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Modeling and metrological analysis of an X-ray diffractometer for crystal-assisted collimation in particle accelerator

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Abstract. A FEM model of a double-crystal diffractometer and its metrological analysis is proposed for a complete characterization of bent crystals involved in the process of particles collimation in the Large Hadron Collider at CERN, in terms of miscut, bending and torsion angles. The model reproduces the laboratory measurement procedure based mainly on a 2D scanning algorithm and a π rad flip of the crystal under test. In this paper, we briefly present a physical analysis of the diffractometer, uncertainty sources definition, and their effect on the final results. The final goal is to reach a measurement uncertainty of $1\,\mu$rad with a coverage factor k=3.

1. Introduction

Bent crystals as primary collimators change significantly the collimation process in particle accelerators. In traditional collimation, a multi-stage, massive blocks of amorphous material, performs like a geometrical constrains, where at every stage particles are partially absorbed and partially outscattered as showers and non-primary halos onto the following stages. Conversely, bent crystals deflect coherently beam particles, using the channeling mechanism, onto one single dedicated absorber. This particle deflection has the same amplitude of the crystal bending angle, that typically is of several tens of μrad, opposed to the few μrad of the classical carbon collimators [1, 2, 3]. A double-crystal diffractometer, well known and generally present in literature in various areas of research [4, 5, 6], can be used for the bent crystals characterization. FEM model is critical to conduct a feasibility analysis; for this reason, it can be adapted to different wavelengths, crystal orientations or technical specifications, automatically constructing the geometry in order to cut the doublet present in the X-ray source, as the measurement setup is optimized in terms of width of the final spot on the detector to obtain the best resolution.

In this paper, A FEM model of a double-crystal diffractometer and its metrological analysis is proposed for a complete characterization of bent crystals involved in the process of particles collimation in LHC at CERN, in terms of miscut, bending and torsion angles. The FEM model is able to reproduce the measurement method and estimate the spot full width half maximum

($FWHM$) on the X-ray detector in different working condition. The entire measurement procedure is constituted by a 2D scanning algorithm and a π rad flip of the bent crystal, as described in [7]. During the measurement both an angular and a linear scan are performed and diffraction occurs only when the Bragg condition is locally verified. An uncertainty analysis is carried out to estimate the measurement uncertainty on the characteristic parameters.

2. FEM model

One of the key point for the diffractometer design is the presence of a doublet in the X-ray source: using a silver anode, the peak occurs for a k_α atomic transition, around 22 keV. It is composed by two lines: $k_{\alpha1}$ with double intensity of the $k_{\alpha2}$. The doublet presence broads the spot width and reduces the final resolution. The slit is positioned at an appropriate distance from the monochromator in order to cut the $k_{\alpha2}$ radiation. Dynamical theory of diffraction is considered for the monochromator and the bent crystal: the Darwin angular widths are obtained for the [1,1,1] silicon crystallographic planes. The FEM model is realized through *Comsol*: the layout is parameterized to be adaptable and for this purpose all the main components are represented. Measurement procedure and off-center misalignment are implemented through parametric equations, in this way different scenarios can be selected.

