

Ex situ tuning of bendable x-ray mirrors for optimal beamline performance

Wayne R. McKinney,^{1*} Valeriy V. Yashchuk,¹ Daniel J. Merthe,¹ Nikolay A. Artemiev,¹
and Kenneth Goldberg²

¹Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California, 94720

²Center for X-Ray Optics, Lawrence Berkeley National Laboratory, Berkeley, California, 94720

Abstract

We extend analytical and numerical methods recently developed at the Advanced Light Source (ALS) optical metrology laboratory (OML) for optimal tuning and calibration of bendable x-ray optics based on ex situ measurements with surface slope profilers [Opt. Eng. 48(8), 083601 (2009); Proc. SPIE 8141, 8141-19 (2011)]. We minimize the rms variation of residual slope deviations from ideal surface figure. Previously, our adjustment assumed the deviations were weighted equally across the optic. In this work, we analyze the case when the mirror length is significant with respect to the imaging conjugate. This corresponds, for example, to high de-magnification by bendable Kirkpatrick Baez mirror pairs, used near the ends of synchrotron and free electron laser beamlines for micro- and nano-focusing that often results in a very short mirror to image distance, of the same order of magnitude as the mirror's length. In this case, contributions to focal distortion of residual errors of mirror surface figure (appearing due to mechanical alignment tolerances, sagittal shaping errors, and the limited number of adjustable parameters inherent in a two-couple bender) strongly depend on position across the optic. Specifically, the downstream deviations from exact shape should be weighted less because the rays have a shorter path to travel to the image. Here, we derive an analytical expression for the weighting function and present a mathematical background for the bending adjustment procedure for optimization of the mirror's beamline performance. The efficacy of the optimization is demonstrated for a short-focus mirror used for diffraction limited focusing at ALS beamline 12.3.2.

Keywords: bendable mirrors, x-rays, x-ray optics, synchrotron radiation, synchrotron beamline, Kirkpatrick-Baez

1. INTRODUCTION

In Refs.¹⁻⁴ an experimental method for optimally setting bending couplers of bendable x-ray optics has been suggested and thoroughly discussed. The method utilizes ex situ optical slope metrology for obtaining characteristic functions of the bending couplings that describe the response of the mirror surface shape to a unit change of the couplings. With the characteristic functions experimentally determined, the surface slope deviation from the desired shape is minimized by optimizing the values of the applied bending couplings. Mathematically, for the optimization of the mirror, linear regression analysis is used assuming an equal contribution of the mirror surface points to the final beamline performance of the optic.

In this report, we extend the method to account for different statistical weights of the surface slope errors for different positions along an x-ray focusing elliptically-shaped mirror. The problem becomes important for beamline applications where the distance from the mirror to the focal plane is comparable with the size of the optic. Such a situation obtains, for example, with the focusing Kirkpatrick-Baez (KB) mirrors used at the ALS beamlines 5.3.1, 10.3.2, and 12.3.2.⁵

The plan for the present report is as follows. In Sec. 2, we will derive an analytical expression that describes a weighting function for an elliptically-shaped focusing mirror. The mathematical formalism of linear regression analysis including a weighting function in the course of optimal setting of bendable mirrors is presented in Sec. 3, and a specific example is given in Sec. 4. Conclusions will be drawn in the last section, Sec. 5.

*wrmckinney@lbl.gov 1-510-486-4395 FAX 1-510-486-4385

<http://opticalmetrology.lbl.gov>

2. ANALYTICAL WEIGHTING FUNCTION FOR AN ELLIPTICALLY-SHAPED FOCUSING MIRROR

As a figure of merit of the optimization of the optic's beamline performance, we use the rms size of the resulting spot in the desired focal plane in the tangential direction. Even though we consider each measured point on the optic, this is not the complete image width that is sometimes called the "full width at zero height," FWZH, of the image.⁶

In the geometrical optics approximation, a surface slope error $\delta\varphi(x)$ at a point x of the mirror surface at the distance of $r'(x)$ from the image focal plane leads to a transverse deviation of the focal position of the corresponding light ray by a value of

$$\delta s(x) = 2 \cdot r'(x) \cdot \delta\varphi(x). \quad (1)$$

Here and below we assume that $x = 0$ corresponds to the mirror center.

