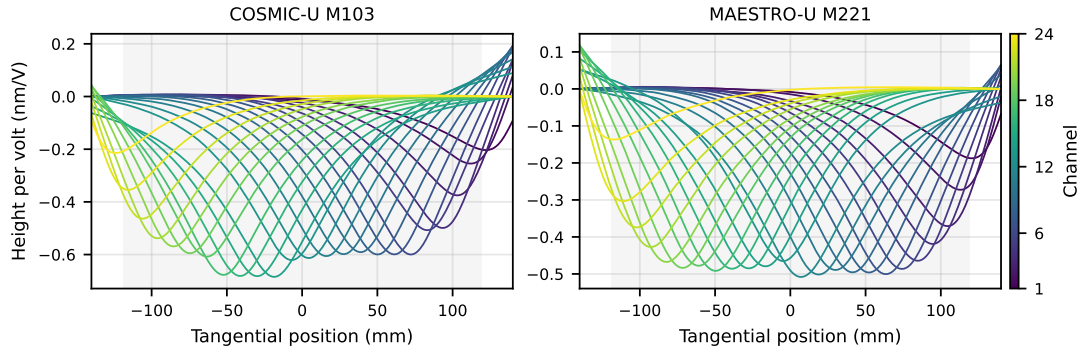


Figure 5. Measured influence functions of the 24 actuators of COSMIC-U M103 (left) and MAESTRO-U M221 (right), as height change per volt, smoothed as used in the simulations. Color denotes the channel. The shaded band marks the ± 119 mm range over which the AXO figure errors are fitted.

once in use, each measurement will be stored on the server with its UID and metadata as it is taken and can enter the simulations directly.

At every photon energy, the builders update the source and the monochromator automatically, replacing the manual widget settings described in Section 2.1. The source size and divergence are computed from the design parameters of the ALS-U electron beam⁵ and of the undulator of each beamline. The grating angles satisfy the grating equation $m\lambda = d_0 (\sin \alpha - \sin \beta)$ together with the VLS defocus condition¹⁶

$$\frac{\cos^2 \alpha}{r} + \frac{\cos^2 \beta}{r'} = m\lambda g_1, \quad (1)$$

where α and β are the incidence and diffraction angles measured from the surface normal, r and r' are the source and image distances of the grating, $d_0 = 1/g_0$ is the central groove spacing, and g_1 is the first VLS ruling

coefficient in the groove-density expansion $g(w) = g_0 + g_1 w + \dots$. The two equations are solved numerically at each energy, and the premirror pitch and its position along the beam follow from the fixed-exit condition. The fixed-focus constant $c_{\text{ff}} = \cos \beta / \cos \alpha$ equals the design value of the grating (Table 2) only at its design energy and varies slightly elsewhere.

With these functions, every study becomes a loop over the builder arguments that runs without manual steps. Energy scans are laid out over the range of each grating, so the photon energies where the gratings switch are included. The measured figure errors are held in memory as height meshes, one per mirror, so a mirror's figure error is switched on or off, or replaced by another measurement, through a single argument. Energy scans, per-mirror on/off studies, and through-focus scans over the operating range of both beamlines are therefore run directly from Python. The builders also record where each ray hits every optic, which gives the beam footprints quoted in Section 2.2 and is used in the AXO correction below.

The AXO correction runs in the same loop. Each AXO is simulated at the grazing angle fitted to its measured shape, with the fit residual as its figure error (Section 2.2). The corrected surface is this residual plus a linear combination of the measured influence functions f_j , with the voltages V_j as coefficients, within an assumed limit of ± 500 V. To correct only the AXO's own figure error, we fit the slopes of the influence functions to the negative of the residual slope over ± 119 mm. In practice, the AXO must also compensate the horizontal errors that the beam accumulates from the mirrors upstream. For this whole-beamline correction, we fit the voltages directly to the beam, using a single trace with the actuators off. In that trace, each ray i hits the AXO at position y_i and the exit slit at x_i . Changing the voltages changes the surface slope under each ray and, to first order, moves the ray at the exit slit to

