Planar channelling of 855 MeV electrons in silicon: Monte Carlo simulations

Andriy Kostyuk\textsuperscript{1}, Andrei Korol\textsuperscript{1,2}, Andrey Solov’yov\textsuperscript{1,3} and Walter Greiner\textsuperscript{1}

\textsuperscript{1} Frankfurt Institute for Advanced Studies, Johann Wolfgang Goethe-Universit"at, 60438 Frankfurt am Main, Germany
\textsuperscript{2} Department of Physics, St. Petersburg State Maritime Technical University, 198262 St. Petersburg, Russia
\textsuperscript{3} A F Ioffe Physical-Technical Institute, 194021 St. Petersburg, Russia

E-mail: kostyuk@fias.uni-frankfurt.de

Received 25 November 2010, in final form 28 February 2011
Published 29 March 2011
Online at stacks.iop.org/JPhysB/44/075208

Abstract

A new Monte Carlo code for the simulation of the channelling of ultrarelativistic charged projectiles in single crystals is presented. A detailed description of the underlying physical model and the computation algorithm is given. The first results obtained with the code for the channelling of 855 MeV electrons in silicon crystal are presented. The dechannelling lengths for (1 0 0), (1 1 0) and (1 1 1) crystallographic planes are estimated. In order to verify the code, the dependence of the intensity of the channelling radiation on the crystal dimension along the beam direction is calculated. A good agreement of the obtained results with recent experimental data is observed.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

In this paper we consider planar channelling of 855 MeV electrons in silicon crystal using a new Monte Carlo code.

Channelling takes place if charged particles enter a single crystal at small angle with respect to crystallographic planes or axes [1]. The particles get confined by the interplanar or axial potential and move preferably along the corresponding crystallographic planes or axes following their shape.

Recent revival of the interest to this phenomenon is due to its growing practical application. In particular, the crystals with bent crystallographic planes are used to steer high-energy charged particle beams entering single crystals. Since its appearance [2] and first experimental verification [3], this idea has been attracting a lot of interest worldwide. Bent crystal has been routinely used for beam extraction in the Institute for High Energy Physics, Russia [4]. A series of experiments on the bent crystal deflection and collimation of proton and heavy ion beams were performed at different accelerators [5–10] throughout the world. The bent crystal method has been proposed to extract particles from the beam halo at CERN’s Large Hadron Collider [11]. The possibility of deflecting positrons [12], electrons [8, 13, 14] and $\pi^-$ mesons [15, 16] has been studied as well.

Another very promising application of the channelling phenomenon is a novel source of hard electromagnetic radiation. A single crystal with periodically bent crystallographic planes can force channelling particles to move along nearly sinusoidal trajectories and radiate in the hard x- and gamma-ray frequency range. The feasibility of such a device, known as the ‘crystalline undulator’, was demonstrated theoretically a decade ago [17, 18] (further developments as well as historical references are reviewed in [19]). The advantage of the crystalline undulator is in extremely strong electrostatic fields inside a crystal, which are able to steer the particles much more effectively than even the most advanced superconductive magnets. This fact allows one to make the period $\lambda_u$ of the crystalline undulator in the hundred or even ten micron range, which is two to three orders of magnitude smaller than that of conventional undulator. Therefore the wavelength of the produced radiation $\lambda \sim \lambda_u/\left(2\gamma^2\right)$ ($\gamma \approx 10^3$–$10^4$ being the Lorentz factor of the particle) can reach the (sub)picometre range, where conventional sources with comparable intensity are unavailable [20].
Initially, it was proposed to use positron beams in the crystalline undulator. Positively charged particles are repelled by the crystal nuclei and, therefore, they move between the crystal planes, where there are no atomic nuclei and the electron density is less than average. This reduces the probability of random collisions with the crystal constituents. Hence, the transverse momentum of the particle increases slowly and the particle travels a longer distance in the channelling regime.

