Ultra-relativistic electron beams deflection by quasi-mosaic crystals

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Abstract. This paper provides an explanation of the key effects behind the deflection of ultra-relativistic electron beams by means of oriented ‘quasi-mosaic’ Bent Crystals (qmBC). It is demonstrated that accounting for specific geometry of the qmBC and its orientation with respect to a collimated electron beam, its size and emittance is essential for an accurate quantitative description of experimental results on the beam deflection by such crystals. In an exemplary case study, a detailed analysis of the recent experiment at the SLAC facility is presented. The methodology developed has enabled to understand the peculiarities in the measured distributions of the deflected electrons. Also, this achievement constitutes an important progress in the efforts toward the practical realization of novel gamma-ray crystal-based light sources and puts new challenges for the theory and experiment in this research area.

In recent years significant efforts of the research and technological communities have been devoted to design and practical realization of novel gamma-ray crystal-based light sources (CLS) that can be set up by exposing oriented linear, bent or periodically bent crystals to beams of ultrarelativistic positrons or electrons \([1,2]\). Brilliance of radiation emitted in a crystalline undulator LS by available beams in the photon energy range \(10^{10}–10^{11}\) MeV, being inaccessible to conventional synchrotrons, undulators and XFELs, greatly exceeds that of laser-Compton scattering LSs and is higher than predicted in the Gamma factory proposal to CERN \([3]\). Manufacturing of CLSs will have significant impact on many research areas in physics, chemistry, biology, material science, technology and medicine, being a subject of current European projects ‘N-LIGHT’ \([4]\) and TECHNO-CLS \([5]\).

So far oriented crystals exposed to beams of charged particles have been already utilized in a number of applications for beams manipulation, such as steering, bending, extraction and focusing, see \([2,6]\) and references therein. These and other newly emerging applications in this research area require high-quality crystals (bent or periodically bent) and collimated beams of ultrarelativistic particles of different energies.

Construction of novel CLSs is a challenging task involving a broad range of correlated research and technological activities \([1,2]\). During the last decade a number of papers published in high-impact journals \([7–13]\) on channeling and channeling radiation experiments with bent crystals at different facilities (SLAC, CERN, MAMI). This paper reports on the important progress in this field providing an explanation of the key effects arising by deflection of ultrarelativistic electron and positron beams by means of oriented ‘quasi-mosaic’ Bent Crystals (qmBC). It is demonstrated that account for specific geometry of qmBC and its orientation with respect to a collimated beam of projectile particles, the beam size and emittance is essential for the quantitative description of the experimental results on the beam deflection by such crystals.

Manufacturing of crystals of different desired geometry is an important technological task in the context of their applications in the gamma-ray CLSs and the aforementioned experiments. The systematic review of different technologies exploited for manufacturing of crystals of different type, geometry, size, quality, etc., is given in \([1,2,6]\). A short summary of several relevant approaches that have been utilized to produce bent crystals is provided in Supplemental Material (SM).

The high-quality qmBCs structures with desirable and fully controllable parameters have been manufactured for the aforementioned channeling experiments by the following means \([14–16]\). When a moment of force is applied to a crystalline material, some secondary curvatures may arise within the solid \([17]\). A well-known secondary deformation is the anticlastic curvature with

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radius \( R_a \) that occurs in a medium subjected to two moments. In particular, it occurs in the perpendicular direction with respect to the primary curvature. When the two curvatures are combined, the deformed crystal acquires the shape of a saddle. In contrast to an amorphous medium, physical properties of crystals may be strongly anisotropic. Another type of the deformation caused by anisotropic effects is the ‘quasi-mosaic’ (QM) curvature \([18,19]\). QM bent crystals belong to a class of bent crystals featuring two curvatures of two orthogonal crystallographic planes.

In order to understand the effects arising during channeling of charged particles through qmBC one should consider the geometry of such a crystal and its orientation with respect to an incident beam. This geometry is shown in Fig. 1. For the sake of clarity, the case of planar channeling is addressed below.

Consider a crystal whose planes, which are parallel to the \((xy)\) plane, experience anticlastic bending with the curvature radius \( R_a \). The center \( O \) of the curvature lies on the \( z\)-axis, which runs through the crystal center. The QM bending deforms the crystal planes parallel to the \((xz)\) plane. In what follows, it is assumed that \( R_a \) and the QM bending radius \( R_{qm} \) greatly exceed the crystal thickness \( L \). These conditions were met for the qmBC samples used in the experiments \([7–13]\). The QM bending angle is defined as follows:

\[
\theta_{qm} = L/R_{qm} \ll 1. \tag{1}
\]

To start with, let us assume an ideally collimated narrow beam (i.e., that of zero divergence and zero beam size in the \( y \) direction, \( \sigma_\phi, \sigma \to 0 \)) incident on the crystal along the \( z \) direction. For a planar channeling, the beam size and divergence in the \( x \) direction do not play important role and thus are not considered below.

