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Simulations of electron channeling in bent silicon crystal

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Abstract. We report on the results of theoretical simulations of the electron channeling in a bent silicon crystal. The dynamics of ultra-relativistic electrons in the crystal is computed using the newly developed part [1] of the MBN Explorer package [2,3], which simulates classical trajectories of in a crystalline medium by integrating the relativistic equations of motion with account for the interaction between the projectile and crystal atoms. A Monte Carlo approach is employed to sample the incoming electrons and to account for thermal vibrations of the crystal atoms. The electron channeling along Si(110) crystallographic planes are studied for the projectile energies 195–855 MeV and different curvatures of the bent crystal.

1. Introduction

Channeling is a phenomenon which is known to arise when a charged particle enter a crystal at angles small enough with respect to crystallographic planes or axes [4]. The particles become confined and forced to move through the crystal preferably along the corresponding crystallographic direction experiencing the collective action of electrostatic field of the lattice ions. The field is repulsive for positively charged particles and, therefore, they are steered into the inter-atomic region, while negatively charged projectiles move in the close vicinity of ion strings or planes.

Under certain conditions [5] the channeling effect persists even if a crystal is bent. In this case, the particle deviates from its initial direction of motion due to extremely strong electrostatic field in the crystal. The field strength is typically of the order of 10^{10} V/cm which is equivalent to the magnetic field of approximately 3000 T. Therefore, bent crystal can steer particles much more effectively than any existing magnet. In particular, in experimental high energy physics the crystals with bent crystallographic planes are used to steer high-energy charged particle beams replacing huge dipole magnets (see, e.g. [10]).

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A comprehensive review of theoretical and experimental achievements in the investigation of the channeling effect in straight and bent crystals one can find in [4, 6–10].

Recently, the crystalline undulator (CU) concept was formulated for producing undulator-like electromagnetic radiation in the sub hundreds of keV up to the MeV photon energy range [11, 12]. In a CU the radiation is emitted by a beam of ultra-relativistic charged particles which undergo channeling in a periodically bent crystal. As a result, in addition to a well-known channeling radiation, there appears the radiation due to the undulating motion of the particles which follow the periodic bending of crystallographic planes. The intensity and characteristic frequencies of the CU radiation can be varied by changing the type of channeling particles, the beam energy, the crystal type and the parameters of periodic bending. We refer to Ref. [13] which represents the underlying fundamental physical ideas as well as the theoretical, experimental and technological advances made during the fifteen years in exploring various features of CUs and its radiation.

Several experimental attempts were made [14] or planned to be made [15] to detect the radiation from a positron-based CU. So far, the attempts have not been successful due to various reasons (see discussion in Refs. [13, 15]). However, quite recently the first signatures showing evidence for the CU radiation were experimentally observed for 195–855 MeV electrons at the Mainz Microtron (Germany) facility [16, 17]. Another set of experiments is scheduled for the year 2013 at the SLAC facility (USA) with 10 – 20 GeV electron beam [18].

Theoretical support of ongoing and future experiments as well as accumulation of numerical data on channeling and radiative processes of ultra-relativistic projectiles in straight, bent and periodically bent crystals must be based on an accurate procedure which allows one to simulate the trajectories corresponding to the channeling and non-channeling regimes. The procedure must include a rigorous description of the particle motion and an efficient algorithm of its numerical realization. It is strongly desirable to make the procedure as much model-independent as possible. This means that the only allowed parameters are those which describe *pairwise* interactions of the projectile with constituent atoms.

