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FOUR-BOUNCE CRYSTAL MONOCHROMATORS FOR THE SIRIUS/LNLS BEAMLINES

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Abstract

Beamlines of new 4th-generation machines present high-performance requirements in terms of preserving beam quality, in particular wavefront integrity and position stability at micro and nanoprobe stations. It brings about numerous efforts to cope with engineering challenges comprehending high thermal load, cooling strategy, crystal manufacturing, vibration sources, alignment and coupled motion control. This contribution presents the design and performance of four-bounce silicon-crystal monochromators for the Sirius beamlines at the Brazilian Synchrotron Light Laboratory (LNLS), which is basically composed of two channel-cut crystals mounted on two goniometers that counter-rotate synchronously. The mechanical design ascertained the demands for the nanoprobe and coherent scattering beamlines - namely, CARNAÚBA and CATERETÊ - focusing on solutions to minimize misalignments among the parts, to grant high stiffness and to ensure that the thermal performance would not impair beam characteristics. Hence, all parts were carefully simulated, machined, and measured before being assembled. The present work introduces mechanical, thermal, diagnostics, and dynamic aspects of the instruments, from the design phase to their installation and initial commissioning at the beamlines.

INTRODUCTION

Carnaúba (CNB) and Cateretê (CAT) are the longest Sirius beamlines. Their scientific programs bring several cutting edge contrasts and imaging techniques for research in numerous science fields. Carnaúba has a sub-microprobe (600-150 nm) and nanoprobe (120-40 nm) experimental stations and covers the energy range from 2.05 to 15 keV. Cateretê's experimental station is followed by a 30 m flight path in-vacuum detector and receives a 30 um² beam in the energy range from 4 to 21 keV. In order to achieve such goals, the beamline instrumentation needs to present exceptional performance [1, 2]. Notably, such beamlines will use a four-bounce crystal monochromator (4CM) to select and scan X-rays with resolution of $\Delta E/E=10^{-4}$.

The main attributes of a 4CM are the high energy resolution and its independency from the beam divergence [3]. The first Sirius' 4CMs are based on cryogenically cooled Si crystals and it introduces a simple concept that prioritizes high mechanical stiffness associated to robust control.

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MECHANICAL DESIGN

The equipment comprises a pair of channel-cut silicon crystals in a horizontal +--+ configuration so that the parallelism between diffraction surfaces is inherently ensured, the downstream beam keeps the same direction of the upstream beam regardless of Bragg's angle, and higher resolution in the selection of X-ray energy is achieved when compared to double crystal monochromators [4]. Table 1 shows the 4CM specifications.

Table 1: Specifications of Carnaúba and Cateretê 4CMs

Parameter	CNB	CAT
Crystal Set	Si (111)	
Angular Range (°)	7-75	4.5-50
Encoder Resolution (urad)	<< 1	
Axes synchronization (urad)	< 10% D.W.	
Crystal Size (mm³)	62x90x50	50x98x62
Channel-Cut gap (mm)	8.0	6.2
Crystal Temperature	125 K	
Beam Size (mm²)	1.5x2.6	0.99 x 0.51
Heat Load from Beam (W)	7	17.4
Base Pressure	<5E-8 mbar	

The rotation of the crystals around Bragg angle is driven by a pair of high-resolution goniometers Aerotech APR-200. Naturally, both axes must rotate in opposite directions. Hard stops and limit switches confine the ranges to avoid damage.

The cooling source is a commercial ST-400 UHV cryostat (Janis) supplied by an open cycle liquid nitrogen flow, capable of dissipating 70 W and linked to the crystals by copper thermal straps (TS), which allows the rotations. Additional copper parts are used to fit the different geometries and follow the crystal rotation movement. The straps are also useful to attenuate vibrations from the cooling system, whereas the goniometers are rigidly fixed on a granite bench, which aims to minimize the amplification of vibrations from the ground, Figure 1.

Each channel-cut crystal is clamped to a titanium frame at three contact zones with flexible links designed to minimize deformation and maximize stiffness. The frame is kept in an intermediary temperature, while the rotary stage below it is kept at environmental temperature, Figure 2 zooms the previous figure, highlighting the crystal frame.