$$x_i(V) = x_i + 2q \sum_j V_j f'_j(y_i), \quad (2)$$

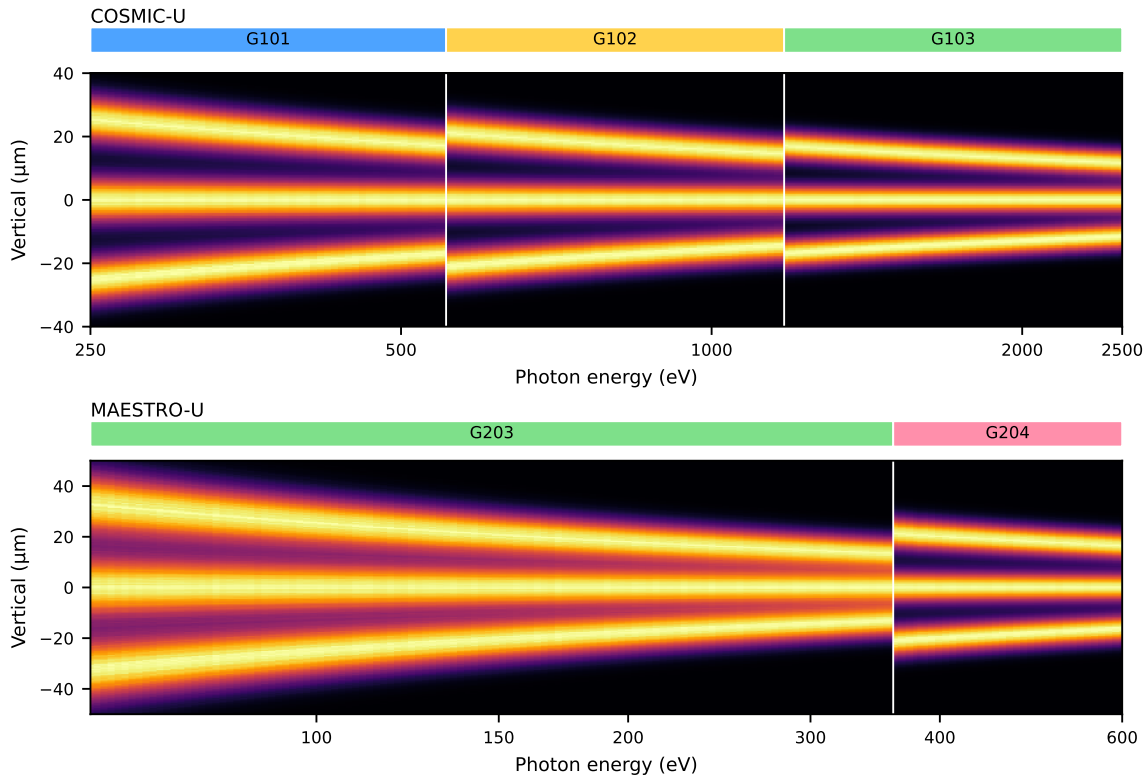


Figure 6. Dispersive-direction (vertical) profile at the exit slit versus photon energy with ideal optics, for a source with three photon energies E and $E(1 \pm 1/R_t)$ (shadow4). **Top:** COSMIC-U, $R_t = 5,000$. **Bottom:** MAESTRO-U, $R_t = 15,000$, with the $c_{\text{ff}} = 2.2$ gratings. Each energy is normalized to its maximum, and the photon energy axis is logarithmic. White lines mark the grating changes; the bar above each map gives the grating.

where q is the image distance of the AXO. The voltages that minimize the mean of $x_i^2(V)$, the squared spot size plus the squared centering error, follow from a linear least-squares fit. This fit uses no figure-error metrology of any mirror and is repeated at each photon energy. In both fits, a small penalty on the voltages keeps them low where the data do not constrain them, and the corrected beamline is then traced again.

