THE HD-DCM-Lite: A HIGH-DYNAMIC DCM WITH EXTENDED SCANNING CAPABILITIES FOR SIRIUS/LNLS BEAMLINES

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Abstract

After successfully designing, installing, and commissioning two units of the High-Dynamic Double-Crystal Monochromator (HD-DCM) at the Brazilian Synchrotron Light Laboratory (LNLS) - Sirius, two more units are now required. Since they demand only a smaller energy range (5 to 35 keV), the total gap stroke of the new instruments can be significantly reduced, creating an opportunity to adapt the existing design towards the so-called HD-DCM-Lite. Removing the large gap adjustment mechanism allows a reduction of the main inertia by a factor of 5, enabling the HD-DCM-Lite to deliver energy flyscans of hundreds of eV reaching 20 cycles per second while keeping fixed exit and the pitch stability in the range of 10 nrad RMS (1 Hz - 2.5 kHz). Hence, an unparallel bridge between slow step-scan DCMs and fast channel-cut monochromators is created. This work presents the in-house development of the HD-DCM-Lite, focusing on its mechanical design, discussions on the ultimate scanning constraints (rotary stage torque, voice-coil forces, interferometers, and encoders readout speed limits and subdivisional errors), and thermal management.

INTRODUCTION

A lighter version of the High-Dynamic Double-Crystal Monochromator (HD-DCM) [1-3] has been designed for two of the new Sirius beamlines at the Brazilian Synchrotron Light Laboratory (LNLS): the QUATI (quick absorption spectroscopy) and the SAPUCAIA (small-angle scattering) beamline. Differently from the two first beamlines that required larger angular (3° to 60°) and energy range (2.3 to 35 keV), these two forthcoming beamlines have smaller energy range requirements – namely, 5 to 35 keV for QUATI and 5 to 18 keV for SAPUCAIA -, allowing a design with an angular range from 5° to 40°. In addition, QUATI also adds the challenge of time-resolved analysis, benefiting from quick energy scans. The new design focus on extending its scan capabilities while preserving stability creating a solution between the current HD-DCM (limited in speed but with fixed-offset and extremely stable) and fast channel-cut monochromators [4], which suffer from offset variation. This work will present the main topics considered during the design of the HD-DCM-Lite.

MECHANICAL DESIGN

The current HD-DCM design was used as starting point for the HD-DCM-Lite because it is an extensively optimized and tested system, proven to reach 10 nrad RMS (root mean square) of pitch parallelism performance (within 1 Hz to 2.5 kHz) [2]. Nevertheless, the design had to be adapted to become capable of meeting the fast energy scan requirements for quick-EXAFS (Extended X-ray Absorption Fine-Structure) experiments. Since only the design variations can be discussed here for conciseness, [1] may be consulted for the full set of specifications.

The total gap range between crystals could be reduced from 9 mm to 2.75 mm, such that the long-stroke (LOS) mechanism (see [1]) could be eliminated, enabling a more compact, easier to assemble and cheaper system. Consequently, the moment of inertia was reduced from 13.5 kg.m² to 2.7 kg.m², allowing higher accelerations, an important upgrade towards fast scan capability.

Another essential step was doubling the torque capability, now reaching 58.2 N.m after substituting the passive bearing by another Aerotech's APR-260DR-180 rotary stage, thus increasing the scanning capabilities. To handle the power dissipation of the two rotary stages in demanding long-term scan trajectories, a water-cooling circuit has been implemented on the stages. The HD-DCM-Lite is shown in Fig. 1 in comparison to the original HD-DCM.

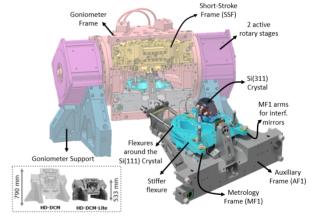


Figure 1: Highlights of the main mechanical design changes and improvements in the HD-DCM-Lite.

From lessons learned [5], this designing opportunity is also taken for improvements in the dynamics of the metrology frame (MF1) supporting the first crystals (CR1s). Increasing its mounting stiffness – by removing the zirconia spacers between MF1 and Auxiliary Frame (AF1) and stiffening the flexures between them - and shortening its "arms" for the interferometer mirrors, the first eigenfrequency should increase from 500 to 800 Hz, reducing the sensitivity to disturbances. Then, to recover the required thermal resistance between the CR1s and the AF1, a complementary set of flexures is added around the CR1s.