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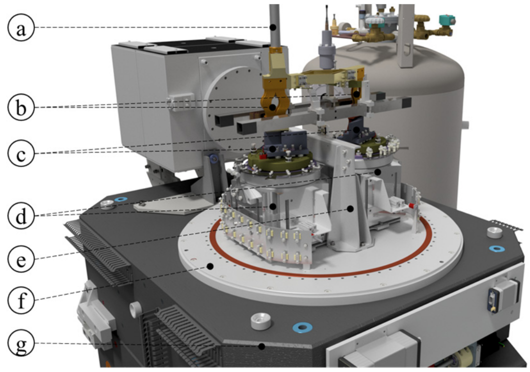

Figure 1: CAD representation of 4CM-CAT. Cryostat (a), copper straps (b), crystals (c), rotary stages (d), linear actuator module (e), vacuum chamber (f), granite bench (g).

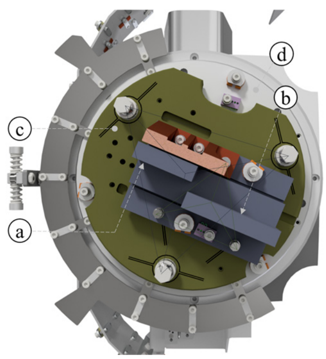

Figure 2: CAD representation of first channel-cut crystal module, containing the first (a) and second (b) diffraction surfaces and the crystal frame (c), which is clamped to the rotary stage (d) at three points 120° spaced.

A linear actuator assembled in a stainless-steel structure is used to move a slit between the two crystals. The slit supports beam diagnostics and acts as a mask to avoid diffractions from other lattice planes. The parts are mounted inside an ultra-high vacuum (UHV) stainless-steel chamber and a liquid nitrogen vessel is placed next to it in order to supply the fluid, Figure 3.

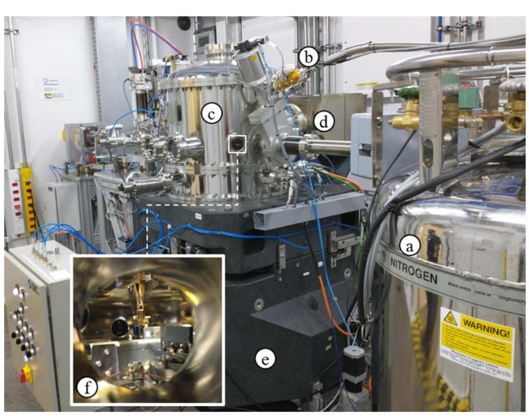

Figure 3: Photography of 4CM-CNB. Liquid nitrogen vessel (a), cryostat (b), vacuum chamber (c), ion pump (d), granite bench (e), and internal view (f).

Alignment

The number of degrees of freedom (DoF) is limited to enhance the stiffness of the system. The DoF for alignment of the entire equipment in relation to the beamline are entrusted to the granite bench (three rotations, Rx, Ry, Rz and two translations Tx, Ty) [5]. Inside the vacuum chamber, the only DoF are Bragg rotations delivered by the goniometers and the translation of the shielding. Therefore, the alignment of the parts, including the parallelism between axis and the positioning of the crystals in relation to Bragg axis, is defined by dowel pins, machining shims, control of screw tightening and metrology.

To ensure the perpendicularity between diffraction planes and rotation axis, with error below 100 µrad, crystals were assembled on their goniometers and the crystallographic orientations were aligned by using an X-ray diffraction setup providing inputs for tailoring the shims among crystals and their frames.

The parallelism between the axis and the alignment of the entire equipment in the beamline is expected to be achieved with a precision better than ±100 µm (Tx, Ty) and ± 500 µrad (Rx, Ry, Rz) (Fig. 4) when referencing via Laser Tracker.

A script was developed in Python to evaluate the effects of misalignments in the ray-tracing. Figure 4 shows the possible positions of the x-ray beam downstream 4CM-CAT along a full Bragg scan for $1x10^4$ beams reflected by the four crystals subject to random misalignment conditions.

Input	Gap between crystals	6.2±0.05 mm
	Rx, Ry, and Rz (Bench to Lab)	± 500 µrad
	Rx', Ry', and Rz' (Rotary Stages to Bench)	± 500 µrad
	Rx'', Ry'', and Rz'' (Crystal to Rotary Stages)	± 100 µrad

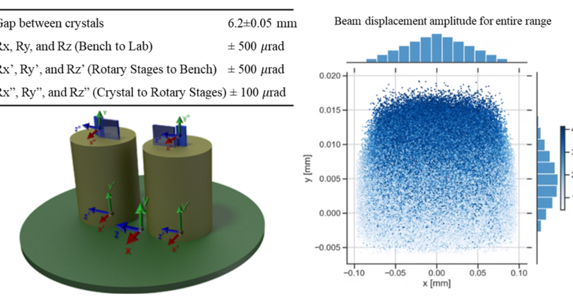

Figure 4: Variations of the virtual source due to random misalignments showed on top-left table. $1x10^4$ cases were considered inside these ranges. The coordinate systems xyz, x'y'z' and x''y''z'' are fixed to bottom flange, bottom part of goniometers and center of rotation of crystals, respectively.

