Optomechanical Optimization for a Sagittaly Bent Double Crystal Monochromator, using Combined Finite Elements and Ray Tracing

Application to the SAMBA Beamline

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Abstract

Designing a second crystal for a sagitally bent Double Crystal Monochromator (DCM) requires dealing with a number of conflicting requirements. Especially when working with high-energy photons, the angular aperture (Darwin width) becomes very narrow (below 10μrad for Si) while simultaneously the bending radius is increasing small (down to 1m for typical beamline dimensions at 40keV). In this situation, the cross-talk between tangential and sagittal curvature becomes a key parameter, and two strategies are generally used to overcome the issue: either using a flat crystal with a specific length/width ratio, or usage of a rib-stiffened crystal. In the frame of the upgrade of the SAMBA beamline DCM, both solutions have been explored, using a suite of scripts connecting a general purpose FEM code (ANSYS) and a ray-tracing code (SpotX). This has allowed a systematic evaluation of a wide number of configurations, giving insight in the interaction between geometric parameters, and ultimately resulting in a twofold increase in the photon throughput at 30keV without comprising neither spectral resolution nor spot size at sample location.

Introduction

During the upgrade of the SAMBA (Spectroscopy Applied to Material Based Absorption) beamline DCM, the second crystal needed to be replaced, along with its bending mechanics. Two improvements were requested by the beamline scientist. Firstly, it was desired to extend the 2nd crystal usable length so that the corresponding (longitudinal) translation stage could be removed, thus improving mechanical stability. Secondly, the photon throughput at high energies had to be as high as possible (preferably no less than 50% at 30keV).

Main Objectives

1. Develop a suite of analysis tools to generate, analyse, and post process crystal designs
2. Explore configurations for the two families of solutions (flat vs ribbed)
3. Confirm final impact on optical performance using ray tracing.