SCANNING CONSTRAINTS

For time-resolved experiments, faster energy scans may enable scientific opportunities in analyzing quick chemical reactions or material phase variations, for example. Therefore, every design decision in the HD-DCM-Lite must consider its impact on pushing the scanning speed to its limits. The following discussion presents the main factors that constrain the scanning capabilities, also predicting how fast the system will be able to go.

Torque and Sensors Constraints

Regarding the rotary stages, scanning speeds can be limited by torque and sensor readout rate for quadrature signals, which, assuming sinusoidal trajectories, can be evaluated according to:

$$f_{\text{max}_{\text{T}}} = \frac{1}{2\pi} \sqrt{\frac{T_{\text{max}}}{AI_{\text{xx}}}} \tag{1}$$

$$f_{max_e} = \frac{\text{res}_e f_r}{2\pi A} \tag{2}$$

In (1), knowing the system moment of inertia I_{xx} and given a desired angular amplitude A, the maximum frequency f_{max_T} that the system can develop is bounded by the maximum torque T_{max} in the rotary stages. This maximum frequency will be different for: the Si(111) and Si(311) crystal sets; the absolute energy values; and the scanning energy amplitude, because they change the amplitude A according to Bragg's law of diffraction.

In (2), the maximum scanning frequency f_{max_e} due to the encoder readout speed depends on its resolution res_e , the angular amplitude A, and the acquisition rate f_r for the quadrature signal. With the current control solution for the HD-DCM using NI's CompactRIO (cRIO) [6], f_r is limited to 10 MHz. Among the options given by the stage manufacturer, two encoders with resolutions of 191 nrad and 19.1 nrad were compared. For some range of energies, it was observed that the encoder with the best resolution would dominate the scanning frequency limits over the torque boundaries, whereas the encoder with 191 nrad of resolution will not add new limits - while preserving acceptable energy resolution - becoming the one selected.

Yet, a sinusoidal trajectory is never completely smooth in real world. For example, when using optical encoders, there are errors within the scale pitch length called Sub-Divisional Errors (SDE). This noise added to the smooth position trajectory creates regions with higher derivative, resulting in an increment of the speed read by the encoder. In this case, the calculations show that this contribution is not more than 1% of the total speed. Still, these accelerations do have some impact in the control dynamics and final stability.

Now, concerning the control of the gap between crystals made by the short-stroke (SHS) (see [1]), its built-in SmarAct's Picoscale interferometer is also currently read as a quadrature signal limited at 10 MHz in cRIO, such that the target speed is limited to 1 mm/s for the current resolution of 0.1 nm. Therefore, the speed in the gap adjustment

(following the rotary stages angle to keep the fixed beam offset) cannot exceed this limit. This sensor also has SDE, but its amplitude is negligible. If required in the short term, the resolution can be worsened, at the cost of some loss in stability performance, to increase speeds. For the long term, work is in progress to handle the PicoScale data as an absolute measurement, without speed limits.

Uniting the torque, encoder and current interferometer limitations, Fig. 2 was constructed to show the first prediction for the HD-DCM-Lite scanning boundaries (the horizontal boundary is related to the balance-mass (BMS) [1] displacement limits, which will be presented later). For low energies, the interferometer is the main constraint (non-linear in energy), whereas torque (linear in energy) limits the higher frequencies. Scanning frequencies above the curves cannot be performed.

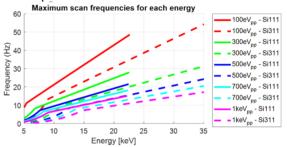


Figure 2: Maximum scanning frequencies constrained by torque, encoder, and interferometer limitations for each crystal set, central energy, and amplitude (peak-to-peak).

Voice-Coil Effort Constraints

In the field of possible trajectories constrained as previously discussed, some representative options were simulated (using a MATLAB® toolbox developed for Dynamic Error Budgeting [5]) to predict the resulting effort at each of the three voice-coil (VC) actuators of the SHS (see [1]), checking for their operational limits and verifying if their dissipated power could compromise the thermal management (detailed in the next session). The worst-case scenario happens for the trajectory with highest possible frequency, i.e., 54 Hz and 0.2 mrad of amplitude for Si(311), resulting in RMS forces of 0.3 N in the upstream (VC1) and 3.1 N in the downstream VCs (VC2 and VC3).