According to Eq. (1), the contribution of the surface slope error $\delta\varphi(x)$ to the focal error and, therefore the statistical weight of the point x are proportional to the local distance to the focus $r'(x)$. For high quality x-ray optics, $r'(x)$ can be approximated with high accuracy by the value corresponding to the ideally shaped mirror (no surface slope errors).

The ideal shape of an elliptical mirror can be described with a set of parameters (see, for example, Ref.⁷): the distance from the object focal plane (defined by the point F_1 in Fig. 1) to the mirror center r_0 , the distance from the image focal plane (the point F_2 in Fig. 1) to the mirror center $r'_0 = r'(x=0)$, and the value of the grazing incidence angle $\alpha_0 = \alpha(x=0)$. Figure 1 depicts the parameterization of the elliptical surface. The angle β_0 in Fig. 1 is the angle of rotation of the coordinate system connected with the mirror (x, y) with respect to that of the generated ellipse (X, Y)

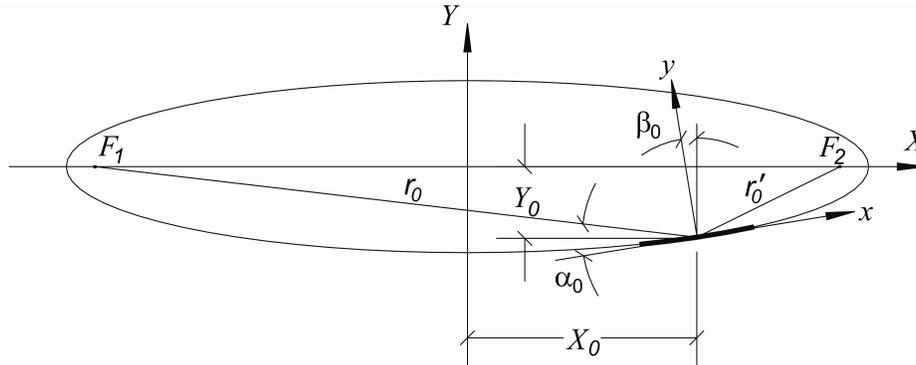


Figure 1: Definition of parameters describing an elliptically shaped mirror.

The canonical parameters of the corresponding ellipse

$$\frac{X^2}{a^2} + \frac{Y^2}{b^2} = 1 \quad (2)$$

are given by (see. e.g., Ref.⁷)

$$2a = r_0 + r'_0, \quad (3a)$$

$$b^2 = a^2(1 - \varepsilon^2), \quad (3b)$$

$$Y_0 = -\frac{r_0 r'_0 \cos(2\alpha_0)}{2a\varepsilon}, \quad (3c)$$

$$X_0 = a\sqrt{1 - Y_0^2/b^2}, \quad (3d)$$

where ε is the eccentricity of the ellipse is given by:

$$\varepsilon^2 = \frac{r_0^2 + r_0'^2 + 2r_0 r'_0 \sin(2\alpha_0)}{4a^2}, \quad (3e)$$

and we assume here that $r_0 > r'_0$.

The relation between the canonical parameters (3) and the corresponding focal distances are:⁸

$$r(X) = a + \varepsilon X \quad \text{and} \quad (4a)$$

$$r'(X) = a - \varepsilon X. \quad (4b)$$

Equations (4) can be transformed to the coordinate system related to the mirror:

$$r(x) = a + \varepsilon(X_0 + x\cos\beta_0) = r_0 + \varepsilon x\cos\beta_0 \quad \text{and} \quad (5a)$$

$$r'(x) = a - \varepsilon(X_0 + x\cos\beta_0) = r'_0 - \varepsilon x\cos\beta_0, \quad (5b)$$

where⁷

$$\cos\beta_0 = \cos\alpha_0/\varepsilon. \quad (6)$$

Therefore, we finally have:

$$r(x) = r_0 + x \cdot \cos\alpha_0 \quad \text{and} \quad (7a)$$

$$r'(x) = r'_0 - x \cdot \cos\alpha_0. \quad (7b)$$

3. PROCEDURE FOR SETTING OF BENDABLE MIRRORS FOR OPTIMAL BEAMLINER PERFORMANCE

According to Eq. (1), the function given by Eq. (7b) allows the transformation of the surface slope errors measured *ex situ* to the corresponding expected errors of the focal positions of the rays reflected in the point x of the mirror. Optimization of beamline performance of the mirror consists in minimization of variance of the focal positions rather than minimization of the least mean square of the residual surface slope variation.