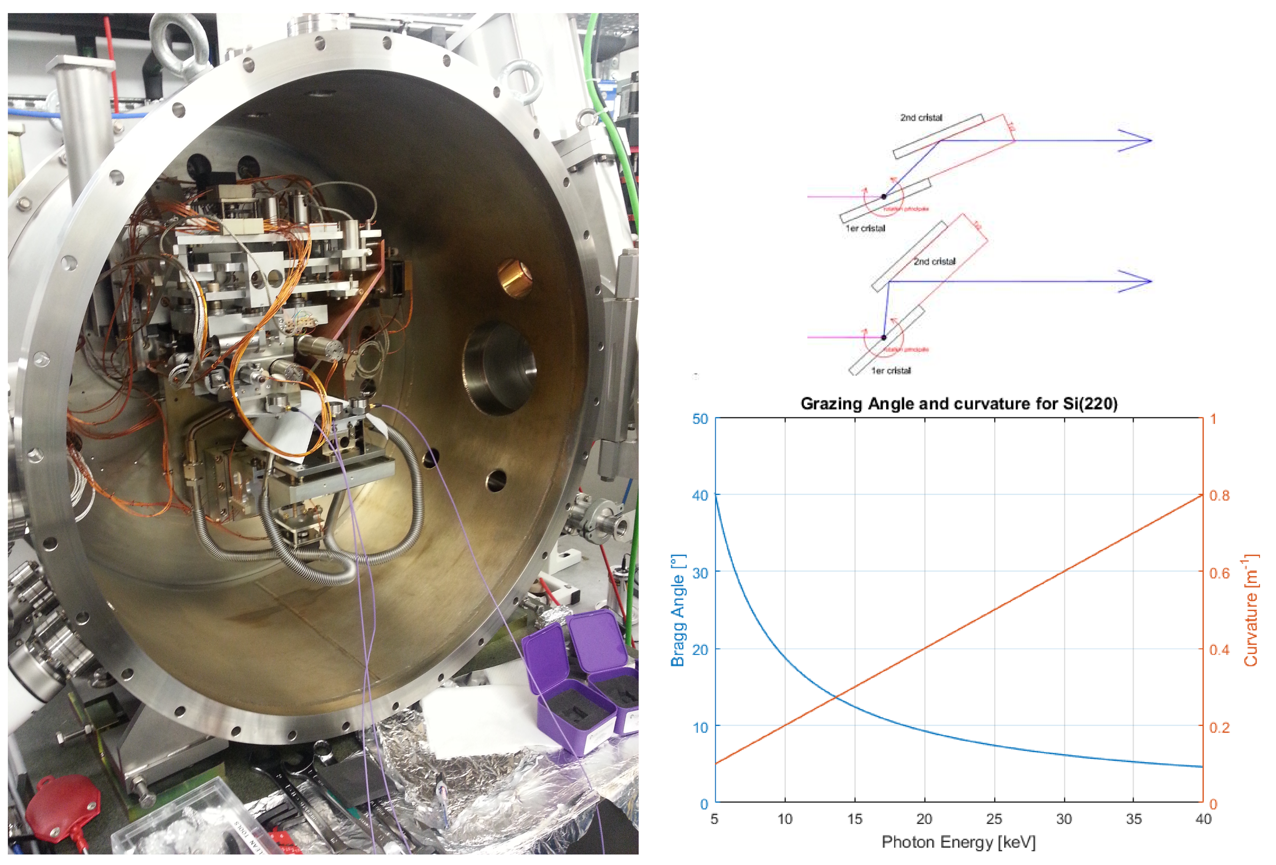

Figure 1: DCM overview and working principle

Methods

Because of the relatively large design space, a numerical Design Of Experiment (DOE) approach has been used, the 4 parameters being the crystal width and length and ribs spacing and height. For each parameter, 3 values have been used (low, base, high), resulting in a 3^4 DOE. Moreover, the results needed be obtained for various photon energies and beam position along the crystal length, hence a systematic and efficient approach was required.

STEP 1: FE Models generation and Analysis (ANSYS)

ANSYS Parametric Design Langage (APDL) scripts have been used to generate, solve, and post process the results for each design, at 3 working energies (5, 20 and 30keV). 3D deformed shapes are then exported on a rectangular grid, as ASCII files.

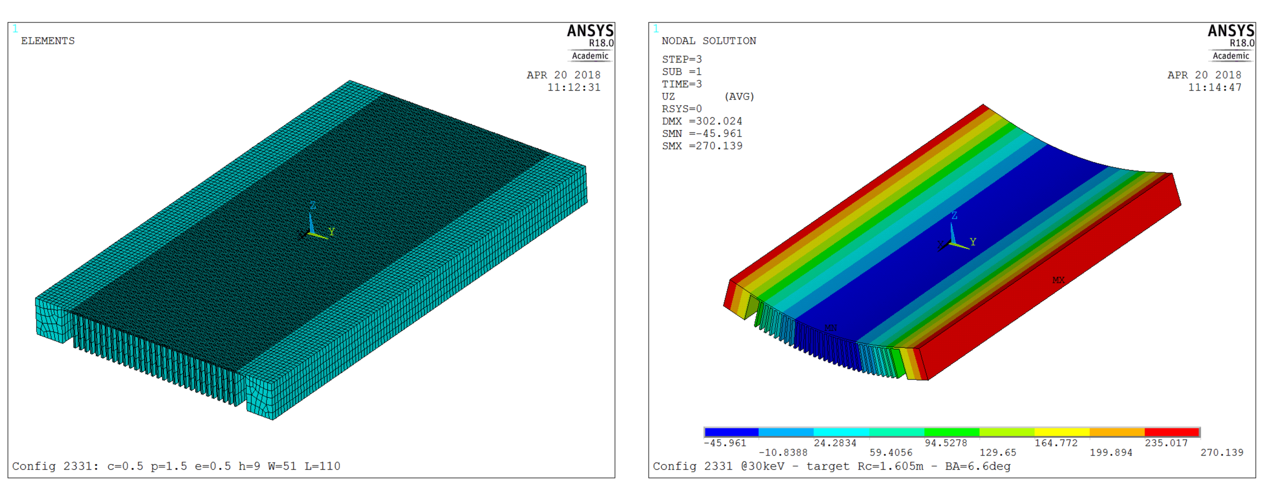

Figure 2: Exemple FEM and corresponding deformed shape @30keV

STEP 2: Optical surface shape analysis (MatLab)

