MECHANICAL DESIGN OF NEW DUAL PINHOLE MINI-BEAM COLLI-MATOR WITH MOTORIZED PITCH AND YAW ADJUSTER **PROVIDES LOWER BACKGROUND** FOR X-RAY CRYSTALLOGRAPHY AT GMCA@APS *

Shenglan Xu, Nagarajan Venugopalan, Oleg Makarov, Sergey Stepanov and Robert F. Fischetti GM/CA and XSD. Advanced Photon Source.

Argonne National Laboratory, Argonne, IL60439 USA

Abstract

The GM/CA-developed, quad-mini-beam collimator [1, 2, 3], advanced rastering and vector data-collection software tools [4], have enabled successful data collection on some of the most challenging problems in structural biology. This is especially true for membrane-protein crystals grown in lipidic cubic phase, where crystals are typically small, fragile, and "invisible" when cryo-cooled. There are two main sources of X-ray scattering (besides the sample) that reach the detector, contribute to background and limit data resolution. These are scattering within the collimator that escapes the exit aperture and air-scattering of the direct beam before it terminates in the beam-stop. Scattering from the collimator can be reduced by decreasing the exit aperture size. A quad mini-beam collimator was built consisting of 5-, 10-, 20- and 150 µm beam defining apertures with 50-, 70-, 100- and 300 µm exit apertures, respectively. Previous collimators were positioned in the X-ray beam by two motorized translational motions and two manual angular adjustments via a kinematic mount. The individual beams were selected by recalling stored translational positions. The pitch and yaw angular adjustments were manually pre-adjusted to one optimal position for all four apertures. Due to reduced tolerance in the new design, aligning each of the pin-hole combinations to high-precision required motorizing both translational and angular motions. The novelty of the new mechanical design is the compactness and positional stability of the structure. The new collimator positioning system consists of three frames, four C-flex bearings, two actuators and two high precision stages. The two pairs of commercial flex bearings function as a universal joint.

INTRODUCTION

Since 2007, GM/CA has provided micro-diffraction capabilities at both 23-IDD and 23-IDB beamlines through versatile collimator systems. A robust, monolithic quadcollimator provided user-selectable beam sizes of 5, 10, 20 µm or "full beam" (~25 x ~75 µm FWHM). These quad collimators were positioned in the X-ray beam by two motorized translational motions and two manual angular adjustments via a kinematic mount. The individual beams were selected by recalling stored translational

Beam Lines

positions. The pitch and yaw angular adjustments were manually pre-adjusted to one optimal position for all four apertures (Figure 1). An active beam stop of 1.0 mm diameter is typically positioned about 35 mm downstream of the sample. A prototype collimator with 5 µm beam defining and 150 µm exit aperture was developed for scanning X-ray micro diffraction studies of tissue architecture. This collimator in combination with a 0.5 mm beam stop resulted in a 30% background reduction, prompting us to develop dual pin-hole collimators for reduced background.



Figure 1: Close up of the Quad collimating system installed at the beamline end station. Two high resolution micro translation stages are combined to form an XY system for the collimators alignment. The travel range is 15 mm for both horizontal and vertical. The design resolution is 0.007 µm and the repeatability is 0.1 µm. The whole system stability is $+/-0.1 \mu m$.

DUAL PIN-HOLE COLLIMATOR

Design of Dual Pinhole Collimator

The dual pinhole collimator design significantly reduces the X-ray scattering that escapes the collimator, Figure 2. The collimator assembly has a steel scatter guard body that hosts an entrance and exit sub-assembly. Both subassemblies consist of a steel cap and a Platinum pinhole

THAA03

9th Edit. of the Mech. Eng. Des. of Synchrotron Radiat. Equip. and Instrum. Conf.MEDSI2016, Barcelona, SpainJACoW PublishingISBN: 978-3-95450-188-5doi:10.18429/JACoW-MEDSI2016-THAA03

aperture. The pinhole of the entrance sub-assembly acts as the X-ray beam defining aperture while the pinhole of the exit sub-assembly captures the scatter from the beam defining aperture and air scatter within the collimator body. The steel cap upstream of the beam defining aperture prevents back scatter from escaping the collimator body, while the steel cap down-stream of the exit aperture further reduces the scatter escaping the collimator.



Figure 2: GMCA dual- pinhole mini-beam collimator assembly.

Quad Mini-beam Collimator with Dual Pinhole

The dual pinhole concept was incorporated into a quad, uni-body collimator, Figure 3. The collimator includes four sets of pinholes. Three sets are for mini-beams and one trims the full beam in the horizontal direction to allow a 0.5 mm diameter beamstop to be used. The history of the development of the GMCA quad collimator is illustrated in Figure 4.



Figure 3: GMCA Quad - dual- pinhole Mini-beam Collimator Assembly.