More recently, an electron-based crystalline undulator was proposed [21]. On one hand, electrons are less preferable than positrons. Due to their negative charge, the electrons are attracted by the lattice ions and, therefore, are forced to oscillate around the crystal plane in the process of channelling. The probability of collisions with crystal constituents is enhanced. Thus, the dechannelling length is smaller by about two orders of magnitude in comparison to that of positrons at the same conditions. On the other hand, the electron beams are easily available and are usually of higher intensity and quality. Therefore, from the practical point of view, electron-based crystalline undulator has its own advantages and deserves a thorough investigation.

There is another reason why electron channelling needs a thorough analysis. This is the disagreement between theory and experimental data. For example, the Baier–Katkov–Strakhovenko formula for the dechannelling length (equation (10.1) in [22]), \( L_d \), predicts \( L_d = 23 \mu m \) for 1.2 GeV electrons in the Si (1 1 0) planar channel, while the value extracted from experimental data is \( L_d = 28 \mu m \) [23]. At 855 MeV, the formula yields \( L_d = 15.7 \mu m \) versus \( L_d = 18 \mu m \) obtained from a model-dependent analysis of the experimental data [24]. These discrepancies are rather small and can be attributed to different definitions of the dechannelling length used by experimental and theoretical groups.

For lower energies, the discrepancy is much more dramatic: \( L_d = 6.7 \mu m \) calculated versus \( L_d = 31 \mu m \) measured [25] and \( L_d \approx 1 \mu m \) calculated versus \( L_d = 36 \mu m \) measured [26] for electron energies 350 MeV and 54 MeV, respectively.

Clearly, further theoretical and experimental investigations of the electron channelling are necessary (see also [27]). No accurate theoretical description of the electron deflection by bent crystals or the electron-based crystalline undulator is possible until an adequate and model-dependent analysis of the experimental data is available.

To build such a model, we developed a new Monte Carlo code that allows us to simulate the particle channelling and calculate the emitted radiation. In contrast to other channelling codes [28–30], our algorithm does not use the continuous potential approximation. This novel feature is especially beneficial in the case of negatively charged projectiles, which channel in the vicinity of the atomic nuclei, where the continuous potential approximation becomes less accurate.

In this paper we present the first results obtained with our code. We have studied the channelling of 855 MeV electrons in a straight single crystal of silicon along three different crystallographic planes: (1 0 0), (1 1 0) and (1 1 1).

The probability of collisions with crystal constituents is enhanced. Thus, the dechannelling length is smaller by about two orders of magnitude in comparison to that of positrons at the same conditions. On the other hand, the electron beams are easily available and are usually of higher intensity and quality. Therefore, from the practical point of view, electron-based crystalline undulator has its own advantages and deserves a thorough investigation.

Figure 1. An example of a ‘snapshot’ of a silicon atom as it is seen by an ultrarelativistic projectile moving along the z-axis. The larger and smaller circles represent the nucleus and the electrons, respectively. The dashed line shows the Thomas–Fermi radius of the atom.

The probability density to see the atomic electrons at positions \( \vec{r}_1, \vec{r}_2, \ldots, \vec{r}_Z \) (Z is the atomic number) is given by squared absolute value of the wavefunction of the atom:

\[
\psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_Z) = |\psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_Z)|^2.
\]  

Instead of using the exact wavefunction, we approximate it by a spherical symmetric probability distribution that on average reproduces the electrostatic potential of the atom in Molière’s approximation [31]. Our approach ignores nonsphericity of electron orbitals as well as anticorrelations, due to Coulomb’s repulsion and Pauli’s principle, between electron positions.

The interaction of the projectile with an atomic constituent is considered as a classical scattering in a Coulomb field of a static point-like charge. A projectile with electric charge \( q_p \) and initial speed \( v \) along the z-axis attains, after interaction...
with a static charge $q_i$, a transverse momentum

$$\Delta \vec{p}_\perp = -q_i \vec{r}_\perp / v_r \perp,$$  

(2)

where $\vec{r}_\perp$ is the vector connecting the projections of the projectile and the static charge onto the $(x,y)$ plane.