These RMS forces do not include the offset effort necessary to have the SHS at the exact nominal gap value to start scanning, which is a crucial aspect in the HD-DCM-Lite, since there is no compensation by the LOS module. Considering the limits at 5° and 40°, with gap values of 9.03 mm and 11.75 mm, and the natural sag variation related to the SHS weight, up to more 3.1 N is required for each VC. Finally, these effort contributions must be added to a final one: the force necessary to correct angular misalignments and parasitic torques (passively introduced after baking and cryocooling procedures) between the SHS and the MF1. With the experience gathered with the existing HD-DCMs and considering a safety factor, the resulting worst-case misalignment correction could reach 3 mrad, demanding additional 1.3 N for VC1 and 1.8 N for VC2 and VC3.

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Uniting all contributions, maximum values of 4.7 N for VC1 and 8.0 N for VC2 and VC3 are obtained, which, according to Akribis' AVM-40-HF-6.5 datasheet [7], is still within 50% of the maximum continuous force specification (at 100°C). Thus, using the force sensitivity constant of 20.7 N/A and the resistance of 11.31 Ω , the power consumption for VC1 could reach 0.6 W, and 1.7 W for VC2 and VC3 individually, totalling 4.0 W.

Balance-Mass Displacement Constraints

The last factor to be considered is the balance-mass (BMS) displacement. As the VCs act to position the SHS with respect to the MF1, the reaction forces are directed to the BMS, which responds passively over its mounting stiffnesses, with the possibility of collisions against the mechanical hard-stops, creating disturbances and stopping the system. The solution was to increase the stiffness of the folded leaf-springs that constrain the BMS. Yet, although smaller displacements now occur for the same reaction forces and higher forces are allowed, the consequence in dynamics is shifting the eigenfrequencies from 6.1 Hz to 25.8 Hz and from 9.0 Hz to 38.0 Hz for the gap and pitch/roll degrees of freedom (DoFs), respectively. This means that the BMS is now slightly less efficient as a dynamic filter, but still compatible with the overall mechatronic architecture, as verified in the dynamic models.

Then, still using the same model and following the analyses of the VC efforts, i.e., considering offset, scanning and misalignment-related effects, a few representative cases were selected to investigate the displacement of the BMS in all three DoFs with respect to both its mounting frame and the SHS. As the BMS is now relatively stiffer, for the lower scanning frequencies its displacements remain within only a small fraction of the tolerable ranges of a few millimeters and milliradians. As it might be expected, the limits are found as the displacements quickly increase near the BMS resonances. Thus, respecting the constraints in Fig. 2, a new constraint of at least 24 Hz must be considered, with simulation results suggesting that even higher frequencies still below 38 Hz may become feasible.

To conclude, with simplified mechanics, the predictions for the HD-DCM-Lite pitch stability show the even better static performance of 5 nrad RMS (1 Hz - 2.5 kHz), which may be maintained even for some scanning conditions with appropriate control strategies, but also leaves some margin for occasional scanning disturbances.

THERMAL MANAGEMENT

As in the mechanical design, the thermal management of the HD-DCM-Lite was also based on the HD-DCM [8]. Here, the beam power load inputs are 54 W for QUATI and 80 W for SAPUCAIA. Aside from keeping all components functioning within nominal temperatures, the main objective is to keep the CR1s cryogenically cooled at 78 K – as not to damage them with the high-power densities –, and the lattice parameter of the 2nd crystals (CR2s) close to that of the hotspot in the CR1s, to prevent energy mismatching. For modelling purposes, the ideal temperature

was considered as 155 K as a mean value for different operating conditions or modes of the system.

A lumped-mass thermal model was developed in Simulink®. The conductances were simulated via Ansys® for each connection separately as a geometric factor to include non-linear temperature effects. The model also included radiation, which was obtained using Gebhart factors [9] from a view factor matrix simulated in Ansys Fluent® from a simplified model. The contact resistances were estimated according to [10, 11]. The Simulink® model was a timedomain transient solution for the system, using look-up tables to get the temperature-dependent conductivity for the nodes, and an algebraic thermal radiative heat flux output at each time step, from the Gebhart factors. With this model, it was possible to obtain the desired high-conductivity braid specifications [12] for the CR2s. Only one braid was necessary in this design, resulting in less contact resistances and better cooling performance.