At the crystal entrance, the angle \( \theta_e \) between the beam direction and a tangent line to the QM bent plane depends on the beam displacement \( h \) along the \( y \)-axis:

\[
\theta_e(h) = \frac{h}{R_a} - \frac{\theta_{qm}}{2} = \Delta h/R_a \tag{2}
\]

where \( \Delta h = h - h_0 \) with

\[
h_0 = \theta_{qm}R_a/2 \tag{3}
\]

being the displacement for which the entrance angle \( \theta_e = 0 \), i.e., the tangent line is parallel to the \( z \)-axis.

A probability of a particle to be accepted into the channeling mode becomes significant if \( \theta_e \) does not exceed Lindhard’s critical angle \( \theta_c \), i.e., the maximum incident angle consistent with the channeling condition formulated within the continuous potential model \([20]\). Then, using (2) one finds the maximum value of \( \Delta h \)

\[
\Delta h_{\text{max}} = \theta_cR_a, \tag{4}
\]

so that the channeling condition is met for the particles with \( h \) within the interval \( h_0 \pm \Delta h_{\text{max}} \).

At the crystal exit, the angle \( \theta_e \) between the tangent line and the beam direction is related to \( h \) via

\[
\theta_e(h) = \theta_e(h) + \theta_{qm}. \tag{5}
\]

Hence, the projectiles that are accepted at \( y = h \) and channel through the whole crystal are deflected by the angle lying within the interval \( \theta_e(h) \pm \theta_{c} \).

The particles that enter having \( \Delta h < 0 \) can experience either volume capture or volume reflection \([21,22]\) in the crystal. The geometry analysis for these regimes is given in SM. The particles that enter with \( \Delta h > \Delta h_{\text{max}} \) are neither accepted nor experience the volume reflection but experience multiple scattering which becomes closer to the scattering in the amorphous medium as \( \Delta h \) increases.

Consider now a Gaussian beam, with width \( \sigma > 0 \) and divergence \( \sigma_\phi > 0 \) that is incident on the crystal being centered at \( y = h \). For a beam centered at \( h \), most of its particles enter the crystal having the transverse coordinates lying within the interval from \( h - \sigma \) to \( h + \sigma \) and the corresponding incident angles \( \theta_e \). Therefore, the distribution of deflected particles becomes a superposition of different propagation scenarios discussed above.

Below in the paper, we demonstrate that it is important to know the values of \( \sigma \) and \( \sigma_\phi \) as well as of \( R_a \) quite accurately to be able to interpret results of the experiments on beam propagation through oriented qmBC crystals.

In what follows, we focus on the analysis of the experiment at SLAC \([8]\), although the physics discussed and the conclusions drawn are applicable to other aforementioned experiments with oriented qmBC. In the experiment, a 60 \( \mu \)m thick Si(111) qmBC was exposed to a 6.3 GeV electron beam. To deduce the values of \( \sigma \) and \( \sigma_\phi \), one can rely on the following description provided in the cited paper: (i) “... a beam width of < 150
μm (1σ) in the vertical and horizontal plane,” and (ii) “The beam divergence was inferred...to be less than 10 μrad.” The QM bending radius of the (111) planes was quoted as \(R_{qm} = 15\) cm. It was mentioned that some measures had been taken “to reduce the anticlastic deformation” although the explicit value of \(R_a\) was not indicated. Indirectly, one can estimate \(R_a\) basing on the data presented in [14]. This paper, cited in Ref. [8], discusses the QM bending of Si(211), i.e., it refers to a different geometry in which the (111) planes experience the anticlastic bending rather than the QM one. For this geometry, the value \(R_a = 366\) cm on the center of the sample was measured. In our simulations we considered \(R_a\) as a parameter varied within the interval 100 – 300 cm. Using the aforementioned value of \(R_{qm}\) in (1), one finds \(\theta_{qm} = 400\) μrad. Fixing \(R_a\) and taking into account that for a 6.3 GeV electron Lindhard’s critical angle is 80 μrad [8], one calculates \(h_0\) and the maximum displacement \(\Delta h_{max}\).