The total transverse momentum attained by the projectile in the collision with the atom is a vector sum of (2) over all atom constituents. The absolute value of the projectile momentum remains unchanged. This means that the projectile energy losses for ionization or excitation of the atom are neglected. Indeed, the ionization losses of high-energy electrons or positrons in matter are very small (see, for example, figure 27.10 in [32]).

The above procedure is approximate. It is valid if the scattering angle $\vartheta = |\Delta \vec{p}_\perp|/p$ is small. In the opposite case, not only formula (2) but also the representation of the atom as a collection of static charges becomes wrong. However, accurate description of the large angle scattering is not important for modelling of the channelling processes. First, such processes are rare. Second, if the projectile is scattered by an angle that is much larger than the critical Lindhard’s angle $\vartheta_t$, [1], its probability to return to the channelling regime is negligible. Therefore, the trajectory of a projectile after a large-angle scattering is out of our interest and the precise value of the large scattering angle does not matter.

On the other hand, the scattering by $\vartheta \lesssim \vartheta_t$ is important for a proper modelling of the channelling phenomenon. Lindhard’s angle for ultrarelativistic projectiles is typically in the submiliradian range. The described procedure as well as formula (2) are valid for such small scattering angles.

The ‘snapshot’ model is applied not only to each atom but also to the crystal as a whole. The thermal motion of the atoms is even slower than the motion of atomic electrons. Therefore, the projectile sees the atomic nuclei ‘frozen’ at random positions in the vicinity of nodes of the crystal lattice. The probability distribution of the position of the nucleus relative to the node can be approximated by a three-dimensional normal distribution with the variance equal to the squared amplitude of thermal vibrations of the crystal atoms.

Although the crystal constituents are considered as static point-like charges, and the model looks like completely classical construction at the first sight, the quantum properties of the crystal are properly taken into account: the probability distributions of electrons and nuclei are found from the quantum theory.

In contrast, the quantum aspects of the projectile motion are indeed completely ignored. Our code performs calculation of trajectories of the projectiles in the crystal. Calculation of a particle trajectory implies that its coordinate and momentum can be measured simultaneously. Let us estimate the validity domain of this approximation.

The notion of trajectory makes sense in the case of a channelling particle if one is able to determine the particle coordinate $y$ and the transverse momentum $p_y$, with accuracies $\delta y$ and $\delta p_y$, that are much smaller than the channel width $\Delta$ and typical value $p_y^{ch}$ of the transverse momentum of a channelling particle. On the other hand, the product $\delta p_y \delta y$ cannot be smaller than $\hbar$ due to Heisenberg’s uncertainty principle. We obtain, therefore, the following inequality:

$$p_y^{ch} \Delta \delta y \gg \hbar.$$  

(3)

The transverse motion of the projectile can be described by the laws of dynamics of a nonrelativistic particle with the mass $E/c^2$. Here $E$ is the projectile energy and $c$ is the speed of light. The transverse kinetic energy of the channelling particle cannot exceed the depth of the interplanar potential well $U_{\text{max}}$:

$$\left(\frac{p_y^{ch}}{E/c^2}\right)^2 < U_{\text{max}}.$$  

(4)

Combining (3) and (4) one sees that the projectile can be considered classically if its energy $E$ is sufficiently large:

$$E \gg \frac{(hc)^2}{2d^2U_{\text{max}}}.$$  

(5)

Putting $U_{\text{max}} = 20$ eV and $d = 1 \text{ Å}$ one obtains $E \gg 0.1$ MeV. However, the sign $\gg$ in this inequality has to be understood as ‘at least three orders of magnitude larger’. To show this, let us consider a simple example of a parabolic potential well of depth $U_{\text{max}}$ and width $d$:

$$U(y) = U_{\text{max}} \left(\frac{y}{d/2}\right)^2.$$  

(6)

The oscillation frequency in such potential for a particle with mass $E/c^2$ is $\omega = c\sqrt{U''(0)/E}$, where $U''$ is the second derivative of the potential energy with respect to $y$. From (6) one finds $U'' = 8U_{\text{max}}/d$. The number of quantum levels in the potential well is

$$n \approx \frac{U_{\text{max}}}{\hbar \omega} = \frac{d}{2\hbar c\sqrt{U_{\text{max}}E/2}}.$$  