Most of the existing codes, capable to simulate channeling process, can be categorized as following. Some of them (see, for example, Refs. [19–21]) are based on the concept of the continuous potential [4]. This approximation, being adequate in describing the channeling motion, becomes less accurate and more model-dependent when accounting for uncorrelated scattering events. The accurate description of the latter is essential for a quantitative analysis of the dechanneling and rechanneling processes. Other group of the codes [22–24] utilizes the scheme of binary collisions which assumes that the motion of a projectile at all times is influenced by the force due to the nearest atom. Computer facilities available at present allow one to go beyond this limitation and to account for the interaction with larger number of the crystal atoms. Such an extension of the binary collisions algorithm was implemented in the recent code for electron channeling described in Refs. [27]. The code, however, was based on the specific model for electron–atom scattering which results in a noticeable overestimation of the mean scattering angle. In more detail this topic was addressed in Ref. [1] (see also comments in Section 3).

To simulate propagation of ultra-relativistic particles through media, the channeling process in particular, one can approach and algorithms used in modern molecular dynamics codes (see Ref. [2] for the comparative review of the codes). The latter allow one to model the dynamics of various molecular system by efficient numerical integration of classical equations of motion for all atoms in the system. The interaction between atoms is implemented in terms of interatomic potentials, the types and parameters of which can be chosen from a broad range to ensure the most adequate quantitative description of the simulated molecular system.

Recently, the molecular dynamics concept was applied to describe the motion of a single projectile in the static field of atoms which constitute a scattering medium [1]. For this purpose we have used the MBN EXPLORER software package [2, 3] and supplied it with additional module

which treats classical relativistic equations of motion and generates the crystalline environment dynamically in the course of particle propagation. This module, combined with the variety of interatomic potentials implemented in MBN EXPLORER, makes the program a unique tool for studying relativistic phenomena in various environments, such as crystals, amorphous bodies, biological medium. Verification of the code against available experimental data was carried out for 6.7 GeV projectile electrons and positrons in channeling in straight Si(110) channels [1].

In the present paper we present the results obtained with the new code [1] on the Monte Carlo simulation of the channeling of electrons along the (110) crystallographic plane in straight and bent single silicon crystal. The calculations were performed for $\varepsilon = 195, 345, 600$ and 855 MeV electrons which correspond to the experimental conditions at the Mainz Microtron (Germany) [30]. We have restricted the current analysis to the bent crystals with constant curvature, although these results will help one to estimate the reasonable parameters of periodically bent crystal channels and, therefore, will facilitate future simulations and experimental study of the electron-based crystalline undulator.

2. Physical model for channeling

Upon entering a crystal, a particle with the charge q experiences an electrostatic field $U(\mathbf{r})$ of the crystalline environment. To compute the motion of projectiles in the latter potential, we employ the relativistic classical dynamics and solve the following pair of equations

$$d\mathbf{r}/dt = \mathbf{v}, \quad d\mathbf{p}/dt = -q\partial U/\partial \mathbf{r} \quad (1)$$

for the particle coordinate $\mathbf{r}(t)$ and velocity $\mathbf{v}(t)$ as the functions of propagation time t . The momentum $\mathbf{p}$ relates to the velocity $\mathbf{v}$ according to the relativistic expression $\mathbf{p} = m\gamma\mathbf{v}$, where m is the mass of the particle, $\gamma = [1 - (v/c)^2]^{-1/2} = \varepsilon/(mc^2)$ is the Lorentz factor, ε is the projectile energy and c is the speed of light.

To incorporate the many-body interaction of the projectile with the crystalline constituents, the potential U is represented by the sum of atomic potentials U_{at} ,

$$U(\mathbf{r}) = \sum_j U_{\text{at}}(\mathbf{r} - \mathbf{R}_j), \quad (2)$$

where $\mathbf{R}_j$ is the position vector of the j -th atom in the crystal. The atomic potentials are evaluated according to the Molière approximation [25]. The computations with MBN EXPLORER can also be performed, if demanded, employing a more elaborated Pacios approximation for the atomic potentials [26].

Formally, the sum in Eq. (2) is carried out over all atoms of the sample. However, the atomic potentials decay with increasing distance from the atoms, and the decay becomes exponential when the distances exceed the atomic sizes. This allows one to restrict the number of atoms interacting with the projectile by accounting only for those separated from the projectile by distances shorter than some cut-off distance. Selection of these atoms for a given location of the projectile is facilitated by a linked cells algorithm implemented in MBN EXPLORER [2, 3].