This study shows that the variations over the entire range according to the specified alignments values could achieve 20% of the beam size downstream the 4CM. Gap variations from machining process cause the major contribution for horizontal deviations whereas perpendicularity error among rotary stages and floor are dominant for vertical movements.

The offset calibration is achieved by matching reflections of the first and third surfaces to the white beam and by maximizing the intensity in the diagnostics between the channel-cuts and in the visualization device downstream.

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Cooling

The high-power photon density from an X-ray synchrotron beam can deform the surfaces of the optical elements and affect the beam quality. The difference of temperature among the diffraction surfaces of the monochromator crystals leads to dissimilar distances between adjacent lattice planes (d-spacing), impairing the photon flux downstream. Moreover, the overall deformation on the footprint results in variations in terms of size and position of the focal point of the beamline, where the samples are usually placed [6, 7]. Such deformations are minimized when the crystals are maintained at cryogenic temperatures, where silicon has high thermal conductivity and low coefficient of thermal expansion (CTE). This effect is illustrated for 4CM-CNB by Figure 5. The smaller the crystal deformation the smaller the beam size at the focus and its position deviation along the X-Ray beam direction (Z)

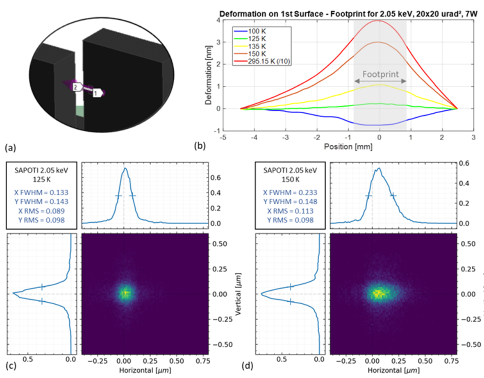

Figure 5: Deformation along the 1st crystal surface of 4CM-CNB (a) due to thermal effects for different bulk temperatures made on Ansys for a 1.6 x 2.7 mm² 7W footprint at 2.05 keV (b). Values for 295.15 K are divided by 10. Raytracing of the diffracted X-Ray beam at experimental station downstream 4CM for crystals at 125 K (c) and 150 K (d) made on Shadow.

A lumped model was applied to design the parts to keep the crystals temperatures close to 125 K [8], which is expected to be achieved after the update of the thermal straps [9]. The cryostat and cryogenic infrastructure are analyzed in a dedicated work [10].

Control

The movements of all axes are controlled by a high-performance Delta Tau (Faraday) motion control solution. On the other hand, the temperature monitoring and control is overseen by a CompactRio (National Instruments) device. The position feedback system consists in a rotary scale TONIC Renishaw with resolution of 26.62 nrad. The control system used is the PowerBrickLV (Delta Tau) which allows kinematics transforms, thus being possible to control Bragg's angle with less than 50 nrad RMS positioning error (from 1 Hz to 2.5 kHz) and to maintain the synchronism of the stages during 600 eV/s movement within 3 urad RMS [11].

PRELIMINARY CHARACTERIZATION

Some preliminary characterizations were accomplished to evaluate the performance with beam. Figure 6 shows an experimental rocking curve obtained by fixing the first set at 9.75 keV and scanning the second set to calibrate small offset among the crystals at the CNB 4CM. The FWHM of the rocking curve matches the expected value, which is a convolution of the total intrinsic reflection width (~27 urad) and the small beam divergence (17 urad)

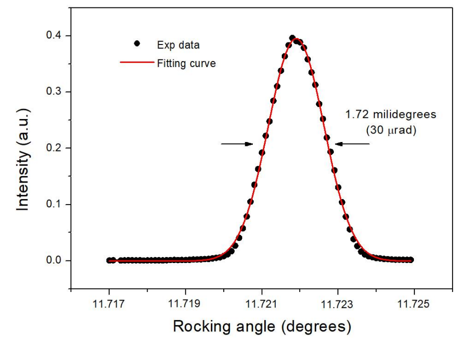

Figure 6: Rocking curve.