(7)

Solving (7) for $E$ yields

$$E \approx \frac{16\pi^2}{2d^2U_{\text{max}}} (hc)^2.$$  

(8)

The right-hand sides of (5) and (8) coincide up to the factor of $16\pi^2$. The classical description is valid if the number of levels is sufficiently large. Taking $n = 10$ one obtains $16\pi^2 = 1600$. Hence, our model can always be applied to ultrarelativistic heavy projectiles. It is applicable in the case of light projectiles if their energy is in the hundred MeV range or higher. The applicability conditions for an electron projectile may be somewhat stricter than for positrons, because the planar potential well is narrower in the case of negative particles. In this paper we apply the model to electron projectiles at energy $E = 855$ MeV. In this case the classical approximation is expected to be satisfactory.

The process of radiation emission by the projectile is also treated classically. The energy $E$ per unit interval of the radiation frequency $\omega$ per unit of the solid angle $\Omega$ emitted by the projectile is calculated according to formula (14.65) from [33]:

$$\frac{d^3E}{d\omega \ d^2\Omega} = \frac{q_p^2}{4\pi^2 c^3} \left\{ \int_{\tilde{n}}^{\tilde{n}_u} dt \tilde{n} \times \left[ (\tilde{n} - \beta(t)\times \dot{\beta}(t)) / (1 - \tilde{n} \cdot \dot{\beta}(t))^2 \right] \times \exp \left\{ \frac{i\omega}{c} \left[ \gamma(t) - \tilde{n} \cdot \dot{r}(t) \right] \right\} \right\}^2.$$  

(9)
Here \( \mathbf{n} \) is a unit vector pointing from the crystal to a distant observation point, \( \mathbf{r}(t) \) is the projectile coordinate as a function of time and \( \beta(t) \) and \( \beta'(t) \) are respectively its velocity and acceleration divided by the speed of light: \( \beta(t) = \mathbf{r}(t)/c \), \( \beta'(t) = \mathbf{v}(t)/c \). The integration over the time \( t \) is taken from the moment \( t_{\text{in}} \) of entering to the moment \( t_{\text{out}} \) of exiting the crystal by the projectile.

The classical approach is valid for relatively soft radiation: the photon energy has to be much smaller than the energy of the projectile.\[ r_i = a_{\text{TF}} \hat{r}_i, \quad i = 1, \ldots, Z. \] Here, \( a_{\text{TF}} \) is the Thomas–Fermi radius of the atom:
\[ a_{\text{TF}} = \frac{0.8853}{Z \alpha^3} a_{B}, \] with \( a_{B} \) being Bohr’s radius, and \( \hat{r}_i \) is found by solving the following transcendental equation:
\[ \chi(r_i) = \frac{Z e}{r} \chi \left( \frac{r}{a_{\text{TF}}} \right). \]

The screening function \( \chi \) satisfies the conditions
\[ \chi(0) = 1, \quad \lim_{r \to \infty} \chi(r) = 0, \] so that the potential has the Coulomb form \( (Ze)/r \) in the vicinity of the nucleus but is fully screened out by the electron cloud at large \( r \).

We use the Molière screening function [31], which has the form
\[ \chi(\mathbf{r}) = \sum_{j=1}^{3} a_j \exp(-\beta_j \mathbf{r}) \] with numerical parameters having the values
\[ a_1 = 0.35, \quad a_2 = 0.55, \quad a_3 = 0.1, \quad \beta_1 = 0.3, \quad \beta_2 = 1.2, \quad \beta_3 = 6.0. \]