Therefore, the simplest way to upgrade the existing OML algorithm and software^{1,2} to allow for optimization based on beamline focusing performance of a mirror is to pre-process the measured slope distribution $\varphi(x)$ according to Eq. (1) and Eq. (7b) in order to generate the corresponding traces of ray deviation functions in the focal plane:

$$s(x) = 2r'(x) \cdot \varphi(x) = 2(r'_0 - x \cdot \cos\alpha_0) \cdot \varphi(x). \quad (8)$$

The corresponding desired trace is

$$s_0(x) = 2(r'_0 - x \cdot \cos\alpha_0) \cdot \varphi_0(x), \quad (9)$$

where $\varphi_0(x)$ is the surface slope distribution of a mirror with the ideal elliptical shape. We add the word functions, for they are not exactly ray deviations. If they were, then the exact function to which we optimize would be identically zero since we wish to focus to a point image. Note that the trace of transverse deviations is $\delta s(x) = s(x) - s_0(x)$.

The rest of the optimization algorithm stays the same. Three position traces measured with different bender couplings,

$$(C_A, C_B), (C_A + \Delta C_A, C_B), \text{ and } (C_A, C_B + \Delta C_B), \quad (10)$$

are used to calculate the bender's characteristic functions:

$$f_A^*(x_i) = \frac{s(x_i; C_A + \Delta C_A, C_B) - s(x_i; C_A, C_B)}{\Delta C_A}, \quad f_B^*(x_i) = \frac{s(x_i; C_A, C_B + \Delta C_B) - s(x_i; C_A, C_B)}{\Delta C_B}. \quad (11)$$

Linear regression analysis with the functions $f_A^*(x_i)$ and $f_B^*(x_i)$ is applied to best fit the measured position distribution to the ideal one:¹⁻³

$$s(x_i; C_A, C_B) - s_0(x_i) \approx \delta C_A \cdot f_A^*(x_i) + \delta C_B \cdot f_B^*(x_i) + C_0. \quad (12)$$

4. APPLICATION TO ALS BEAMLINE 12.3.2

We choose to apply the new adjustment protocol to the vertical mirror of the KB pair from ALS Beamline 12.3.2. The mirror was successfully adjusted by the previous *ex situ* method in the OML less than 1 μ rad rms deviation from the exactly required tangential elliptical cylinder. Once on the beamline, KB mirrors are typically adjusted further, and it is generally assumed that this is due to imprecision in the control of the geometry of installation. As we will show, however, the best adjustment for a case like this one is not to adjust the mirror *ex situ* exactly as before. Note that the best tangential ellipse is still the ideal goal. However, we wish to show that unavoidable errors from fabrication and assembly tolerances are best not evenly distributed to minimize the rms deviation from the exact ellipse without consideration of the weighting function described above.

Table 1 shows the parameters of this case. Note the extremely short mirror center to image distance r' and its relation to the length of the mirror, which is 102 mm.

Table1: Defining parameters of vertical KB mirror from Beamline 12.3.2

object to mirror center, r	2223.6 mm	grazing angle, α_0	3.51 mrad
mirror center to image, r'	135.5 mm	mirror length	102 mm

The mirror's adjustment in the OML is summarized in Table 2, below. Three scans were taken with standard nominal adjustments of the bending springs between scans, see Eq. (10). In order to get accurate values of the characteristic functions the encoders were moved approximately 200 steps, even though the final adjustments turned out to be less than this amount. Going farther than the expected final adjustments for the two trial adjustments gives better estimates for the characteristic functions because of the presence of noise in the LTP slope data. These three scans were then used to predict optimal settings under the previous assumptions using regression analysis. The scan number indicates the time order of the scans, (2899, 2900, 2901, 2902). The order in the table shows the order that they are sent to the algorithm,

(2900, 2899, 2901) in order to match the equations of the analysis, Eq. (10). In this specific case, normal procedure was not followed, as the downstream bending couple was varied first. However, since the characteristic functions, and their corresponding encoder adjustments appear symmetrically, the reversed series of adjustments is easily compensated by carefully keeping track of the reversal in the numerical output, see Eq. (12).