The module for channeling simulations, implemented in MBN EXPLORER, has been designed to describe the crystalline structure acting on a moving projectile "on the fly" in the course of integrating the dynamical equations (1). This is achieved by introducing a "dynamic simulation box" which shifts following the propagation of the particle (see Ref. [1] for more details). Within the simulation box, the equilibrium positions of the crystal nodes are determined according to the lattice structure under study. Then, the thermal vibrations of the crystal are accounted for by displacing the atoms with respect to the equilibrium positions. For each atom, a displacement Δ_i along a given Cartesian axis $i = x, y, z$ is selected randomly according to the normal distribution

$$w(\Delta_i) = (2\pi u_T^2)^{-1/2} \exp[-\Delta_i^2/2u_T^2], \quad (3)$$

where u_T is the amplitude of the thermal vibrations. For a Silicon crystal at the room temperature $u_T = 0.075 \text{ \AA}$ [6].

To study the channeling motion along a particular crystallographic plane one needs to specify the orientation of the crystal with respect to the incoming particles. To do this, we introduce the laboratory reference frame with the z -axis along the beam. In the case of a straight crystal we orient the crystallographic plane parallel to the (xz) -plane. A care is taken to avoid accidental orientations of crystallographic axes along the beam, as this is also done in the most common experiments in order to exclude the axial channeling. To simulate a bent crystal, the coordinates x', y', z' of each lattice node are obtained from the coordinates x, y, z of the same node in the straight crystal according to the relations $x' = x$, $y' = y + \delta(z)$, $z' = z$, where

$$\delta(z) = R - \sqrt{R^2 - z^2} \quad (4)$$

is the shape of the bent crystallographic plane and R is the bending radius.

A convenient parameter showing impact of the curvature R^{-1} on the channeling for the particles with the energy ε is the ratio C of two opposite forces acting on the projectile: the centrifugal force ε/R and a maximal interplanar force $F_{\max}$ stabilizing the motion of the particle transversely to the crystallographic planes. The value $C = 0$ corresponds to the straight crystal and $C = 1$ is the critical value at which the potential barrier between the channels disappear. The value $F_{\max}$ has been estimated withing the continuous approximation for the planar potentials and found to be 6.67 GeV/cm for the electron channeling along the 110 plane in Silicon crystal. We use the latter value as the reference to introduce the bending parameter

$$C = 1.57 \times 10^{-4} (\varepsilon_{\text{MeV}} / R_{\text{cm}}), \quad (5)$$

where ε_{MeV} is the electron energy in MeV and R_{cm} is the bending radius in cm.

Having specified the orientation and bending of the crystal with respect to the beam direction, we use a Monte Carlo approach to sample the beam electrons. The particles are assumed to enter the crystal at $t = 0$ with $z = 0$ and the aperture (x, y) coordinates being randomly selected from the intervals $-1.5d \leq x \leq 1.5d$ and $-0.5d \leq y \leq 0.5d$, where d is the interplanar distance (e.g., $d = 1.92 \text{ \AA}$ for the Si (110) planes). The corresponding initial velocities are set to be $v_x = v_y = 0$ which correspond to the ideal case of a zero-emittance beam. Thus, at the entrance the particles are directed along the crystalline planes, and the particular sampling of the initial y -coordinates covered uniformly the interplanar extension for the channel which can guide the particles into the crystal. With the above initial conditions, the dynamical equations (1) are integrated numerically employing the forth-order Runge-Kutta algorithm. The integration proceeds until z exceeds the length L of the crystalline sample.

3. Numerical results

Using the approach described in the preceding section we have simulated propagation of the electrons and positrons with energies $\varepsilon = 195, 345, 600$ and 855 MeV along the (110) planes in straight and bent single crystal of the length L from 25 up to 300 micron. Most of the simulations have been performed for $L = 75 \text{ }\mu\text{m}$.