To take into account quantum and thermal oscillations of the atoms in the crystal, the atomic nuclei is placed not exactly in the lattice node but is shifted from it by a random vector \( \hat{r} \). Each component of the random vector is normally distributed:
\[ w(\rho_k) = \frac{1}{\sqrt{2\pi \alpha(T)}} \exp \left[ -\frac{1}{2} \left( \frac{\rho_k}{\alpha(T)} \right)^2 \right], \quad k = x, y, z. \]
Here \( \alpha(T) \) is the average oscillation amplitude. We used the value \( \alpha(T) = 0.075 \) Å in our calculations, which corresponds to the room temperature [34].
The trajectory of the projectile is modelled as follows. The particle moves along straight line segments between the points where its coordinate $z$ coincides with the $z$ coordinate of one of a crystal constituent: an electron or a nucleus. At this point the transverse momentum of the projectile is changed according to equation (2). Then the projectile is moved further along a straight line segment corresponding to the transverse momentum $\vec{p}_z + \Delta \vec{p}_z$ until its $z$ coordinates coincide with that of the next crystal constituent and a new modification of the particle momentum is performed.

A crystal constituent is taken into account if it belongs to the lattice node located within a cylinder of radius $40 \alpha_{\text{TF}}$ around the particle. Initially, the axis of the cylinder is the straight line along the direction of the projectile momentum at the point of entering the crystal. The length of the cylinder is approximately 200 Å. When the particle approaches the end of the cylinder, a new cylinder is built as an extension of the old one but along the direction of the new particle momentum. The procedure continues until the end of the crystal is reached. As a result, the cylinders form a 'pipe' filled by the crystal lattice and the particle channels inside it as it is shown in figure 2.

Substantial computer time is saved due to the fact that only the part of the crystal lattice inside the 'pipe' is modelled and the rest of it is ignored. The simulation takes about 0.8 s per 1 μm of the particle trajectory on a 3 GHz CPU core.

After the projectile trajectory is simulated, the radiation spectrum is calculated. The integral in (24) is approximated with a sum over the trajectory points:

$$\frac{d^3 \mathcal{E}}{d(h\omega) d^2 \Omega} = \frac{\alpha}{4 \pi^2} \sum_j \left( \frac{\delta \vec{p}_j}{D_{j-1}} + \frac{(\vec{p}_j - \vec{n})(\delta \vec{p}_j \cdot \vec{n})}{D_j D_{j-1}} \right) \times \exp\left( \frac{\phi_{j-1} + \phi_j}{2} \right),$$

(24)

where $\delta \vec{p}_j$ is an increment of $\vec{p}$ between two successive trajectory points: $\delta \vec{p}_j = \vec{p}_j - \vec{p}_{j-1}$ and $\alpha$ is the fine structure constant. The denominators $D_j$ are found from the formula $D_j = 1 - (\vec{p}_j \cdot \vec{n})$ and the phases $\phi_j$ are given by the expression

$$\phi_j = \frac{\alpha}{c} \left[ ct_j - \vec{n} \cdot \vec{r}_j \right].$$

(25)

Dividing (24) by $h\omega$ yields the formula for the number of photons.

4. Simulations

The calculations were performed for $E = 855$ MeV electrons in a single crystal of silicon for three crystal orientations corresponding to channelling along $(100)$, $(110)$ and $(111)$ planes. The simulated positions of the crystal constituents and the potential energy of the projectile electron in the field of crystal planes in continuous approximation. The plots in the right column serves an illustrative purpose only, the continuous potentials are not used in the calculation algorithm.

4. Simulations

The calculations were performed for $E = 855$ MeV electrons in a single crystal of silicon for three crystal orientations corresponding to channelling along $(100)$, $(110)$ and $(111)$ planes. The simulated positions of the crystal constituents and the potential energy of the projectile electron in the electrostatic field of crystal planes are shown in figure 3.

Initially, the projectiles had zero transverse momentum. This corresponds to the ideal case of a zero-emittance beam entering the crystal strictly parallel to the coordinate axis $z$. The transverse position of the projectile at the entrance of the crystal was chosen randomly, homogeneously distributed along the channel width. Then the trajectory of the particle was simulated as described in the previous section. The simulation
of the trajectory was terminated if the particle went through the crystal: \( z > L_{cr} \), or if the deviation of the projectile from its initial direction became too large: \( |\mathbf{p}_L|/|\mathbf{p}_z| > 100/\gamma \) (here \( p_L \) and \( p_z \) are respectively the transverse and the longitudinal momenta and \( \gamma \) is the Lorentz factor of the projectile.)