Table 2: Adjustment details of the vertical KB mirror from Beamline 12.3.2 under the previous method without weighting. Note that the downstream encoder was varied first, a departure from the usual method. The software algorithm is symmetrical with respect to the order of variation, and the results are correct irrespective of which bending couple is varied first, as long as the scans are sent to the algorithm in the correct order, and the reversal is tracked.

NO WEIGHTS		upstream encoder	downstream encoder	predicted change upstream	predicted change downstream	rms difference from exact ellipse, measured
Prediction triplet	Scan 2900	-153.35	280.68			17.70 μrad
	Scan 2899	-153.39	+80.77			1.63 μrad
	Scan 2901	46.62	+280.85			27.82 μrad
Prediction applied to this scan	Scan 2902	-132.30	+70.05	$\Delta_{up} = -37.25$ add to 2902	$\Delta_{down} = +33.50$ add to 2902	1.75 μrad
Final settings	predicted \rightarrow	-169.45	+103.54		predicted \rightarrow	0.50 μrad

We now proceed to show our ex post facto analysis with the new method of this work, including the weighting function. We repeat the method from Table 2 in Table 3, only this time all the scanned slope data and the slope of the exact ellipse are converted into ray deviation functions by Eqs. (8) and (9), which are then sent to exactly the same computer code as before. In effect, we subtract a set moving perfect rays from a set of moving deviated rays in order to get the size of the image. This is a consequence of the fact that Eqs. (8), and (9) assume a constant incidence angle, which is not really the case, but does not affect the final result.

Table 3: Adjustment details of the vertical KB mirror from Beamline 12.3.2 under the new method with weighting.

WITH WEIGHTS		upstream encoder	downstream encoder	Ray error predicted change upstream	Ray error predicted change downstream	rms difference from exact ellipse	predicted rms width of the image
Prediction triplet, applying transformation to slope measurements	Scan 2900	-153.35	280.68				
	Scan 2899	-153.39	+80.77				
	Scan 2901	46.62	+280.85				
Prediction applied to this scan	Scan 2902	-132.30	+70.05	$\Delta_{up} = -71.02$ add to scan 2902	$\Delta_{down} = -24.80$ add to scan 2902		
Prediction with weights		-203.32	+45.25		predicted \rightarrow predicted \rightarrow	0.59 μrad (0.50 μrad without weights)	0.15 μm rms (0.37 μm rms without weights)
Results from in situ alignment	Merthe et al. ⁹	-204	+264				

Adding the weighting changes the predicted adjustments, as seen by comparing the data in Table 2, and Table 3. The predicted rms deviation from exact tangential elliptical cylinder only rises from 0.50 to 0.59 μrad , a relatively small change. However, in exchange for this small increase, the predicted rms width of the image goes from 370 nm to 150 nm which is exactly what was measured at the beamline after in situ alignment.⁹ Moreover, the upstream prediction is, within experimental error, exactly the final adjustment of the upstream bender in situ.⁹ The only difference between our ex post facto set of predictions is the difference between the setting of the downstream bender from this work, and the in situ methods. Note, however, that we specifically de-emphasized the downstream part of the mirror in the weighting because the rays have less distance to travel, and hence the mirror can be allowed to deviate more from the exact elliptical figure at the downstream end. In order to confirm our analysis we can use the developed model, Eqs. (8), (9), and (12) to find the predicted slope errors for the un-weighted and weighted cases. This is shown in Fig. 2, below.