The Monte Carlo approach to sampling the incoming particles and including the thermal fluctuations of the crystalline lattice yields a manifold of different trajectories. By analyzing the dependencies $y(z)$ for each trajectory one concludes whether the channeling occurs and, if so, what parts of this trajectory are in the channeling mode. The analysis is similar to that used for the straight crystal [1], whereas now the shape of bent channels is described by Eq. (4).

Although the particles are initially directed along the crystalline planes, not all of the trajectories show the channeling. Thus, the important parameter to estimate is the acceptance

$$A = N_{\text{acc}} / N_0, \quad (6)$$

which is the ratio of the number N_{acc} , of particles captures into the channeling mode at the crystal entrance (the accepted particles) to the total number N_0 of the simulated trajectories (the incident particles). In general, the acceptance depends on the angular distribution of the particles at the entrance, in particular it decreases drastically for the incident angles exceeding the Lindhard's critical angle. In our simulations the incident beam has zero emittance, i.e. the projectiles are collimated "optimally" to get into the inside of the crystal. Therefore, the acceptance we calculate represents an upper bound estimate for a possible experimental outcome.

Fig. 1 shows the acceptance of the electrons of different energies directed into the Si(110) channels. It is seen that for the same values of the bending parameter C the acceptance does not vary noticeably with the electron energy. Notice that the bending parameter is energy dependent itself, and the same values of this parameter correspond to larger bending radius with increasing energy (see Eq. (5)). For each electron energy studied in Fig. 1, the acceptance is maximal for the straight channel ($C = 0$) and decreases with C due to increasing centrifugal force acting on the projectile at the entrance.

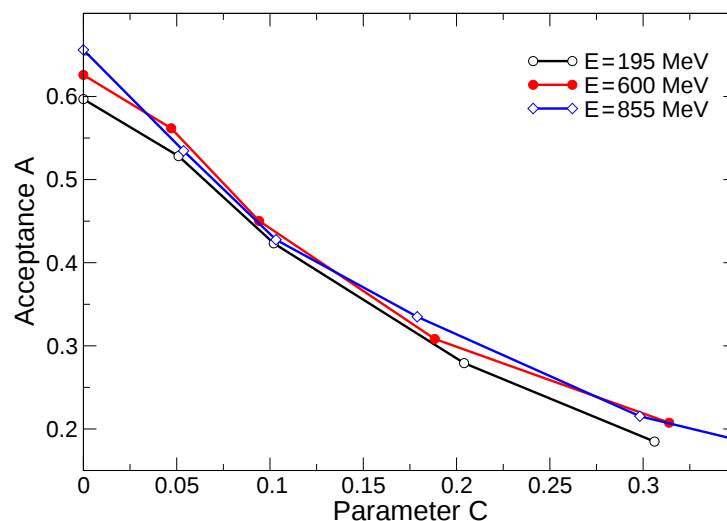


Figure 1. Acceptance A of the planar Si (110) channel as a function of the bending parameter C for several energies of electrons as indicated.

To describe the channeling properties quantitatively, we have computed the numbers $N_{\text{ch0}}(z)$ and $N_{\text{ch}}(z)$ of the electrons that are in the channeling mode at distance z from the crystal entrance. The former quantity stands for the number of electrons that propagate to z channeling in the channel where they were accepted at the entrance. The quantity $N_{\text{ch}}(z)$ is the number of electrons that are in the channeling mode inside the crystal, irrespective of the channel which guides the electronic motion at given z . With increasing z the number $N_{\text{ch0}}(z)$ decreases as the accepted electrons leave the entrance channel, i.e. a *dechanneling* takes place. In the contrast, the number $N_{\text{ch}}(z)$ can increase when the electrons, including those not accepted at the entrance, can become channeling in some other channel as a result of *rechanneling*. The latter process results from random collisions with the crystal constituents experienced by the electrons that have left the channeling regime. The collisions can occasionally scatter the projectiles into the crystalline channels. If the scattering is accompanied by a reduction in the transverse energy, the projectile can become re-channeled.