Numerical modeling of the channeling and related phenomena beyond the continuous potential framework can be carried out by means of the multi-purpose software package MBN EXPLORER [24–26] and a supplementary special multitask software toolkit MBN STUDIO [27]. The MBN EXPLORER was originally developed as a universal computer program to allow multiscale simulations of structure and dynamics of molecular systems.

MBN EXPLORER simulates the motion of relativistic projectiles along with dynamical simulations of the crystalline environment [25]. The computation accounts for the interaction of projectiles with separate atoms of the environment, whereas a variety of interatomic potentials implemented supports rigorous simulations of various media. Overview of the results on channeling and radiation of charged particles in linear, bent and periodically bent crystals simulated by means of MBN EXPLORER can be found in [1,2,6,26].

To model propagation of particles through qmBCs, further development of the algorithm for the atomistic simulations of the crystalline media has been performed in this work. The implemented algorithm enabled simulations of a qmBC defined through a transformation of the unperturbed crystalline medium by three curvatures (primary, anticlastic and QM), positioning of the qmBC with respect to the beam direction and the relativistic molecular dynamics in such environment. The results reported below have been obtained by means of this newly implemented algorithm.

The main outcome of numerical analysis carried out in this Letter in connection with the SLAC experiment is shown in Fig. 2, which compares the current simulations with the experimentally measured intensity of the deflected electron beam as well as with the result of the DYNECHARM++ simulations. The latter intensities were obtained by digitalizing the data, which are presented in arbitrary units in Fig. 3 in [8], followed by the background (ca 1.4 a.u.) subtraction. The resulting experimental values were rescaled to provide the unit area within the interval −0.3...0.55 mrad of the deflection angle. The ratio experiment-to-DYNECHARM++ was kept as in the original figure.

The simulated and measured angular distributions have the characteristic pattern of the two well pronounced peaks interlinked by an intermediate region. The left peak in the vicinity of \(\theta = 0\) describes a fraction of particles propagating though the qmBC in the forward direction. These particles experience multiple scattering resulting in broadening of the initial distribution of the beam particles. Small shift of the peak toward negative angles is due to the volume reflection of the particles from the bent planes. As discussed in SM, this effect becomes more pronounced at the entrance points within the region \(-h_0 < h < h_0\). The right peak is formed by the particles accepted to the channeling regime at the entrance and deflected to the angle \(\theta_s(h)\) according to Eq. (5). Our simulations have shown that the position of the channeling peak is determined by the value \(h\) corresponding to the beam center at the entrance point and the width of the peak is determined by the distribution of \(\theta_s(h)\) for the particles of the beam and by Lindhard’s angle. The peak is also influenced by the dechannelling process that is responsible for the formation of the distribution of the deflected particles in the region between the two peaks.

As mentioned, the angular distribution is very sensitive to the choice of the beam size \(\sigma\), bending radius \(R_a\) and the entrance coordinate \(h\). The current simulations presented in Fig. 2 correspond to a particular set of these parameters; \(\sigma = 75\) μm, \(R_a = 300\) cm and \(h = 675\) μm. It has been established that these values provide close agreement with the experimentally measured distribution. We noted that in Ref. [8] the exact value of \(\sigma\) has been specified, whereas the values of \(R_a\) and \(h\) as well as their impact on the profile of the distribution have not been mentioned at all. Same refers to the results of the DYNECHARM++ simulations.

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1 The quoted value of \(\theta_s\) is calculated in Ref. [8] using the Doyle-Turner potential [23]. It corresponds to the crystal temperature \(T = 300\) K. The results of simulations presented in our paper refer to the same temperature.
Fig. 3  Simulated distributions obtained for the beam size $\sigma = 150 \, \mu m$ and divergence $\sigma_s = 10 \, \mu rad$ but different values of the displacement $h$ and anticlastic radius $R_a$. Left panel refers to $h = h_0$. The $h$ values indicated in the right panel correspond to $\theta_s(h) = 0.44 \, mrad$. All dependencies are normalized to unit area. See also explanation in the text and Fig. S2 in SM.

Figures 3 and 4 illustrate the impact of variation of $\sigma$, $R_a$ and $h$ on the angular distribution. The symbols with error bars stand for the experimental data obtained as described above.