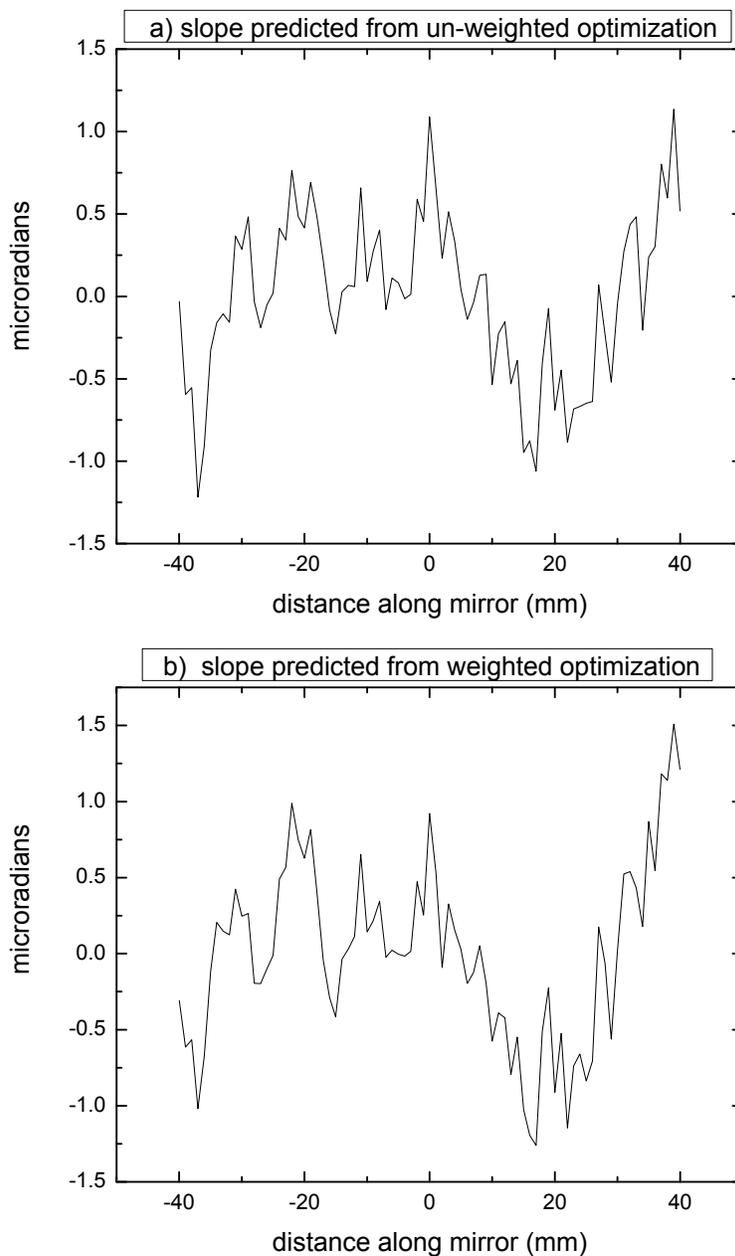


Figure 2. Predicted differences of (mirror slope - exact elliptical slope) for the two cases: a) un-weighted, and b) weighted.

The data in the figure above confirm our numerical results. The slope of the downstream end on the right hand side is steeper, and the deviations on the more important upstream side are smaller. This is more strikingly shown by Fig. 3, below where the predicted ray intercept coordinates for each point are plotted with respect to the corresponding point on the mirror. The rms values of 150 and 370 nm are clearly seen to correlate with the point by point data.

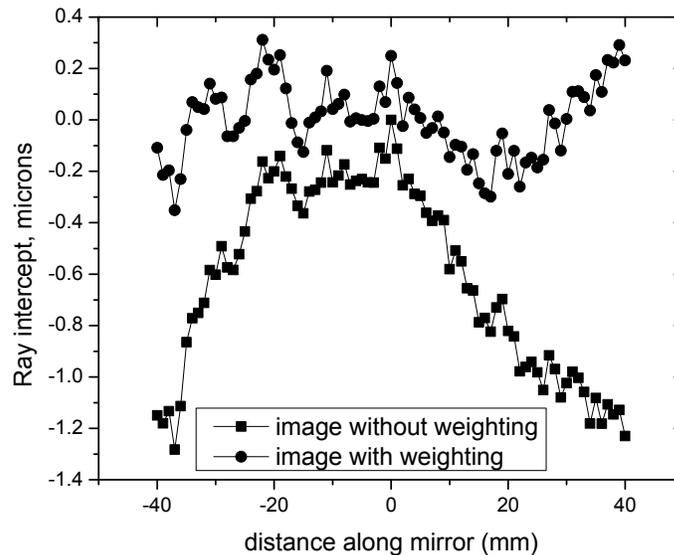


Figure 3. Predicted ray intercept coordinates in the image plane for the two cases of no weighting, and weighting. Note that the final adjustment corresponds to a "bird"-like shape of the mirror, seen here as a third-order polynomial distribution in the ray intercept.