Fable 1: Dual Collimator Pinhol

Collimator	Beam Defining Aperture (μm)	Exit-pinhole Aperture (μm)
1	5	50
2	10	70
3	20	100
4	150	300

Development of the Design of Quad Collimator on GMCA Beamlines



Figure 4: Development history of GMCA quad minibeam collimator.

COLLIMATOR POSITIONING WITH MOTORIZED PITCH AND YAW ADJUSTER



Figure 5: Schematic diagram of the assembled new dual pinhole mini-beam collimator with motorized pitch and yaw adjuster. Backscatter guards with pinholes are inserted in the square-shaped scatter guard. The exit holes are smaller for mini beams. The pinhole selects the central part of the focused beam.

Collimators with small exit apertures require not only X and Y translations to select a particular beam size, but also adjustment of the pitch and yaw angles to center the exit aperture. This necessitated developing a new collimator positioning system with motorized pitch and yaw adjustments, a 3-D model of the collimator positioning system is shown in Figure 5 and two prototype quad collimator assemblies have been built and installed (Figure 6) It consists of: three frames, four C-flex bearings, two actuators and two high precision stages. The two pairs of commercial flex bearings function as a universal joint. The motions of this universal joint are manipulated about the vertical and horizontal axes by two high precision SmarAct actuator stages. Four dual- pinhole collimators are mounted on a block that in turn is mounted on the internal frame. The block's center coincides with the intersection of the two rotation axis resulting in pitch and Yaw motions. The novelty of the new mechanical design is the compactness and positional stability of the structure.

DOI.



Figure 6: New quad mini-beam collimators installed on the GMCA ID stations. The one on the left is on the ID-B station and the other is on the ID-D station.

MINI-BEAM COLLIMATOR WITH SMALL EXIT APERTURES PROVIDES LOWER BACKGROUND

A quad mini-beam collimator was built consisting of 5-, 10-, 20- and 150 μ m beam defining apertures with 50-, 70-, 100- and 300 μ m exit apertures, respectively. Background diffraction patterns (no sample) were systematically recorded for various aperture combinations, and the scattered intensity was radially integrated from the origin to the edge of the pattern, and normalized by the number of pixels.



300/600

Figure 7: Full beam with different beam defining/exit aperture combination.



5µm/250µm

Figure 8: Background scatter for 5µm beam defining aperture.

The 150/300 (beam defining/Exit pinhole aperture) collimator had 27% less background compared to the 300/600 collimator (Figure 7), while the 5/50 collimator had 60% less background compared to 5/250 collimator (Figure 8).

A prototype collimator system consisting of 5µm beam defining apertures with varying exit apertures was constructed to estimate the extent of background reduction; the result is graphically represented in Figure 9. The graphs show a systematic reduction in background across all resolution as the size of the exit aperture was reduced for a 5µm beam defining aperture.



Figure 9: Graphical representation of background scatter for 5µm beam with varying exit apertures.

ACKNOWLEDGMENT

GM/CA@APS has been funded in whole or in part with Federal funds from the National Cancer Institute (ACB-12002) and the National Institute of General Medical Sciences (AGM-12006). This research used resources of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357

REFERENCES

- Fischetti, R.F., Xu, S., Yoder, D.W., Becker, M., Nagarajan V., Sanishvili, R., Hilgart, M.C., Stepanov, S., Makarov, O. and Smith, J.L. (2009) Mini-beam collimator enables micro-crystallography experiments on standard beamlines. JSR 16, 217-225 PMCID 2725011.
- [2] Shenglan Xu, Oleg Makarov, Richard Benn, Derek W. Yoder, Sergey Stepanov, Michael Becker, Stephen Corcoran, Mark Hilgart, Venugopalan Nagarajan, Craig M. Ogata, Sudhir Pothineni, Ruslan Sanishvili, Janet L. Smith, and Robert F. Fischetti;" Micro-Crystallography Developments at GM/CA-CAT at the APS" AIP Conference Proceedings 1234, 897 - 900 (2010).
- [3] Shenglan Xu, Venugopalan Nagarajan and Robert. F. Fischetti "Design and manufacturing of mini beam Collimators for Macromolecular Crystallography at the GMCA CAT at APS" Diamond Light Source Proceedings, Vol 1, e27, page 1 of 4 (Nov.01, 2010).
- [4] Hilgart MC1, Sanishvili R, Ogata CM, Becker M, Venugopalan N, Stepanov S, Makarov O, Smith JL, Fischetti RF. "Automated sample-scanning methods for radiation damage mitigation and diffraction-based centering of macromolecular crystals J Synchrotron Radiat. 2011 Sep;18(Pt 5):717-22. doi: 10.1107/S0909049511029918. Epub 2011 Jul 29.