Each simulated trajectory was analysed to determine the segments corresponding to the channelling and dechanneled regime. The particle was considered to be in the channelling regime from the point of entering the crystal to the point where its crossed one of the two channel boundaries. Then the particle was considered to be dechanneled. If a dechanneled particle changed the direction of the \( \gamma \) component of its velocity two or more times without crossing channel boundaries (i.e. if it made at least one complete channelling oscillation within a channel) it was considered to be rechanneled and remaining in the channelling regime until it crossed one of the channel boundaries again.

The number of the simulated trajectories for the analysis of dechanneled was 40 000, 30 000 and about 28 000 for planar channels (1 1 1), (1 1 0) and (1 0 0), respectively. The dimension of the crystal in the beam direction \( L_{cr} \) was equal to the maximum length of the crystals used in recent channelling experiments [24]: \( L_{cr} = 270.4 \mu m \).

Chanelling radiation was calculated for the plane (1 1 0) and for ‘amorphous’ orientation (i.e. for a crystal oriented randomly avoiding major crystal directions) for seven different values of \( L_{cr} \) ranging from \( L_{cr} = 7.9 \mu m \) to \( L_{cr} = 270.4 \mu m \), 50 000 trajectories were simulated in each case.

5. Definition of the dechanneled length

To make a quantitative assessment of the particle dechanneled process, one needs a definition of the dechanneled length that would be suitable for the Monte Carlo approach.

Let \( z_{d1} \) be the point of the first dechanneled of the projectile. We define the quantity \( N_{ch0}(z) \) as the number of projectile particles for which \( z_{d1} > z \), i.e. this is the number of particles that passed the distance from the crystal entrance to the point \( z \) in the channelling regime and dechannel at some further point. The length \( L(z) \) is the average distance from the point \( z \) to the first dechanneled point:

\[
L(z) = \frac{\sum_{k=1}^{N_{ch0}} (z_{d1}^{(k)} - z)}{N_{ch0}(z)}. \tag{26}
\]

The sum in the numerator is taken over those projectiles for which \( z_{d1} > z \).

Generally speaking, \( L(z) \) depends not only on \( z \), but also on the angular distribution of the particles at the crystal entrance. Nonetheless, as it will be shown below, the kinetic theory of channelling suggests that, at sufficiently large \( z \), \( L(z) \) reaches an asymptotic value that depends neither on \( z \) nor on the initial angular distribution.

From the solution of the diffusion equation (see, for instance, formula (1.38) in [35]), one can obtain the following expression for \( N_{ch0}(z) \):

\[
N_{ch0}(z) = N_0 \sum_{j=1}^{m} A_j \exp(-z/L_j). \tag{27}
\]

Here only coefficients \( A_j \) depend on the initial angular distribution of the particles, while the lengths \( L_j \) depend exclusively on the properties of the crystal channel and the energy, charge and mass of the projectile.

The 1/e dechanneled length \( L_d \) is defined as the largest of the parameters \( L_j \) in (27). The corresponding term dominates the asymptotic behaviour at \( z \gg L_d \):

\[
N_{ch0}(z) \propto N_0 A_d \exp(-z/L_d). \tag{28}
\]

Expression (26) for \( L(z) \) has the following counterpart in the kinetic theory:

\[
L(z) = \frac{1}{N_{ch0}(z)} \int_{z_{d1}}^{\infty} dz_{d1} (z_{d1} - z) \frac{N_{ch0}(z_{d1})}{dz_{d1}}. \tag{29}
\]

Substituting (28) into (29) demonstrates that, indeed, the coefficient \( A_d \) cancels out and \( L(z) \) becomes equal to \( L_d \) in the asymptotic region.

Although the diffusion equation was solved in [35] for a positively charged projectile in harmonic potential approximation, the exponential asymptotic behaviour of \( N_{ch0}(z) \), and, consequently, a constant asymptotic value of \( L(z) \) are a more general result. As is shown in the next section, our simulations demonstrate that it is also valid for electrons.