5. CONCLUSIONS

We have shown that for bent mirrors that have imaging conjugate distances on the same order as the tangential length of the mirror weighting should be used. We have found this weighting function based on the geometry of the exact elliptical figure that is desired. The only change to the previous method is to make a simple linear transformation of the slope data of the triplet (or quadruplet if the predicting triplet is reused for a 4th final tuning file) of slope measurements used for predicting optimum adjustments, and apply the same linear transformation to the exact elliptical slope distribution that is desired. However, the goal of bending to an exact tangential elliptical figure is not abandoned. Since errors of fabrication and assembly always pose some remaining slope deviation from the exact elliptical figure, the bending adjustment, in this case, is best expended on the upstream part of the mirror where the rays have farther to travel to the image. In effect, we have a better result by ex situ optimizing for what is actually desired, rather than a pro forma match to the slope of the exact ellipse. This should result in less need for in situ optimization of the bending couples at the beamline.

Acknowledgements

The authors wish to thank all the members of the Beamline 5.3.1 LDRD team.

The Advanced Light Source is supported by the Director, Office of Science, Office of Basic Energy Sciences, Material Science Division, of the U.S. Department of Energy and by the DOE Laboratory Directed Research and Development Program under Contract No. DE-AC02-05CH11231 at Lawrence Berkeley National Laboratory.

Disclaimer

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor The Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or The Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or The Regents of the University of California.

REFERENCES

- [1] McKinney, W. R., Irick, S. C., Kirschman, J. L., MacDowell, A. A., Warwick, T., and Yashchuk, V. V., "New procedures for the adjustment of elliptically bent mirrors with the long trace profiler," Proc. SPIE 6704, 67040G-12 (2007).
- [2] McKinney, W. R., Kirschman, J. L., MacDowell, A. A., Warwick, T., and Yashchuk, V. V., "Optimal tuning and calibration of bendable mirrors with slope-measuring profilers," Opt. Eng., 48 (8), 083601-8 (2009).
- [3] McKinney, W. R., Anders, M., Barber, S. K., Domning, E. E., Lou, Y., Morrison, G. Y., Salmassi, F., Smith, B. V., and Yashchuk, V. V., "Studies in optimal configuration of the LTP," Proc. SPIE 7801, 780106-12.
- [4] McKinney, W. R., Yashchuk, V. V., Goldberg, K. A., Howells, M., Artemiev, N. A., Merthe, D. J., and Yuan, S., "Design optimization of bendable x-ray mirrors," Proc. SPIE 8141, 81410K-14 (2011).
- [5] Yashchuk, V. V., Merthe, D. J., Goldberg, K. A., Artemiev, N. A., Celestre, R., Domning, E. E., Kunz, M., McKinney, W. R., Morrison, G. Y., Smith, B. V., Tamura, N., and Padmore, H., "Experimental methods for optimal tuning of bendable mirrors for diffraction-limited soft x-ray focusing," Journal of Physics, submitted, SRI-2012 Proceedings (TH-O-P-16), (2012).
- [6] McKinney, W. R., and Howells, M. R., "Design optimization of "straight groove" toroidal grating monochromators for synchrotron radiation," Nucl. Instrum. and Methods 172, 159-156 (1980).
- [7] Howells, M. R., Cambie, D., Duarte, R. M., Irick, S., MacDowell, A. A., Padmore, H. A., Renner, T. R., Rah, S., and Sandler, R., "Theory and practice of elliptically bent x-ray mirrors," Opt. Eng., 39 (10), 2748-2762 (2000).
- [8] Newcomb, S., [Elements of Analytic Geometry], Henry Holt & Co., New York, NY, 135-136 (1884).
- [9] Merthe, D., Kunz, M., Tamura, N., and Yashchuk, V., V., "Effect of In Situ Adjustment on Slope Profiles of BL 12.3.2 Bendable Kirkpatrick-Baez Mirrors," Light Source Beamline Note-1111, Lawrence Berkeley National Laboratory (2012).