By normalizing $N_{\text{ch0}}(z)$ with respect to the number N_0 of all simulated simulated and to the number N_{acc} of accepted electrons we determine the channeling fractions "1" and "2" which characterize the dechanneling process. We also introduce the channeling fraction "3" as the

ratio of $N_{\text{ch}}(z)$ to the number of accepted electrons. The latter fraction is determined by both dechanneling and rechanneling that happen to propagating electrons.

Fig. 2 shows the fractions defined above for the electrons with energy 855 MeV channeling in Si(110). Four separate plots in the figure correspond to different values of the bending parameter. Fraction "1" differs from fraction "2" by a constant factor - the acceptance A , and is included in the plots with an illustrative purpose only. For the same propagation distance z , all three fractions become progressively smaller with increasing the bending parameter. More interesting is to compare fractions "2" and "3". Here, a large enhancement of fraction "3" with respect to "2" is seen for the straight ($C = 0$) channel as well for bent channels corresponding to small values of the bending parameter, $C \lesssim 0.05$. In particular, for the straight channel at the distance $z = 10$ microns the number of electrons channeling in *any channel* exceeds the number of electrons staying in the *entrance channel* by the factor of two, as a result of the dechanneling process. With C increasing, the events of dechanneling become more rare, and the difference between the fractions diminishes (see the plot for $C = 0.2$).

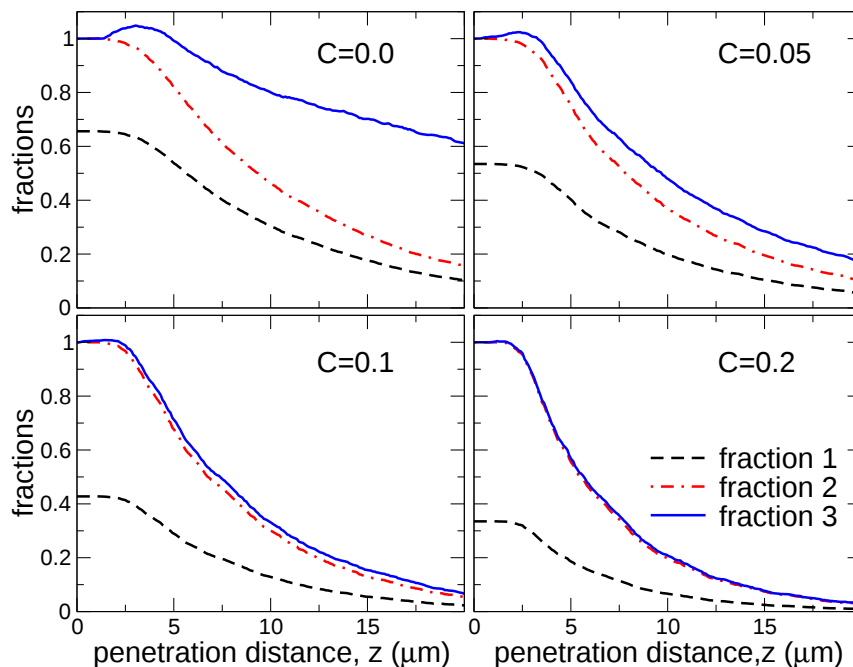


Figure 2. Fractions of channeling electrons with energy 855 MeV for different values of the bending parameter C as indicated. Fractions "1", "2" and "3" designate the ratios $N_{\text{ch0}}(z)/N_0$, $N_{\text{ch0}}(z)/N_{\text{acc}}$ and $N_{\text{ch}}(z)/N_{\text{acc}}$, respectively.