Deformed shapes are read into Matlab, then the best fit cylinder is obtained, and subtracted, giving the geometric *defect*. Then, for each working energy and each working position the following are determined:

1. Ratio of the footprint for wich longitudinal slope is within Darwin Width
2. RMS deviation of the sagittal bending radius

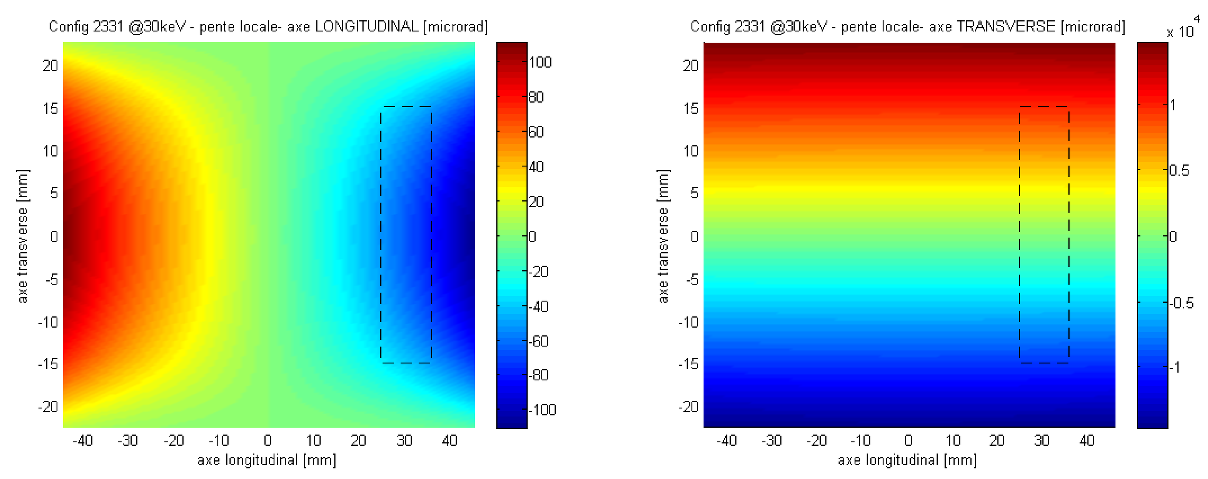

Figure 3: Longitudinal (left) and transverse (right) slopes for best ribbed design @30keV