Finally, to check the scripted results against analytical estimates, we compare them with the expected width of the focused beam for ideal optics. Since the optics in the horizontal and vertical planes of these beamlines are decoupled, the two planes can be treated separately.⁷ Vertically, the grating focuses the beam onto the exit slit with demagnification $1/M = c_{\text{ff}} r/r'$ (Table 2); horizontally, the AXO images the source with $1/M = p/q$, where p and q are its source and image distances. For ideal mirrors, the expected width of the focused beam at the exit slit in each plane is

$$w(E) = \frac{2.355 \Sigma(E)}{1/M}, \quad (3)$$

which is the full width at half maximum (FWHM) of a Gaussian beam. Here $\Sigma(E) = \sqrt{\sigma_e^2 + \sigma_r^2(E)}$ is the source size in that plane, which combines the electron-beam size σ_e and the diffraction-limited photon source size $\sigma_r(E)$.

3. RESULTS

All results in this section are traced with **shadow4**, using 5×10^5 rays and the same random seed (12) in every case for consistency, so that the cases differ only in their optics. We describe the beam size in each plane by the width $w = 2.355 \sigma$, where σ is the intensity-weighted rms of the ray positions. For a Gaussian beam this equals the FWHM of Equation 3. Because each measured profile is one-dimensional (Section 2.2), a mirror's figure error deflects rays only in that mirror's deflection plane and leaves the width in the other plane unchanged (Table 4), so we report the two planes separately. Results at a single energy are given at 1 keV for COSMIC-U (grating G102) and at 300 eV for MAESTRO-U (grating G203).

3.1 Ideal optics

We first trace both beamlines with ideal optics over their full operating range. The builders are called at different photon energies from 250 to 2500 eV for COSMIC-U and from 60 to 600 eV for MAESTRO-U, with the grating angles and the premirror position solved at each energy. The energy grids are laid out over the range of each grating, so they include the grating changes at around 550 eV and 1175 eV on COSMIC-U and at around 360 eV on MAESTRO-U. The simulated widths follow Equation 3 to within 0.02% horizontally and 1% vertically on both beamlines (Figure 8, where they are shown together with the results including the measured figure errors). The small mismatch in the vertical plane arises because Equation 3 uses the design value of c_{ff} for each grating, whereas c_{ff} varies slightly with photon energy. With ideal optics, COSMIC-U meets its $< 10 \times 10 \mu\text{m}$ spot target (Table 1) above 500 eV, and MAESTRO-U meets its $< 25 \times 18 \mu\text{m}$ target above 83 eV, covering most of the design range of each beamline.

The same loop traces the resolving power as well. The source is given three photon energies, E and $E(1 \pm 1/R_t)$, where R_t is the design target: 5,000 for COSMIC-U and 15,000, the low end of the design range, for MAESTRO-U (Table 1). At the exit slit, adjacent energies are separated by one width exactly when the resolving power equals the target, so energies that are resolved show directly that the target is met. Figure 6 shows the resulting dispersive-direction (vertical) profile across both operating ranges. From this profile, the resolving power follows as $E|D|/w_v$, independent of the spacing, where the dispersion D is given by the separation of the outer two energies and w_v is the width of the center energy. It ranges from 8,408 to 11,118 on COSMIC-U and from 19,344 to 30,711 on MAESTRO-U, exceeding the design targets.

To check these values, we compare them with an analytic estimate, the dispersion of the grating divided by the vertical width predicted by Equation 3, both evaluated with the grating angles at each photon energy. Both the simulation and the estimate assume an exit slit matched to the focused beam. At every energy the simulated resolving power agrees with the analytic value to within 0.1% (Figure 8, right).

Table 4. Width $w = 2.355\sigma$ at the exit slit, horizontal (H) and vertical (V), with each mirror’s measured figure error applied alone and together, and position z_w of the horizontal waist from the second moments of the rays, relative to the exit slit (positive downstream). Changes relative to ideal optics are given in parentheses, in percent. COSMIC-U at 1 keV (G102), MAESTRO-U at 300 eV (G203). The AXOs, COSMIC-U M103 and MAESTRO-U M221, are shown before the AXO correction (Section 3.3); grating figure errors are not included.