Then, a sensitivity study for the voice-coils was made, to analyse its power output influence on the CR2s working temperature, in addition to its own. The results can be seen in Fig. 3. As the expected power output is less than 4 W total, this should not impose an additional constraint on the design.

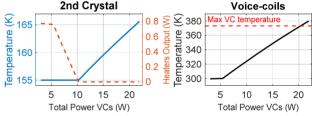


Figure 3: Simulated temperatures of the active 2nd crystal and mean VCs temperature as a function of the VCs power.

CONCLUSION

The predictive design methodology that successfully conceived the HD-DCM is now applied in the development of the HD-DCM-Lite for extended scanning capabilities while maintaining ultra-high stability performance. The competences in design and control, together with toolboxes and libraries, that were developed over the first project have allowed the new machine to be completely designed in-house at LNLS in a short time scale. The prototype is expected to start to be tested still in 2021.

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REFERENCES

- [1] R. R. Geraldes et al., "The New High Dynamics DCM for Sirius," in Proc. 9th Mechanical Engineering Design of Synchrotron Radiation Equipment and Instrumentation Int. Conf. (MEDSI'16), Barcelona, Spain, Sep. 2016, pp. 141-146. doi:10.18429/JACOW-MEDSI2016-TUCA05
- [2] R. R. Geraldes et al., "The Status of the New High-Dynamic DCM for Sirius," in Proc. 10th Mechanical Engineering Design of Synchrotron Radiation Equipment and Instrumentation Int. Conf. (MEDSI'18), Paris, France, Jun. 2018, pp. 147-152. doi:10.18429/JACOW-MEDSI2018-WE-OAMA01
- [3] R. R. Geraldes et al., "Commissioning and prospects of the High-dynamic DCMs at Sirius/LNLS," presented at MEDSI 2020, Chicago, USA, Jul. 2021, paper MOPB03, this conference.
- [4] O. Müller *et al.*, "Quick scanning monochromator for millisecond in situ and in operando X-ray absorption spectroscopy," *Rev. Sci. Instrum.*, vol. 86, no. 9, p. 093905, 2015. doi.org/10.1063/1.4929866
- [5] R. R. Geraldes et al., "Dynamic error budgeting in the development of the High-Dynamic Double-Crystal Monochromator at Sirius Light Source," in Proc. ASPE Topical Meeting 2020, Boston, USA, May 2020.
- [6] M. A. L. Moraes et al., "The FPGA control implementation of the High-Dynamic Double-Crystal Monochromator at Sirius Light Source," presented at ASPE Topical Meeting 2020, Boston, USA, May 2020, unpublished.

- [7] Akribis Systems, "AVM Series," AVM-40-HF-6.5 datasheet, https://www.micromech.co.uk/up-loads/assets/pdf/akribis/voice_coil_motors/akribis_avm_series_datasheet.pdf
- [8] M. Saveri Silva, R. R. Geraldes, A. Gilmour, T. A. M. Ruijl, and R. M. Schneider, "Thermal Management and Crystal Clamping Concepts for the New High-Dynamics DCM for Sirius," in *Proc. 9th Mechanical Engineering Design of Synchrotron Radiation Equipment and Instrumentation Int. Conf. (MEDSI'16)*, Barcelona, Spain, Sep. 2016, pp. 194-197. doi:10.18429/JACOW-MEDSI2016-TUPE15
- [9] B. Gebhart, "Surface temperature calculations in radiant surroundings of arbitrary complexity—for gray, diffuse radiation," *Int. J. Heat Mass Transfer*, vol. 3, no. 4, pp. 341– 346, 1961. doi.org/10.1016/0017-9310(61)90048-5
- [10] P. Marion, L. Zhang, L. Goirand, M. Rossat, and K. Martel, "Cryogenic cooling of monochromator crystals: indirect or direct cooling?", in *Proc. MEDSI 2006*, Hyogo, Japan, May 2006.
- [11] M. S. Silva, "Thermal modelling for the development of a four-bounces crystal monochromator for the Sirius project", University of Campinas, 2019.
- [12] F. R. Lena *et al.*, "Copper Braid Heat Conductors for Sirius Cryogenic X-Ray Optics," presented at MEDSI 2020, Chicago, USA, Jul. 201, paper TUPC14, this conference.