The energy resolution of the 4CM was analyzed in an X-ray absorption spectroscopy experiment at the CNB evaluating the sharp pre-edge peak in the Mn K-edge of $KMNO_4$, Figure 7. The measured FWHM of 1.54 eV is consistent with the convolution of predicted 4CM resolution (0.65 eV) and the intrinsic core hole width of 1.3 eV [12].

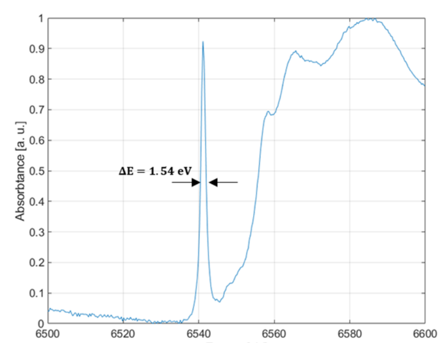

Figure 7: Beamline energy resolution measurement with $KMNO_4$ K edge.

FINAL REMARKS

Cryogenically cooled four-bounces monochromators were developed to meet the needs of Cateretê and Carnaúba beamlines. Preliminary analysis demonstrate reliability and that high resolution performances.

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REFERENCES

[1] H. C. N. Tolentino *et al.*, "Innovative instruments based on cryogenically cooled silicon crystals for the CARNAÚBA beamline at Sirius-LNLS", *AIP Conf. Proc.*, vol. 2054, p. 060026, 2019. https://doi.org/10.1063/1.5084657

[2] F. Meneau *et al.*, "Cateretê, the coherent scattering beamline at Sirius, 4th generation Brazilian synchrotron facility", Coherence at ESRF-EBS, Grenoble, France, 2019.

[3] S Diaz-Moreno *et al.*, "I20; the versatile x-ray absorption spectroscopy beamline at Diamond Light Source", *J. Phys. Conf. Ser.*, vol. 190, p. 012038, 2019.

[4] J. W. M. DuMond, "Theory of the use of more than two successive x-ray crystal reflections to obtain increased resolving power", *Phys. Rev.*, vol. 52, pp. 872-883, Oct. 1937. doi:10.1103/PhysRev.52.872

[5] R. Geraldes *et al.*, "Granite benches for Sirius x-ray optical systems", in *Proc. MEDSI'18*, Paris, France, June 2018. doi: 10.18429/JACoW-MEDSI2018-THPH12

[6] M. Antimonov *et al.*, "On the influence of monochromator thermal deformations on X-ray focusing", *Nucl. Instrum. Methods Phys. Res.,Sect. A,* vol. 820, pp. 164-171, 2016. doi: 10.1016/j.nima.2016.02.103

[7] J. Eckdahl, "Effects of lattice strain in silicon double crystal monochromators", Department of Physics, MAX IV Laboratory, MAXM30, 20181, 2018. http://lup.lub.lu.se/student-papers/record/8947155

[8] M. Saveri Silva, "Thermal modeling for the development of a four-bounces crystal monochromator for the Sirius project", University of Campinas, 2019.

[9] F. R. Lena *et al.*, "Copper braid heat conductors for Sirius/LNLS cryogenic x-ray optics", presented at the 11th Int. Conf. on Mechanical Engineering Design of Synchrotron Radiation Equipment and Instrumentation (MEDSI2020), Chicago, IL, USA, virtual conference, July 2021, paper TUPC14, this conference.

[10] M. Saveri Silva *et al.*, "Cryogenic systems for optical elements cooling at Sirius/LNLS", presented at the 11th Int. Conf. on Mechanical Engineering Design of Synchrotron Radiation Equipment and Instrumentation (MEDSI2020), Chicago, IL, USA, virtual conference, July 2021, paper MOPB02, this conference.

[11] L. Martins dos Santos *et al.*, "The Control System of the Four-Bounce Crystal Monochromators for Sirius/LNLS Beamlines", submitted to 18th International Conference on Accelerator and Large Experimental Physics Control Systems, Shanghai, 2021.

[12] H. C. N. Tolentino *et al.*, "A 2.3 to 25 keV XAS beamline at LNLS", *J. Synchrotron Radiat.*, vol. 8, pp. 1040-6, 2001. doi:10.1107/S0909049501005143