Figure errors	COSMIC-U, 1 keV			MAESTRO-U, 300 eV		
(COSMIC-U / MAESTRO-U)	H [μm]	z_w [mm]	V [μm]	H [μm]	z_w [mm]	V [μm]
none (ideal)	8.22	−1.6	8.56	14.48	−2.2	10.97
M101 / M201	9.31 (+13.3)	21.8	8.56 (0.0)	14.60 (+0.8)	8.1	10.97 (0.0)
M102 / M202	8.22 (0.0)	−1.6	8.68 (+1.4)	14.48 (0.0)	−2.2	10.97 (+0.02)
M103 / M221	8.85 (+7.7)	12.4	8.56 (0.0)	21.02 (+45.1)	−50.4	10.97 (0.0)
M101, M102, M103 / M201, M202, M221	11.24 (+36.7)	35.9	8.68 (+1.4)	18.86 (+30.2)	−40.2	10.97 (+0.02)

Table 5. AXO correction. **Top:** rms height and slope error of each AXO over ± 119 mm before and after the own-mirror fit. **Bottom:** horizontal width w at the exit slit, its change relative to ideal optics, the change of the horizontal divergence, and the largest actuator voltage, at 1 keV (G102) for COSMIC-U and 300 eV (G203) for MAESTRO-U. “Incl. figure errors” has the measured figure errors of M101, M102, and M103 (M201, M202, and M221) with the AXO off; “own mirror” and “whole beamline” add the two fits. Repeating the corrected cases with four other random seeds changes their size relative to ideal by less than 0.1 percentage point.

	COSMIC-U M103, 1 keV				MAESTRO-U M221, 300 eV			
AXO height rms [nm]	8.82 $\rightarrow$ 0.13				34.6 $\rightarrow$ 0.07			
AXO slope rms [nrad]	336 $\rightarrow$ 81				1385 $\rightarrow$ 36			
Beam	w [μm]	Δw [%]	$\Delta\text{div.}$ [%]	$ V _{\text{max}}$ [V]	w [μm]	Δw [%]	$\Delta\text{div.}$ [%]	$ V _{\text{max}}$ [V]
ideal optics	8.22	—	—	—	14.48	—	—	—
incl. figure errors	11.24	+36.7	+0.8	—	18.86	+30.2	+1.5	—
own mirror	9.47	+15.3	+1.1	89	14.61	+0.9	+0.6	146
whole beamline	8.25	+0.4	+1.5	156	14.37	−0.8	+0.7	75

3.2 Including the measured figure errors

Next, the pipeline attaches the measured figure errors (Section 2.2). Because the height meshes are held in memory, each mirror’s error is switched on or off by one argument of the builder, and the same calls give each mirror’s error alone, all of them together, and the full energy scans. The AXOs, COSMIC-U M103 and MAESTRO-U M221, enter with the figure errors left after fitting their installation angle, before any actuator correction. All horizontal results in this section are therefore before the AXO correction, which follows in Section 3.3.

Table 4 lists the widths at the single-energy settings with each mirror’s figure error applied alone and with all of them together. Including the measured figure errors of M101, M102, and M103, the COSMIC-U horizontal width at the exit slit grows by 36.7% at 1 keV; including those of M201, M202, and M221, the MAESTRO-U width grows by 30.2% at 300 eV. Most of this growth is a shift of the focus rather than a blur. On both beamlines the horizontal waist moves tens of millimeters away from the exit slit (Table 4), and at the waist the COSMIC-U spot is close to its ideal size (Figure 7). Such a focus error is what an adaptive mirror is designed to correct.

Over the full operating range (Figure 8, left), the figure errors increase the horizontal width at the exit slit by 25.4 to 44.8% on COSMIC-U and by 21.0 to 30.6% on MAESTRO-U, before the AXO correction. The horizontal divergence changes by at most 0.9% and 1.6%, so the focus error seen at the single-energy settings persists across both ranges.

