HTML ABSTRACT + LINKS

A Ray-Tracing Study of the Dependence of Focal Properties on Surface Figure Error for a Kirkpatrick-Baez (K-B) Mirror System

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Abstract. In the last several years, Kirkpatrick-Baez (K-B) mirror systems have been extensively applied as two-dimensional x-ray focusing elements on x-ray beamlines at low emittance, third generation, synchrotron radiation facilities. The design of the two GM/CA CAT insertion device beamlines at the Advanced Photon Source at Argonne National Laboratory for macromolecular crystallography includes a K-B mirror system situated in each of the experimental stations. Ray-tracing studies have been performed using SHADOW (V2.3.2) to investigate the dependence of the focal distance on the surface figure error obtained from LTP metrology measurements. Additionally, a procedure has been developed to allow one to change the mirror focal positions to provide a beam of given dimensions at a fixed position before or after the focal position. The GM/CA CAT has been established by the National Institutes of Health's (NIH) National Institute of General Medical Sciences (NIGMS), and the National Cancer Institute (NCI) to build and operate a national user facility for crystallographic structure determination of biological macromolecules by X-ray diffraction.

INTRODUCTION

Crystal structures of biological macromolecules are an essential part of our understanding of life processes at the molecular level. The first X-ray diffraction patterns from protein crystals were obtained over 60 years ago using laboratory X-ray sources. In the intervening years there have been many improvements in instrumentation, X-ray sources (including synchrotron radiation sources), focusing optics and detectors [1].

Matching the size and divergence of the X-ray source to the experimental requirements is very important. For instance a smaller beam may result in increased radiation damage during data collection, while a larger beam may results in increased background [2].

The Kirkpatrick-Baez (K-B) [3] mirror systems have been extensively applied as two-dimensional x-ray focusing elements on x-ray beamlines. A simple analytical design procedure to optimize the focused beam size for a crystallography beamline will be presented below.

RAY-TRACING STUDIES FOR GM/CA ID EXPERIMENTAL STATION

The GM/CA CAT facility consists of two insertion device (ID) beamlines and one bending magnet beamline. The layout of the experimental stations for the two ID beamlines is very similar. This study investigates the focal properties of the beamline referred to as ID_in (Figure 1.) which has a slightly higher demagnification ratio. Ray-tracing studies have been performed using SHADOW (V2.3.2) to investigate the dependence of the focal distance on the surface figure error obtained from LTP metrology measurements.

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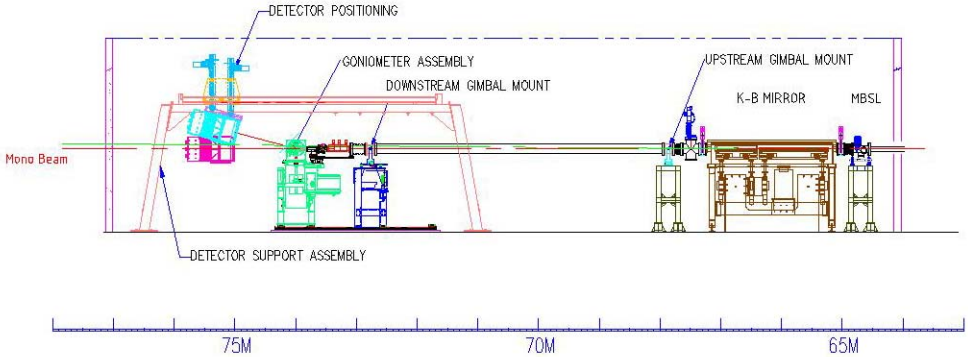

FIGURE 1. Layout of the experimental station for the ID beamlines.

The Shadow input parameters used for the simulations are listed in Table 1. The standard Undulator A consists of 72 magnetic pole pairs. The insertion devices for the GM/CA CAT ID beamlines are a shortened version of the Undulator A which have 62 pole pairs [4].