Fig. 3 shows the fractions $N_{\text{ch}}(z)/N_{\text{acc}}$ of channeling electrons with the energies $\varepsilon = 600$ and 855 MeV for different values of the bending parameter C . Comparing the fractions for same values of C one notices, that the portion of channeling electrons is higher for higher ε . With C increasing the channeling fractions gradually decrease and change the character of the decay at large distances: from the inverse power-law decay at small C to the exponential one at the larger values.

By analyzing the channeling segments for each simulated trajectory we have calculate two characteristic penetration lengths introduced in Ref. [1]. The first one, L_{p1} , is a mean value of the primary channeling segments which start at the crystal entrance. The other length, L_{p2} , is defined as a mean path with respect to all channeling segments, including those which result due to the rechanneling process. Generally speaking, L_{p1} depends on the angular distribution of

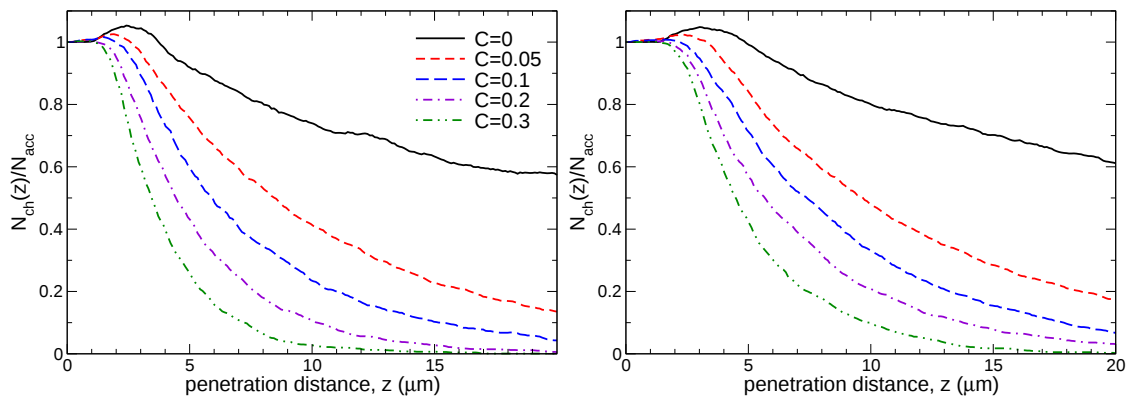


Figure 3. The channeling fraction $N_{\text{ch}}(z)/N_{\text{acc}}$ for $\varepsilon = 600$ MeV (left plot) and $\varepsilon = 800$ MeV (right plot) electrons versus the penetration distance. Different curves correspond to different values of the bending parameter as indicated.

Table 1. Acceptance A and penetration lengths L_{p1} and L_{p2} for different energies ε of electrons channeling in bent Si(110). The results refer to the crystalline sample of the length $L = 75$ μm .

$\varepsilon(\text{MeV})$	R (cm)	C	N_0	A	L_{p1} (μm)	L_{p2} (μm)
195	∞	0	1708	0.583	4.08 ± 0.29	4.08 ± 0.11
	3	0.010	1570	0.575	3.90 ± 0.30	4.08 ± 0.14
	0.6	0.051	1710	0.525	3.91 ± 0.29	3.91 ± 0.23
	0.3	0.102	1550	0.423	3.19 ± 0.25	3.21 ± 0.24
	0.1	0.306	1728	0.196	1.99 ± 0.22	1.99 ± 0.21
600	∞	0	1420	0.609	9.38 ± 0.75	8.70 ± 0.33
	2	0.047	1502	0.560	8.81 ± 0.72	8.25 ± 0.62
	1	0.095	1461	0.446	7.05 ± 0.63	7.12 ± 0.60
	0.5	0.188	1432	0.330	5.28 ± 0.52	5.28 ± 0.52
855	∞	0	1128	0.656	11.90 ± 1.11	11.13 ± 0.53
	2.5	0.054	1462	0.553	9.79 ± 0.81	9.87 ± 0.72
	1.3	0.103	1419	0.423	8.55 ± 0.81	8.50 ± 0.78
	0.7	0.192	1460	0.303	6.59 ± 0.68	6.61 ± 0.68
	0.5	0.268	1504	0.241	5.38 ± 0.55	5.43 ± 0.56
	0.3	0.447	1376	0.134	4.50 ± 0.61	4.48 ± 0.61