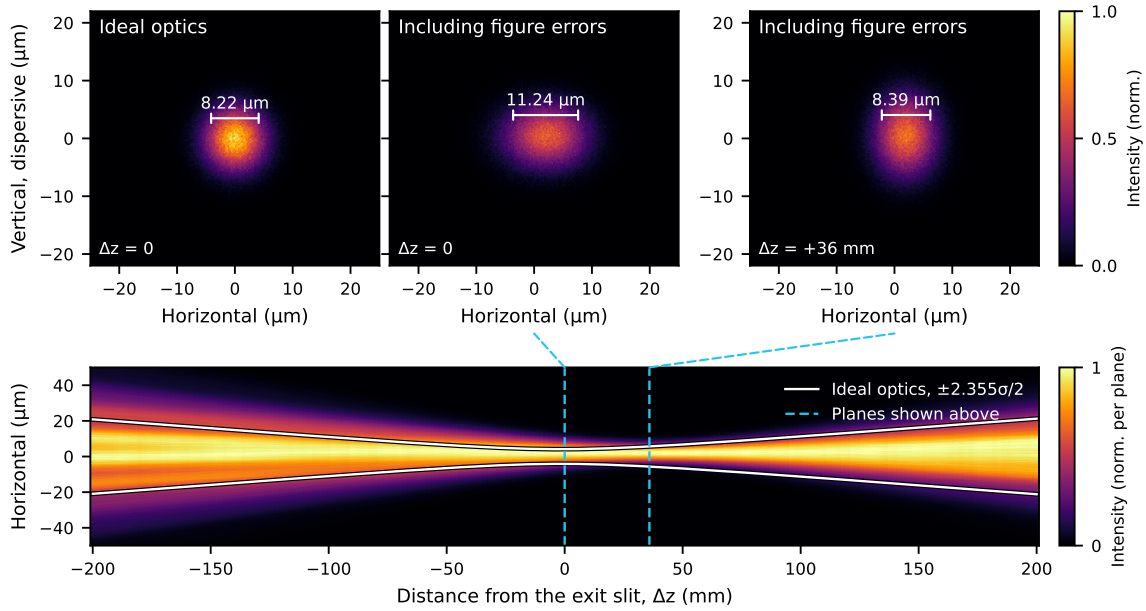


Figure 7. COSMIC-U horizontal focus at 1 keV (**shadow4**, G102). **Top:** spot with ideal optics at the exit slit (left), and including the measured figure errors of M101, M102, and M103 at the exit slit (middle) and at the horizontal waist, 36 mm downstream (right). The spots share one window and one intensity scale, normalized to the ideal peak; bars and labels give the horizontal width w . **Bottom:** horizontal profile including the measured figure errors versus distance from the exit slit, each plane normalized to its maximum; white lines mark the ideal $\pm w/2$ envelope, and dashed lines the planes shown above. COSMIC-U M103 is shown before the AXO correction.

In the vertical plane, only the premirror, COSMIC-U M102 or MAESTRO-U M202, deflects the beam, so its figure error is the only one included that affects the vertical width and the resolving power; grating figure errors are not yet included (Section 4). Its effect is small on both beamlines, and the resolving power stays above the design target at every energy (Figure 8, middle and right).

3.3 With the AXO correction

Above we showed that the measured figure errors mainly move the horizontal focus away from the exit slit. Correcting such errors is the role of the AXO, and the pipeline applies the correction in the same loop as the studies above, using the two fits described in Section 2.3. Because the beam and its footprint on the AXO change with photon energy, we repeat these fits at each energy, as an operator would correct the beam at the energy in use. After either fit, the corrected AXO is traced together with the measured figure errors of the other mirrors.

The own-mirror fit brings the figure error of both AXOs to about 0.1 nm rms or less (Figure 9), below their specifications in Table 3, with every voltage well below the allowed ± 500 V limit (Table 5). Only on COSMIC-U M103 does a small ripple remain, on the scale of the actuator spacing, which the actuators cannot follow.