TABLE 1. Shadow input parameters used for the simulation

Source	
Storage ring energy (GeV)	7
Storage ring current (mA)	100
Emittance	2.97 nm/rad, 1% coupling
Sigma X (cm)	0.0217
Sigma V (cm)	0.001255
Source size - FWHM	507 X 29 μm^2
Insertion device	Shortened Undulator A
Undulator period (cm)	3.3
Number of periods	62
Energy	12KeV (Fundamental)
Geometrical Layout	
White beam slits	@26.7 m from the center of straight section Opening: 2.5 mm x 1 mm
K-B elliptical horizontal focusing mirror	@65.8 m from the center of straight section
mirror size	1050 mm x 60 mm
Grazing angle	4 mrad
K-B elliptical vertical focusing mirror	@66.745 m from the center of straight section
mirror size	600 mm x 60 mm
Grazing angle	3 mrad
Focus position 1 (at sample)	@74.0 m from the center of straight section
Focus position 2 (at detector)	@74.3 m from the center of straight section
Focus position 3 (3m downstream of sample)	@77.0 m from the center of straight section

The Shadow ray tracings simulations were performed with the focal position parameter set at 7400 cm for the following two cases: 1) mirrors with ideal elliptical shapes, and 2) mirrors with slope error imperfections as measured on a real mirror with an LTP interferometer. The beam size in the vicinity of the expected focal point was evaluate by placing several “screens” to either side of 7400 cm. The black curves in Figure 2 show the calculated beam size at the different screen locations. Note that the simulations show that the minimum beam size is within a few millimeters of the expected 7400 cm position.

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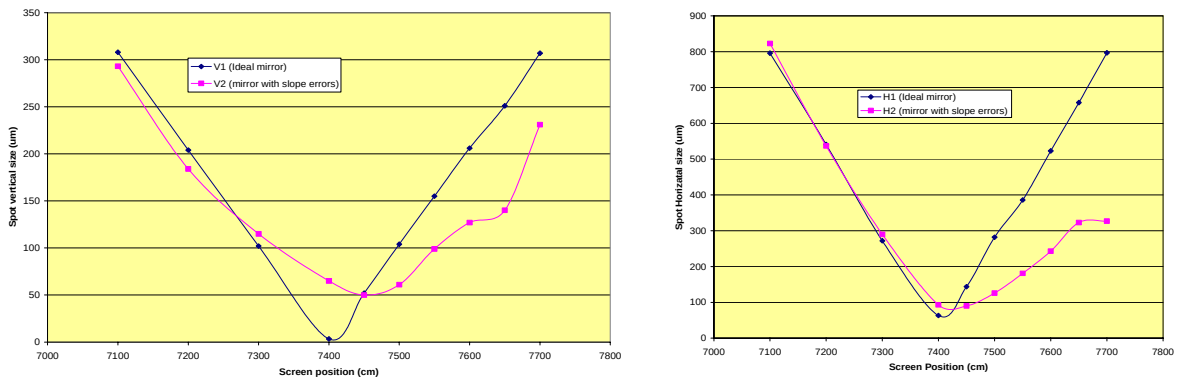
The pink curves in Figure 2 show the calculated beam size at the different screen locations when slope error is included in the simulations. The position where the beam has the minimum size is determined to be at 7435 cm in the vertical direction and 7395 cm in the horizontal direction. The degree of movement of the minimum beam size and the shape around the ideal focal position are strongly dependent on the actual slope errors.

