ISBN: 978-3-95450-207-3 doi:10.18429/JACoW-MEDSI2018-WEPH01

EVALUATION OF ANISOTROPIC SIMULATIONS & REDESIGN OF THE BXDS HIGH ENERGY MONOCHROMATOR BENT LAUE DIFFRACTION CRYSTAL HOLDERS

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Abstract

The Brockhouse X-ray Diffraction and Scattering Sector (BXDS) High-Energy (HE) beamline includes a bent Laue diffraction monochromator. The BXDS HE monochromator achieves energy ranges of 35keV to 90 keV through the bent Laue diffraction of two silicon crystal wafers. Each wafer (460 μm & 1000 μm thick) is bent to achieve specific Sagittal Radius (R_s); subsequent anticlastic Meridional Radius (R_m) results from the anisotropic nature of silicon, creating the desired x-ray focusing parameters. During the initial conditioning of the BXDS HE monochromator spurious diffraction patterns were observed indicating that the crystal holder and crystal integrity failed. Alternative holder designs were evaluated using Finite Element Analysis (FEA; ANSYS) simulations to ensure that appropriate R_s and R_m values were achieved, verification of the crystal holder R_s was completed using contact 3D measurement (FaroArm/Leica T-Probe), and the crystal surface was assessed using 3D optical profiling (Zygo). A superior holder was chosen based on the results, and replaced. The performance of the BXDS HE monochromator has been characterized, indicating the new holder design has achieved x-ray focusing parameters.

INTRODUCTION

Each Si wafer is bent against a precisely machined cryogenically cooled block to achieve specific R_s; a subsequent anticlastic R_m results from the anisotropic nature of Si creating the desired X-ray focusing parameters [1–3]. The theoretical design values for the BXDS HE mono bending radius are found in Table 1), and describe values required for desired focus [1], Si (111) reflection for 35keV, Si (422) & Si (533) reflections for 60-90keV.

Table 1: Theoretical Radius of Curvature

Energy (Si thickness)	R_s [m]	R_m [m]
35keV (460μm)	0.37	-28.0
60-90keV (1000μm)	0.72	-37.0

BACKGROUND

The original BXDS HE crystal holder system was composed of two precisely machined blocks (specifically R_s, with dimensions from Table 1).

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During the initial conditioning of the BXDS HE mono spurious beam shapes were observed from both crystals. The patterns indicated that the crystal holder and crystal integrity had failed. The fluorescing patterns were observed during the initial low flux beam conditioning, suggesting that the crystal fracture resulted during cryogenic cool-down of the stage prior to x-ray attenuation.

The crystal assemblies were removed from the HE mono and inspected. Fractures for both wafers were observed (see Fig. 1), as well the crystal wafer had bonded to the indium foil, suggesting that the wafer was over constrained when assembled.

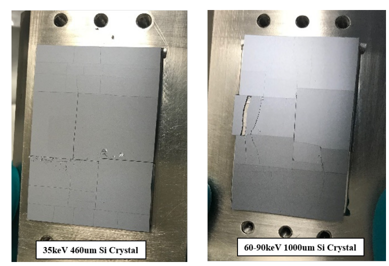

Figure 1: The fractured crystals after being removed. The silicon wafers fractured along the lattice planes (vertically & horizontally). The fractures per area were highest around the locations where the crystals were pressed against the indium foil and the cooling block.

The originally implemented design over-constrained the crystal, resulting in fractures and unusable beam (i.e. unfocused). Therefore, an evaluation of the crystal holders was required.

Objectives

1. Review the current holder design.
2. Confirm the radius induced when clamped against the cooling block & the effect of different clamps on the anticlastic radius.
3. Determine the expected performance (focusing, flux, etc.)

ANISOTROPIC SIMULATION

Initially a review of the original crystal holder was simulated using finite element methods (ANSYS 18.0) and evaluated to determine the resulting R_s & R_m. All simulations used anisotropic material properties for Si (111), and applied non-linear large deformation theory [4–7].

The original mask simulation results demonstrated an immediate issue; the R_m could not be achieved with the

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current style of clamping due to being over constrained by the mask clamped along the entire crystal surface. It was clear that the revised clamping system would require minimal contact.

Three variants of clamped holder styles were developed and evaluated (see Fig. 2). Each design emulated the best practice Laue benders [1, 3]. The variation in clamp designs were intended to maintain the appropriate holding force, bending the crystal wafer against the cooled block to allow the beamline focusing performance (R_s), and to allow the crystal to achieve the anticlastic bend (R_m) .

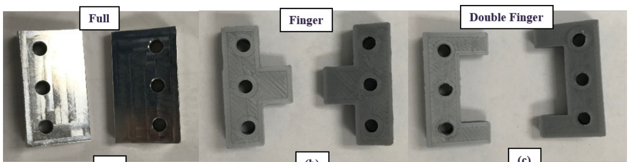

Figure 2: Three clamping styles that were evaluated for use within the BXDS HE mono. (a) the Full clamp applies a line contact to the crystal surface (AL6061), (b) the Finger clamp applies a small line contact force to the center of the crystal (rapid-prototype), (c) the Double Finger clamp applies two small line contact forces to the outer edges of the crystal (rapid-prototype).

The radius of curvature was calculated (ANSYS 18.0) to find deformation maps for each of the directions of interest (R_s & R_m). Data from the deformation paths (see Fig. 3) along each direction were fitted using Least Squared Method to a circle [8]. The results for each clamping style are summarized in Table 2. The Double Finger clamp was found to produce the best simulated curvatures that closely matched theory. Verification with the Zygo Nexview surface profiler indicated otherwise.