A corrected AXO, however, does not by itself give an ideal beam, because the beam also carries the errors of the mirrors upstream. On MAESTRO-U, where these add little, the own-mirror fit already brings the spot close to its ideal size (Table 5). On COSMIC-U, on the other hand, the focus error from M101 remains, and the spot stays clearly larger than ideal at every photon energy (Figure 10). Fitting the voltages to the beam removes this upstream error together with the AXO's own. On both beamlines, the horizontal width then follows the ideal curve over the full operating range, within 0.6% on COSMIC-U and slightly below it on MAESTRO-U, with no actuator above 300 V.

4. DISCUSSION

The pipeline in Figure 2 turns each **shadow4** model into a function of the photon energy, the grating, the figure error of each mirror, and the voltages of the AXO. The studies in Section 3 are therefore loops over these

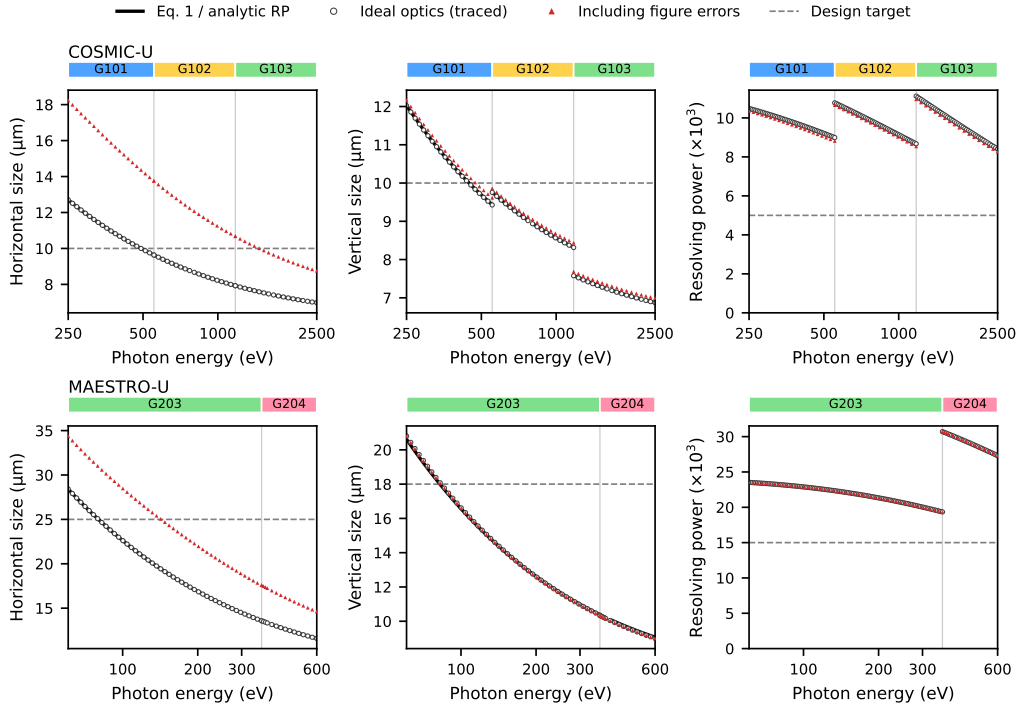


Figure 8. Beam size and resolving power at the exit slit versus photon energy (shadow4). **Top:** COSMIC-U. **Bottom:** MAESTRO-U. **Left:** horizontal width. **Middle:** vertical width. **Right:** resolving power. Lines: Equation 3 and the analytic resolving power; circles: ideal optics; triangles: including the measured figure errors of M101, M102, and M103 (COSMIC-U) or M201, M202, and M221 (MAESTRO-U), with the AXOs before correction and grating figure errors not included. Dashed lines: design targets. The bar above each panel gives the grating; gray lines mark the grating changes. In the MAESTRO-U vertical and resolving-power panels, the markers and lines coincide (differences below 0.1%).

arguments rather than sequences of widget edits: energy scans across every grating, per-mirror on/off studies, and the whole-beamline AXO correction refitted at each photon energy. Because the builders also record where each ray hits each optic, that correction needs only one trace with the actuators off and no figure-error metrology of any mirror. New inputs enter in the same way, as another height mesh on an optic or another argument of a builder, and the next steps below are of this kind.