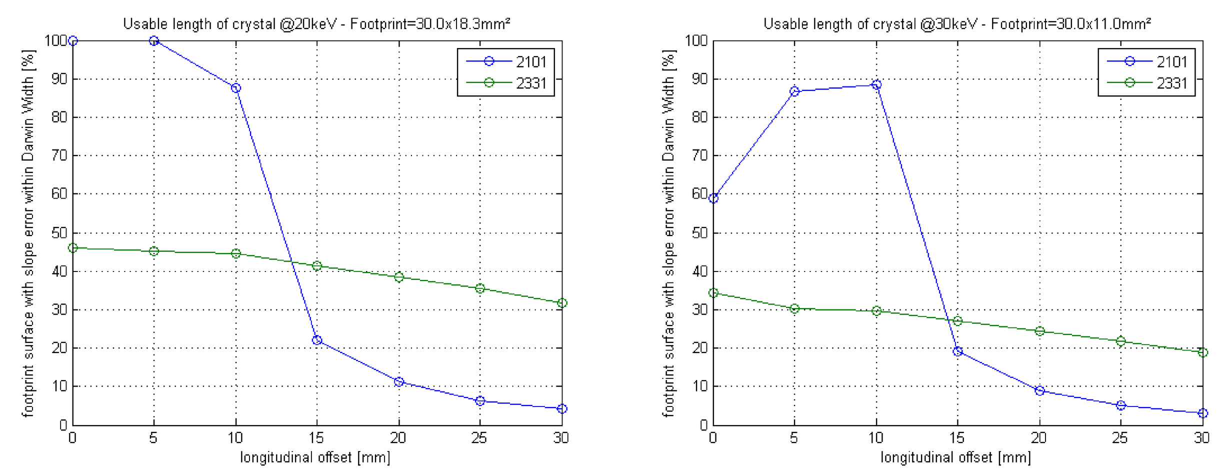

Figure 4: Photon throughput for best flat (2101) and ribbed (2331) configurations at 20 (left) and 30keV (right)

STEP 3: Optical performance final estimation (SpotX)

A complete optical model of the beamline is build using SpotX. At first, no defect is accounted for. This configuration serves as a reference. Then, the defect for two most promising configurations are included, and the analysis is repeated. For each case, one estimates the footprint dimensions (Full Width at Half Maximum), the energy resolution, and the total photon flux.

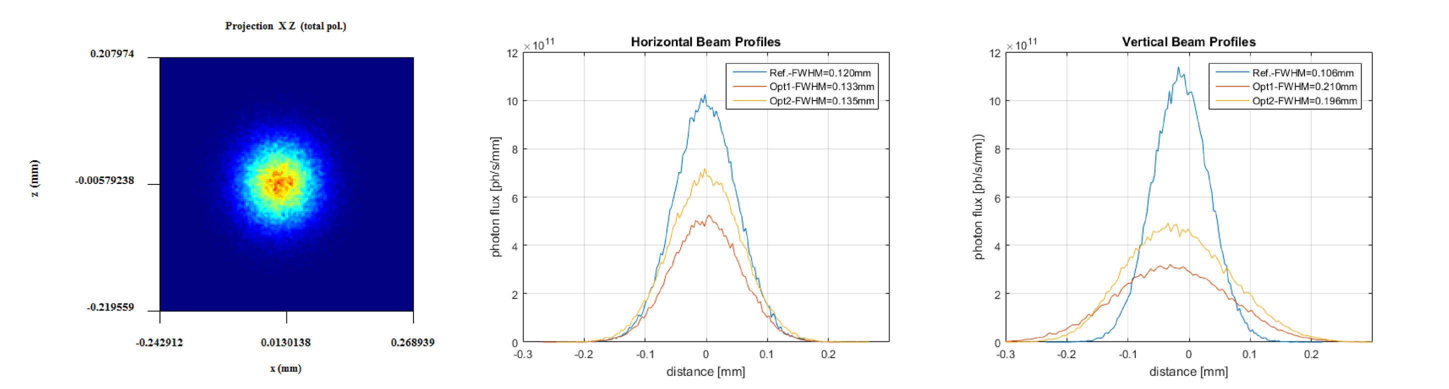

Figure 5: Beam footprint for reference configuration (left) Beam H/V profiles (center/right) @ 30keV

Results

The ray tracing results confirm the comparatively better performance of the flat design, in terms of photon throughput.

Config	FWHM-H [μm]	FWHM-V [μm]	FWHM-E [eV]	Flux [$10^{10} ph/s$]
Reference	120	105	2.55	12.8
Best Ribbed	129	219	2.79	7.2
Best Flat	138	206	2.62	10.1
Target	<150	<300	<3.0	>6.4

Table 1: Optical figures of merit as calculated by SpotX

Conclusions and Outlook

- Using a DOE approach, it was shown that a substantial increase in photon throughput was possible, by minor modifications of the crystal geometric features.
- The ribbed design provides nearly homogenous flatness along the length, while the flat design is only usable at the very center.
- When beam footprint is longitudinally centered on the crystal, flat design is significantly superior. (This comes at the price of needing a dedicated translation)
- For the ribbed design, aberrations due to the local variation of the bending radius ("microlenses" effect) were found to be insignificant at the focus position.