the particles at the entrance. Our simulations, performed for of the zero emittance beams, yield an upper bound estimate for this length. However, the rechanneling electrons are statistically distributed over the incident angles that do not exceed the Lindhard critical angle. Therefore, the length L_{p2} can be thought for quantifying the penetration depth for a beam with non-zero emittance.

Either one from L_{p1} and L_{p2} provides an estimate of the *dechanneling length*. Our results on these quantities for different electron energies and bending parameters are presented in Table 1. Within the statistical uncertainties, the values for both lengths yield the same estimates for the dechanneling length. Also included in this table are the numbers N_0 of the simulated trajectories along with the corresponding acceptances A .

It is worth noting that the values of dechanneling lengths reported in the table noticeably exceed those estimated earlier for $\varepsilon = 855$ MeV electrons channeled in straight [27, 28] and bent [29] Si (110) channels. The calculations performed in the cited papers were based on

the peculiar model of the elastic scattering of an ultra-relativistic projectile from the crystal constituents. The model assumes that due to the high speed of the projectile, its interaction interval with a crystal atom is short enough to substitute the atom with its “snapshot” image: instead of the continuously distributed electron charge the atomic electrons are treated as point-like charges placed at fixed positions around the nucleus. Next, the model implies that the interaction of an ultra-relativistic projectile (e.g., an electron) with each atomic constituent can be reduced to the classical Rutherford scattering. In Ref. [1] it was demonstrated, that such a “snapshot” model noticeably overestimates the mean scattering angle in the process of elastic scattering in a single electron-atom collision. Qualitatively, it is clear that substituting a “soft” electron cloud with a set of point-like static electrons must lead to the increase of the scattering angle simply because each electron acts as a charged scatterer of an infinite mass. As a result, the projectile experiences, on average, harder collisions with electrons as compared to the case when they are continuously distributed in space. The mean square angle for a single scattering is a very important quantity in the multiple-scattering region, where there is a large succession of small-angle deflections symmetrically distributed about the incident direction. In particular, the mean square angle due to soft collisions defines the diffusion coefficient which, in turn, is proportional to the dechanneling length (see, for example, Refs. [8,30]). It was noted in Ref. [1] that the “snapshot” approximation underestimates the dechanneling length of 855 MeV electrons in straight Si (110) by approximately 30 per cent. Comparing the L_{p1} and L_{p2} values presented in Table 1 for $C > 0$ with the data from Ref. [29] one concludes that the discrepancy becomes more pronounced for larger values of the bending parameter.

Let us introduce another characteristic length, the total channeling length L_{ch} , which can be used to quantify the channeling process. This quantity is defined as an average length of all channeling segments per trajectory. Due to the rechanneling process, the total channeling length L_{ch} is an increasing function of the crystal length L . Under the assumption that the probability of rechanneling does not depend on the penetration length one can expect that $L_{ch} \propto \sqrt{L}$ for $L \gg L_{p1}, L_{p2}$. In this limit the number of rechanneling events is large enough to justify the diffusion approach in estimating L_{ch} . The calculated values of L_{ch} (open circles) versus L for 855 MeV electrons in straight Si(110) along with the fitting curves are presented in Figure 4. The solid line stands for the dependence $L_{ch} = 3.68\sqrt{L}$ which seems to be adequate for large values of L but overestimates L_{ch} in the range $L < 100$ micron. The dashed line stands for the best fit which is described by the formula $L_{ch} = 2L^{0.61}$.