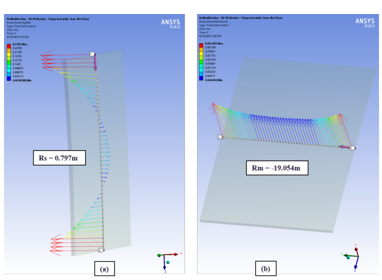

Figure 3: Total deformation results for the Full clamping style of the 1000 µm crystal. (a) the Sagittal path (b) the Meridional path.

VERIFICATION OF CLAMPING METHOD

Two test holders were machined (35keV & 60-90keV stages) so that measurements on the Zygo Nexview profiler could be completed on the crystal surfaces, and so that measurements could be made for various pretension forces for clamping. The crystals were clamped in place using the three clamping styles (Full, Finger, Double Finger), and

Table 2: Three Clamps Simulation Results for 1000µm Si Crystal

Clamp Style	R_s [m]	R_m [m]
Full	0.797	-19.054
Finger	0.771	-13.296
Double Finger	0.754	-48.458

then measured (Table 3) on the Zygo profiler for R_s & R_m, repeated tests were conducted to assess the variability of tightening.

Table 3: Zygo Nexview Profiler Measurements Results for Si Crystals (460 µm top & 1000 µm bottom)

Clamp Style	R_s [m] (±SD)	R_m [m] (±SD)
Full	0.414 (0.121)	-22.066 (9.196)
Finger	0.375 (0.003)	+28.174 (7.719)[1]
Double Finger	0.367 (0.003)	-10.128 (0.859)
Full	0.688 (0.003)	-32.951 (8.459)
Finger	0.694 (0.001)	-64.289 (14.268)
Double Finger	0.699 (0.003)	-23.609 (3.512)

A further analysis of the 1000 μm Si crystal profile at three locations (see Fig. 4) along sagittal curvature plane illustrates the subtle parabolic curvature results.

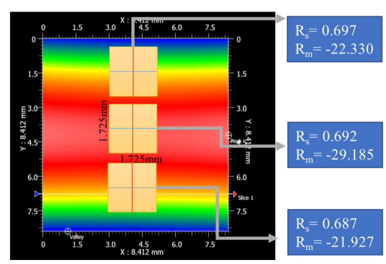

Figure 4: Evaluation of three locations of the Full clamp style using the 1000 µm Si crystal.

The parabolic curvature using the Full clamp was found from both the ANSYS Simulations and the Zygo Profiler. This observation is an unfortunate result likely from the static clamping method. Fortunately, the desired curvature areas was found to exceed the incident beam size creating the desired focusing of the full beam.

REDESIGN IMPLEMENTED

Once evaluation was complete, the Full clamp resulted in the most promising R_s & R_m for both of the 1000 µm & 460 µm Si crystals. The Full clamp was installed on the crystal holders, three Belleville washers were stacked in a parallel configuration for each screw (see Fig. 5), silver paint (Conductive Silver Paint, SPI 05001-AB) was used

[1] Interestingly, the Finger clamp for 460µm Si resulted in a +ve R_m

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as interstitial material between the Si Crystal and copper holder.

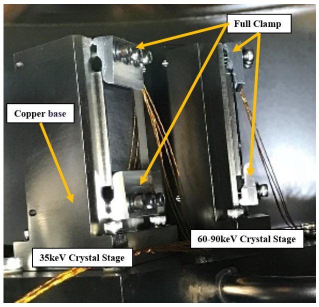

Figure 5: Currently operating within the BXDS HE Mono.

CURRENT PERFORMANCE

The performance of the BXDS HE monochromator has been characterized (see Fig. 6), indicating the new holder design has achieved x-ray focusing parameters that currently approximate the theoretical requirements, but most importantly have produced good initial diffraction from samples.

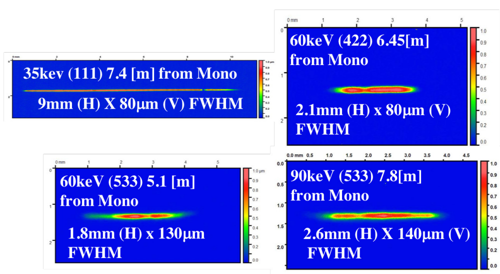

Figure 6: Beam profiles measured with current Full clamp.

The current flux measurements (Table 4) produced from the BXDS HE Mono (In Vacuum Wiggler limited to 8.4 mm gap.

Table 4: Flux Performance for BXDS HE Mono Crystals

Energy	Ion Chamber Flux [ph/s]	% of theory
35keV (460 μm)	1.34 x 10^{13}	22.27
60keV (1000 μm)	2.08 x 10^{12}	61.07
90keV (1000 μm)	8.1 x 10^{9}	4.5

CONCLUSION

With the initial unusable performance from the BXDS HE mono, an evaluation of the crystal holder was required. By removing the over constrained original mask, the Full clamp allowed the crystal to naturally bend achieving acceptable R_s & R_m.

The study conducted of the BXDS HE mono crystal holder demonstrates a simple method of reproducing Laue bent diffraction using two clamps that hold the Si crystal over a precisely machined radius. The design changes have resulted in good X-ray focusing and have demonstrated good diffraction results.

FUTURE WORK

Thermal equilibrium analysis for crystal performance under high heat loads would greatly benefit the understanding of how each crystal behaves. The thermal analysis would consider the attenuated heat, evaluate effective differences/optimization of cooling applied to various clamping methods.

Ultimately, a dynamic bender would be ideal to achieve closer theoretical focusing values, allowing for immediate optimization of the crystal focus. A comparison between a dynamic system and the static system proposed in this work, would be useful to future designers.

ACKNOWLEDGEMENTS

Thank you to Brian Yates, David Muir, John Campbell, and David Smith. Thank you to the BXDS Technical Group.

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