In the vertical plane, the main missing input is the gratings. Their figure errors, and any deviation of their groove density from the design ruling, act directly on the dispersed beam at the exit slit and therefore on the resolving power, which in the present results is affected only by the premirror.

In the horizontal plane, the next input is the heat load on COSMIC-U M101 and MAESTRO-U M201, whose finite-element deformations can enter as further height meshes. A wave-optics study with influence functions of a prototype AXO showed that the adaptive mirror can correct a heat-load curvature of the first mirror down to a radius of about 2 km.⁷ The whole-beamline fit can now test this with the measured influence functions of the delivered mirrors. The fit assumes that these influence functions are linear and stable within ± 500 V, whereas piezoelectric actuation shows cross-talk, creep, and hysteresis,¹⁷ so measuring these effects on both AXOs would refine the model.

The whole-beamline fit in Section 3.3 minimizes the spot size at the exit slit, but the objective of the fit is itself a choice that the pipeline leaves open. With the waist back on the exit slit, the corrected beam keeps the magnification set by the curvature of the first mirror. Its divergence is therefore slightly larger than that of the ideal beamline, and on MAESTRO-U its spot slightly smaller (Table 5, Figure 10, right). Fitting the voltages to a target that weighs spot size against divergence would let the correction be tuned to what each experiment needs. For coherent beams, the natural target is the wavefront itself, which a ray trace does not describe. One

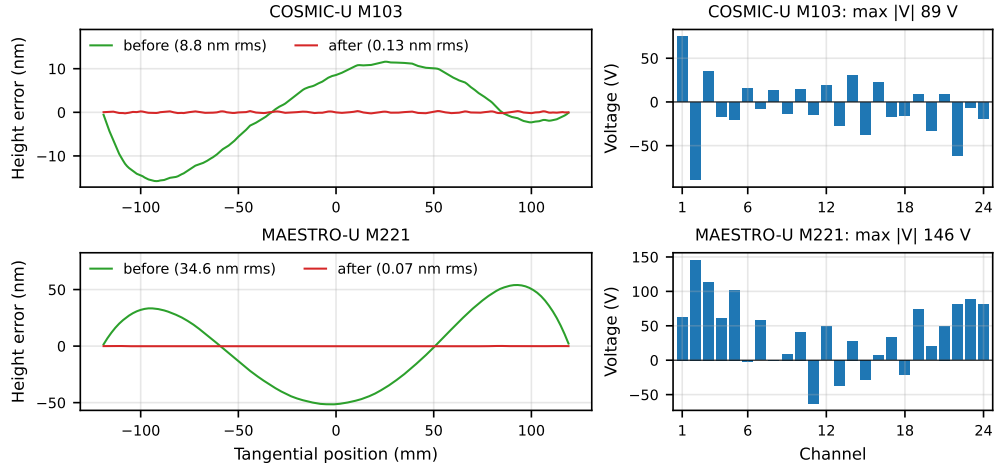


Figure 9. Own-mirror AXO fit. **Left:** figure error of COSMIC-U M103 (top) and MAESTRO-U M221 (bottom) over ± 119 mm, before correction (as in Figure 4) and after, with the rms values in the legend. **Right:** fitted voltages of the 24 actuators.