4. Concluding remarks

Using the newly developed code [1], which was implemented as a module in the MBN Explorer package [2], we have performed the Monte Carlo simulations of trajectories of ultra-relativistic electrons in oriented (110) straight and bent single Si crystal. The description of the particle motion is given in classical terms by solving the relativistic equations of motion which account for the interaction between the projectile and the crystal atoms. The probabilistic element is due a random choice of transverse coordinates and velocities of the projectile at the crystal entrance as well as by accounting for the random positions of the crystal atoms due to thermal vibrations.

The calculations were carried out for several values of the bending radius R and crystal length L . The chosen energies 195, 600 and 855 MeV of electrons are of interest in connection with the ongoing experiments with electron beams at Mainz Microtron [16,17].

The simulated trajectories are used as the input data for numerical analysis of channeling conditions and properties. The calculated data include the channel acceptance as a function of the bending parameter C and of electron energy ε ; the number of primarily channeled particles N_{ch0} and the number of particles in the channeling mode N_{ch} as functions of the penetration distance z . By comparing the dependencies $N_{ch0}(z)$ and $N_{ch}(z)$ we have demonstrated the

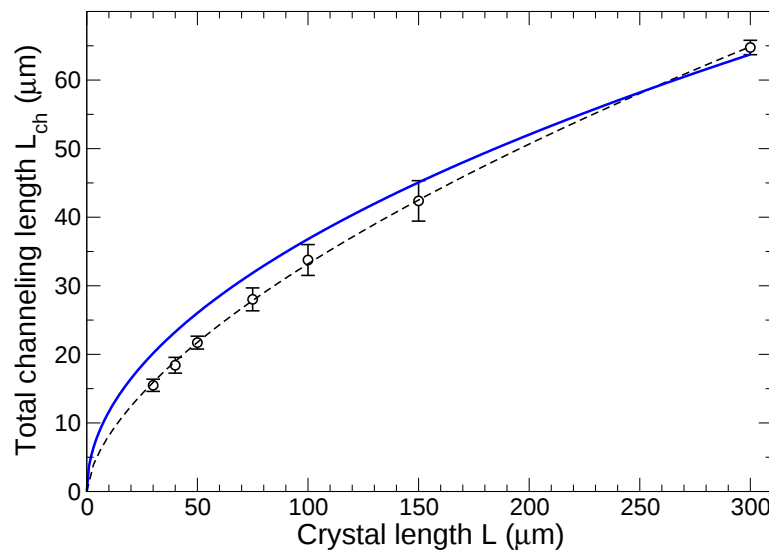


Figure 4. Total channeling length L_{ch} for 855 MeV electrons in straight Si(110) channel versus crystal length. Open circles stand for the calculated values, solid and dashed curves present the dependencies $L_{ch} \propto L^{0.5}$ and $L_{ch} \propto L^{0.61}$, respectively. See also explanations in the text.

important role of rechanneling for projectile electrons.

By analyzing the simulated trajectories we estimated of the electron dechanneling lengths for various ε and C . The obtained results, which are summarized in Table 1, are more accurate than those calculated recently [27, 29] since the latter data were based on the erroneous model of ultra-relativistic electron–atom elastic scattering. We have demonstrated that the model overestimates the mean scattering angle,

Finally, we have performed quantitative analysis of the total length L_{ch} of all channeling segments per a simulated trajectory. This quantity can be measured experimentally by analyzing the radiation emitted within a large cone, $\theta \gg \gamma^{-1}$, as a function of the crystal length. As a prime further step in application of the simulated trajectories we plan to perform the calculations of the emission spectra in a broad range of the photon energies. This will allow us to carry out comparison with the available experimental data and to analyze the influence of the crystal bending on the spectra. Similar calculations are to be performed for the case of positron channeling.

Another important set of calculations concerns simulation and analysis of the channeling process and computation of the emission spectra from sub-GeV electrons and positrons in crystalline undulators. The results of this work, which is currently in progress, will be published elsewhere.

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