Figure 3 shows the distribution for a beam with $\sigma = 150 \, \mu m$ incident on the crystal bent with different anticlastic radius as indicated. In the left panel, each simulation refers to the beam centered at $h = h_0$ and thus most of the accepted particles are deflected by the angle $\theta_{qm}$ resulting in the channeling peak centered at about 0.40 mrad, which is less than in the experiment (ca 0.44 mrad). The peak intensity increases with $R_a$ in accordance with the geometrical arguments discussed above. Indeed, for $R_a = 100 \, cm$, the maximum displacement $\Delta h_{\text{max}} = 80 \, \mu m$ is nearly two times less than $\sigma$ resulting in a small fraction of the accepted particles. Since $\Delta h_{\text{max}} \propto R_a$ (see Eq. (4) and Fig. S2 in SM), then for $R_a = 300 \, cm$, the value of $\Delta h_{\text{max}}$ exceeds $\sigma$ leading to the higher intensity. The qmBC geometry provides also a qualitative explanation of the changes occurring to the left peak. For the smallest radius, the inequality $\Delta h_{\text{max}} < \sigma$ suggests that large number of particles enters the crystal having the transverse coordinate (i) larger than $h_0 + \Delta h_{\text{max}}$, and (ii) lower than $h_0 - \Delta h_{\text{max}}$. The former particles contribute mainly to the amorphous-like distribution, whereas the latter ones can undergo the volume reflection giving rise to the intensity at $\theta_s < 0$. As $R_a$ increases, the numbers of particles of both types decrease making the peak narrower and less intensive.

Aiming at bringing the channeling peak position closer to the measured one another run of simulations has been performed with the same values of $\sigma$ and $R_a$ but different set of initial coordinates of the beam center. The distributions shown in Fig. 3 right refer to $h > h_0$ that correspond to $\theta_s = 0.44 \, mrad$ for each $R_a$ indicated. It is seen that although the channeling peaks are shifted to the right, they, simultaneously, loose the intensity. Apart from this, the left peaks become more powerful being centered at $\theta_s = 0$ due to the increase in the number of particles moving in the forward direction at the expense of the volume-reflected ones. All these modifications can be explained in terms of the qmBC geometry.

Two panels in Fig. 4 correspond to two sets of $R_a$ and $\sigma$. In each panel, the simulations have been performed for different values of the beam center $h$ at the entrance. Vertical lines in Fig. S1 in SM allow one to compare the $h$ values indicated with the boundaries $h_0$ and $h_0 + \Delta h_{\text{max}}$.

The left panel presents a case study in which $\Delta h_{\text{max}} = 160 \, \mu m$ is comparable to the beam size so that for any entrance point within $[h_0, h_0 + \Delta h_{\text{max}}]$ a large fraction of the particles is not accepted resulting in a noticeable decrease of the right peak. The curve with $h = 400 \, \mu m$ corresponds to the case $h = h_0$ when
half of the beam enters the crystal having Δh < 0. In this domain, the volume reflection can occur shifting the main maximum toward negative angles. As h increases, the numbers of both channeling and volume reflected particles decrease leading to the shift of the both maxima to the right as well as to the change in their heights. At h = 600 μm, which corresponds to Δh > Δh_{max}, most of the beam particles do not comply with the channeling condition but experiencing multiple scattering as in amorphous medium. As a result, the main peak becomes more powerful being centered at θ_{0} = 0.

To increase the channeling fraction, one can rely on a larger value of the anticlastic radius and on a narrower beam. For R_{0} = 300 cm, Fig. 4 right, the quantities h_{0} and Δh_{max} are 600 and 240 μm, respectively. The latter value together with the reduced beam size (σ = 75 μm) suggest that a much bigger fraction of the particles can be accepted provided the condition 0 < Δh < Δh_{max} − σ is met. The best agreement with the experiment has been found for h = 675 μm (open circles). This dependence is shown in Fig. 2 in the form of a histogram.

The quantitative analysis of the angular distribution of ultrarelativistic electrons deflected by oriented qmBCs presented in our paper demonstrates the good agreement with experimental data reported in [8]. It has been achieved by accounting for (i) the specific geometry of such crystals and their orientation with respect to the projectile beam and (ii) the realistic beam size and divergence. Remaining discrepancies can be attributed to the uncertainty in concrete values of the beam characteristics and of the entrance coordinate h of the beam center as well as to the effects not included into the current simulations (e.g., quantum effects in multiple scattering in crystals [29], energy spread of the beam particles, beam intensity). It is highly desirable that such information is provided when presenting the experimental data since it allows for its independent unambiguous theoretical and computational validation. Important issue concerns also accurate measurement and computational analysis of the characteristics of radiation that accompany passage of ultra-relativistic projectiles through oriented crystals. Such knowledge is essential for better planning of accelerator-based experiments and for full interpretation of their results.

**Data Availability Statement** This manuscript has no associated data or the data will not be deposited. [Authors’ comment: All data generated are included into this published article. The data presented in this manuscript can be available upon reasonable request to the authors.]

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**Author contributions**

All authors contributed equally to the paper.

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