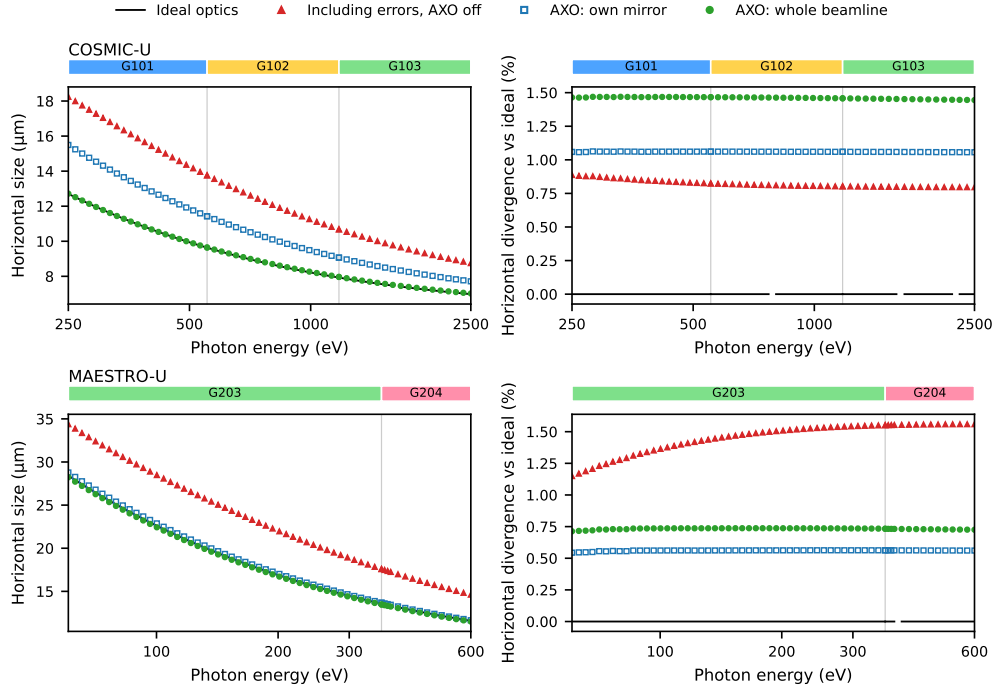


Figure 10. Horizontal beam at the exit slit versus photon energy with the AXO correction (*shadow4*). **Top:** COSMIC-U. **Bottom:** MAESTRO-U. **Left:** horizontal width w . **Right:** horizontal divergence relative to ideal optics. Line: ideal optics; triangles: including the measured figure errors of M101, M102, and M103 (M201, M202, and M221) with the AXO off; squares: own-mirror fit; dots: whole-beamline fit, repeated at each photon energy. The bar above each panel gives the grating; gray lines mark the grating changes.

thing to try is to propagate the same beamline models with a wavefront-propagation code such as *srw*,¹⁸ which OASYS 2.0 also provides, and to fit the voltages to the wavefront.

The whole-beamline correction also links the simulation to measurement. The fit in Equation 2 uses only where each ray hits the AXO and where it arrives at the exit slit. The same information can be measured on the beamline, by scanning a narrow aperture along the mirror while recording the beam position at the exit slit, or

all at once with an X-ray wavefront sensor.^{19,20} Such measurements would take the place of the modeled beam in the fit, so that the voltages at each photon energy come from the beam itself, and they would give a direct diagnostic of the beam during commissioning. Each measurement, whether of the beam, the alignment, or the AXO response, can be loaded back into the model in the same way as the metrology. A model kept up to date in this way is the digital twin introduced in Section 1, and the builders and the AXO fit described here are its starting point.

5. CONCLUSION

We have built scripted models of the COSMIC-U and MAESTRO-U beamlines from their OASYS 2.0 models and used them in three steps: with ideal optics, including the measured figure errors, and with the AXO correction. With ideal optics, the simulated beam size and photon energy resolving power agree with the analytical estimates over the operating range of each beamline. Including the measured figure errors mainly moves the horizontal focus away from the exit slit, so that before the AXO correction the horizontal width at the exit slit grows by 36.7% on COSMIC-U at 1 keV and by 30.2% on MAESTRO-U at 300 eV. Such a focus error is what the AXO is designed to correct. Fitting the AXO voltages to the beam of the whole beamline, at each photon energy, brings the width to 0.4% above ideal on COSMIC-U and 0.8% below it on MAESTRO-U, and keeps it close to its ideal value across both operating ranges. Further inputs, such as grating metrology, heat-load deformations of the first mirrors, and beam measurements during commissioning, can enter the pipeline in the same way, toward a digital twin of each beamline.

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