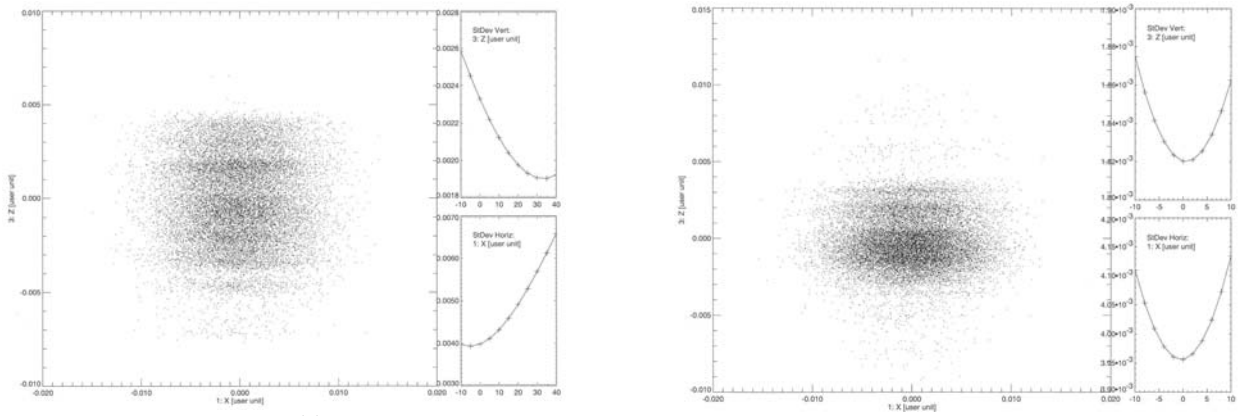
Additional simulations demonstrate that the horizontal focus size is less sensitive to the position along the beam direction. This is due to the fact that the horizontal source size is considerably larger than the vertical source size.



(a) (b

FIGURE 2. Results of the ray-tracing simulation. a.) Vertical and b) Horizontal spot size along the beam direction at different screen positions.

The K-B mirrors with an ideal elliptical shape focused at 7400 cm (sample position). However, adding slope error in to the simulation shits the focal position. Figure. 3a shows that by using the "Ray-Prop controls" function, we can easily find the real focus position (i.e., minimum size). Fig. 3b showed that by manipulating the K-B bending radius iteratively, the x-ray spot size at the sample position can be minimized by forcing the vertical mirror to focus at 7365 cm and the horizontal mirror to focus at 7405 cm.



(a) (b)

FIGURE 3. Shadow ray tracing beam profiles at 7400 cm and "Ray-Prop controls" side bar plots. a) focal position parameter set at 7400 cm, b) focal position parameter optimized to shift minimum focal size to 7400 cm.

Table 2 illustrates the effect of changing the K-B mirror focus position on the beam size obtained at the sample position (74 m). This allows the beam size to be controlled easily. For instance, a beam size of 100 µm x 100 µm can be obtained by a K-B horizontal focus position at 7410 cm and a vertical focus position at 7500 cm, and a beam

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size of 200 µm x 200 µm can be obtained by a K-B horizontal focus position at 7280 cm and a vertical focus position at 7180 cm.

Table 2. Sample at 74 M, K-B focus different position

	Spot size of Sample position at 74m	
K-B focus at position (cm)	**Horizontal size (µm)**	**Vertical size (µm)**
7000	1329	347
7050	1037	344
7100	788	410
7150	578	354
7200	401	136
7250	245	88
7300	143	59
7350	126	54
7400	93	66
7450	167	76
7500	272	107
7550	357	136
7600	436	254
7650	518	290
7700	592	192

CONCLUSIONS

We have performed ray-tracing studies using SHADOW (V2.3.2). The results show that the size and the shape of the focus spot are strongly dependent on the slope error of the K-B mirrors. In the case where slope errors were included, the minimum beam size moves downstream by about 350 mm from the theoretical focus position (without slope errors). Using the "Ray-Prop controls" function, we can easily find the position of the minimum focal size. By manipulating the K-B bending radius iteratively, the x-ray spot size on the sample position can be fine tuned to any desired value.

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REFERENCES

1. Nave, C., "Matching X-ray source, optics and detectors to protein crystallography requirements" Acta Cryst. D55, pp. 1663-1668. (1999).
2. Perrakis, A., Cipriani, F., Castagna, J.C., Claustre, L., Burghammer, M., Riekel, C. and Cusack, S., "Protein microcrystals and the design of a micro-diffractometer: current experience and plans at EMBL and ESRF/ID13" Acta Cryst. D55, pp. 1765-1770 (1999).
3. Kirkpatrick, P. and Baez, A.V., J Optical Soc. of Am. 38 (9) pp. 766-774 (1948).
4. Dejus, R.J., Vasserman, I.B., Sasaki, S. and Moog, E.R., "Undulator A Magnetic Properties and Spectral Performance" ANL/APS/TB-45 (2002).

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