3. Simulation results

As first step, an angular scan is performed around the range $\theta_{B,k_{\alpha1}} - 50\,\mu\text{rad} \leq \theta \leq \theta_{B,k_{\alpha1}} + 50\,\mu\text{rad}$, with 1 μrad steps. For each angular position, the total energy impinging the detector (integral of the spot area) is assessed as a function of the particular tilting angle. In the $k_{\alpha2}$ cutting condition, the spot obtained is shown in Fig. 1(a). In the case the cutting condition is not verified, another spot related to the $k_{\alpha2}$ radiation is present. It comes out from the
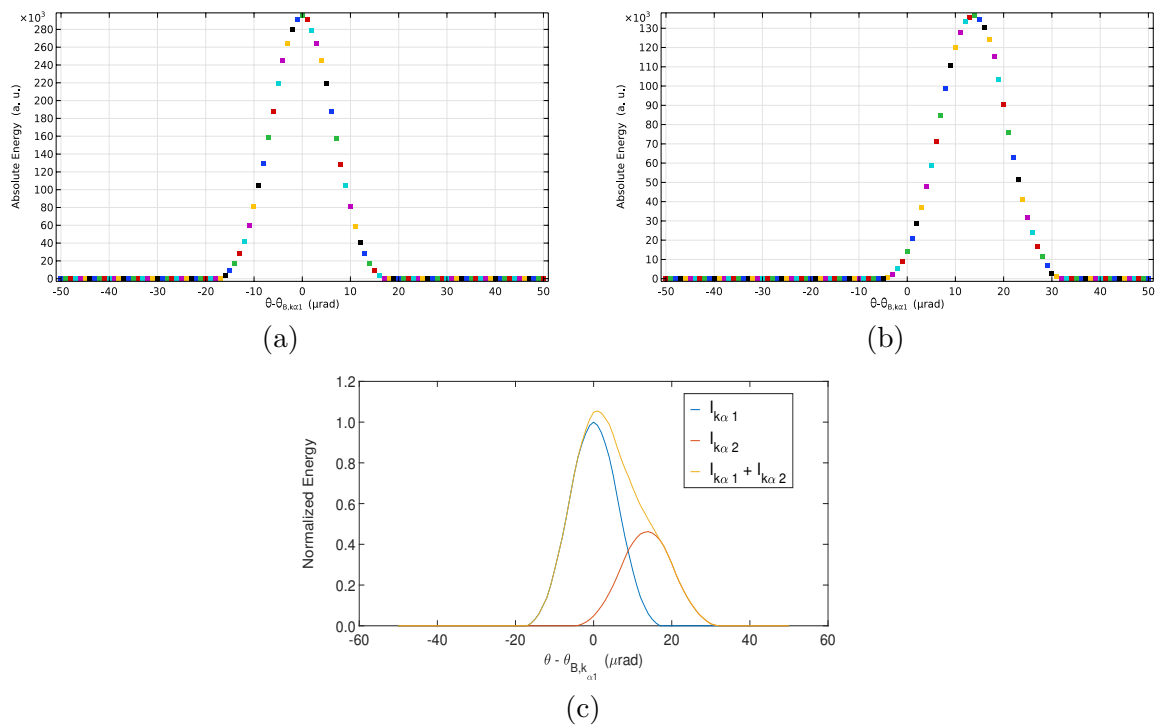
Figure 1. (a) The spot for the $k_{\alpha1}$ radiation, (b) the one for $k_{\alpha2}$, and (c) their sum.

monochromator and hits the crystal under test with an angle equal to $\theta_{B,k_{\alpha2}}$ (Fig. 1(b)): it

will impact on a different location of the bent crystal which, due to its bending, leads to a second peak shifted of the bending angle between the two impact points. The presence of this second peak, that superposes with approximately half the amplitude to the first one, increases the *FWHM* of the total spot shown in Fig. 1(c). The linear scan allows instead to estimate the crystal's center (Fig. 2(b)) and its bending angle (Fig. 2(c)). The scanning is performed along the direction perpendicular to the crystal surface, with a 25 µm step. When each angular scan finishes, the crystal's linear position changes: as mentioned before, its curvature leads to a spot shift, that directly depends from the linear step, which is of the order of 3.83 µrad. *Comsol* returns as *FWHM* for the $k_{\alpha 1}$ spot a value of 14.7 µrad, 15.8 µrad for the $k_{\alpha 2}$ and 20.9 µrad for their superposition.

(a)

(b)

(c)
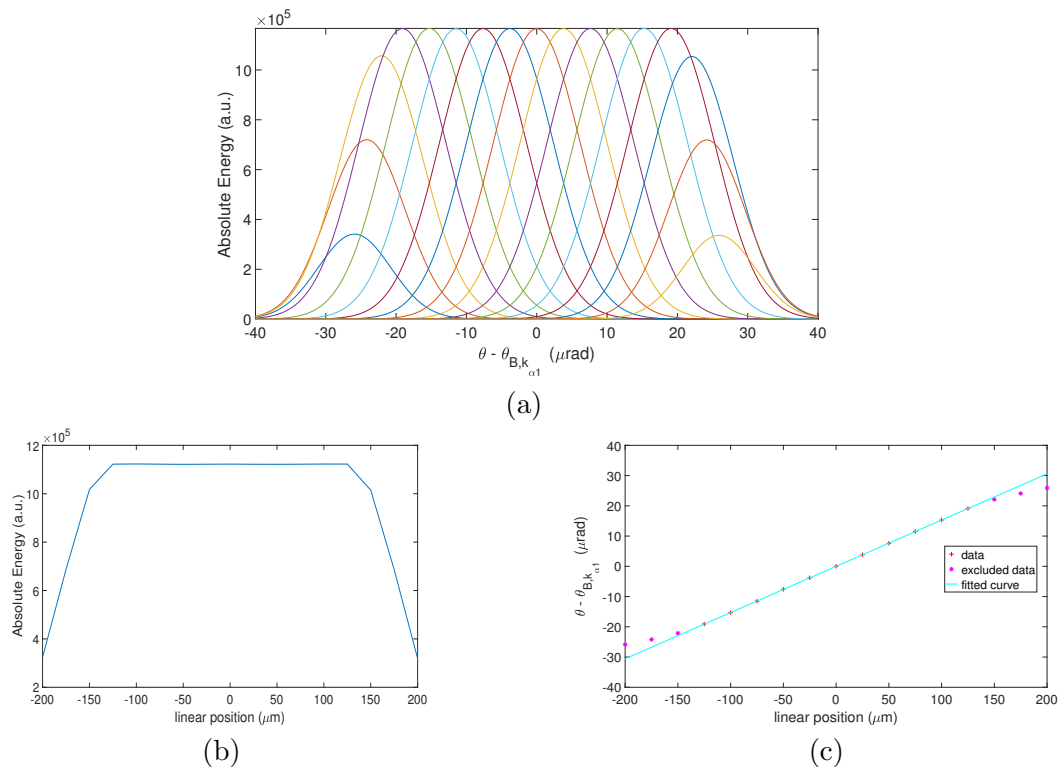
Figure 2. Complete 2D scan, with angular steps of 1 µrad and linear steps of 25 µm (a); Peak maxima vs linear positions to assess total crystal extension and center (b); and linear fit for bending angle determination (c).

4. Uncertainty analysis

Different sources were considered to estimate the final measurement uncertainty with a coverage factor k=3, such as vertical and horizontal misalignments, linear steps angular deviations, effective miscut angle, saddle shape, impact point variation due to crystal's center estimation, rotational axis off-center, and so on. The linear and rotational stages positions and their technical specification are designed to reduce their impact. The presence of an autocollimator allows to compensate the offset uncertainty due to a notideality of the rotational flip axis. Assuming a standard deviation on the angular position of 0.35 µrad, for each point present in Fig. 2(c), a *Monte Carlo* analysis is performed to obtain the envelope of the all possible best fit curves [8, 9]. For a 4 mm crystal thickness along the beam, the extrapolated value is centered around the expected value (54.74 µrad) with an expanded uncertainty $U = k \cdot u_c = 1$ µrad, as shown

in Fig. 3. To obtain a good linear fit, centered around the expected value, the first three and last three spots are excluded from the evaluation, since they are related to an X-ray beam that partially impacts on the crystal (Fig. 2(a) and 2(c)) and this introduces a non-linear error.
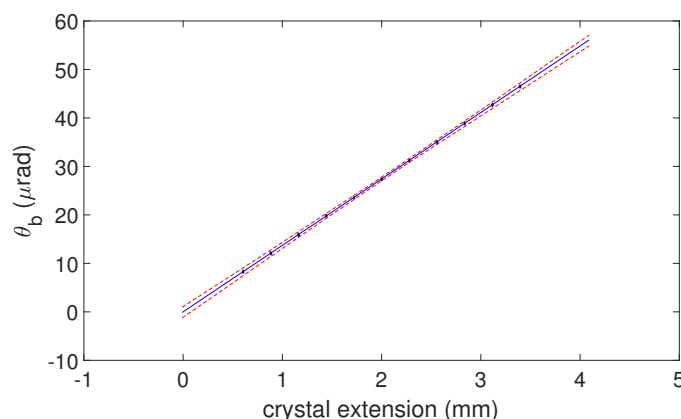
Figure 3. Linear fit for the bending angle determination with the envelope of the all best fit curves.

5. Conclusion

The FEM Model here discussed, allowed us to estimate the spot *FWHM* for each angular scan, replicating the measurement method, and also the effect of a second peak present in the X-ray source. Geometrically we were able to cut this second undesired peak, in order to obtain the best resolution. It also allowed to see a different behavior for the spots related to beams that partially impact on the crystal: these points could be neglected for the linear fit. Furthermore, some uncertainty sources were estimated both using the FEM model and geometrical considerations: this allowed to determine the technical specification for the motion stages involved in the measurement procedure to obtain the target uncertainty. Future improvements could be considered for the measurement method introducing more degree of freedom.

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