Hence, in our Monte Carlo procedure the dechanneled length \( L_d \) is defined as the asymptotic value of \( L(z) \) in the region where it ceases to depend on \( z \).

6. Analysis of the results

The ratio \( N_{ch0}(z)/N_0 \) as a function of \( z \) is shown in figure 4 for three different crystal channels. This fraction decreases rather fast and, as expected, has an exponential asymptotic behaviour.

The quantity \( L(z) \) (26) for the same channels is plotted in figure 5. Indeed, \( L(z) \) becomes constant (within the statistical errors) at large \( z \) corresponding to the exponential behaviour.
of the curves of figure 4. The asymptotic values, $L_\lambda$, are listed in table 1.

Only the particles that remained in the channelling regime from their entrance to the crystal were considered in figures 4 and 5. The fraction of these particles decreases fast. In contrast, the fraction $N_{\text{ich}}(z)/N_0$ of the particles that are in the channelling regime at the point $z$, regardless of their previous channelling status, decreases rather slowly (see figure 6). The reason for this is the rechannelling process. Random collisions with the crystal constituents can occasionally reduce the transverse energy $p_y$ of the projectile $y$ at which rechannelling is clearly seen. According to our results, the fraction of rechannelling is higher for negative than for positive particles.

Rechannelling occurs more often for electrons than for positively charged particles. This is due to the fact that the random scattering is more intense in the vicinity of the crystal plane. For positively charged particles this means that the scattering is most probable near the maximum of the potential energy $U(y)$. Even if a collision occurs to reduce the component $p_y$ of the projectile momentum to zero, the transverse energy $E_y$ still remains in the vicinity of the top of the potential barrier. The range of $p_y$ at which the particle returns to the channelling regime is zero at the maximum of the potential and is small in the vicinity of it. Therefore, the probability of the rechannelling is small.

The asymptotic behaviour of the curves in figure 6 can be explained in the following way. At sufficiently large $z$, the distribution of the dechannelled particles with respect to the transverse momentum $p_y$ is similar to that in an amorphous medium and can be approximated by the Gaussian function:

$$w(p_y) = \frac{1}{\sqrt{2\pi\sigma(z)}} \exp \left[ -\frac{1}{2} \left( \frac{p_y}{\sigma(z)} \right)^2 \right]$$

(31)

In contrast, the potential minimum for negatively charged particles is located near the crystal planes. This means that the random collisions are most probable near the minimum of the potential energy, where there is a wider range of $p_y$ at which $E_y$ drops below the potential barrier. Hence, the probability of rechannelling is higher for negative than for positive particles.

Typical trajectories of electrons are shown in figure 7, where rechannelling is clearly seen. According to our results, a particle rechannels on average 4.8 times on the length of the crystal $L_{cr} = 270.4 \mu m$ into the channel (1 0 0). For the channels (1 1 0) and (1 1 1) the corresponding numbers are respectively 4.4 and 3.5.

The asymptotic values, $L_\lambda$, are listed in table 1.

Table 1. Monte Carlo results for the 1/e dechannelling length $L_\lambda$ for three different crystal channels. The results for initial beam and rechannelled particles coincide within the statistical errors.

| Crystal plane | Initial beam | Rechannelled particles |
|---------------|-------------|------------------------|
| (1 1 1)       | 13.57 ± 0.12 | 13.69 ± 0.07          |
| (1 1 0)       | 8.26 ± 0.08  | 8.38 ± 0.05           |
| (1 0 0)       | 6.38 ± 0.07  | 6.40 ± 0.05           |

Figure 5. The quantity $L(z)$ (26) that becomes equal to the dechannelling length at large penetration depth $z$. The thin lines show the statistical errors.

Figure 6. The fraction of channelling particles as a function of the penetration depth $z$ for different crystal channels (solid lines). The thick dashed lines show the corresponding asymptotes $\propto z^{-1/2}$.

Figure 7. Examples of simulated trajectories. Only initial segments corresponding to $z < 30 \mu m$ are plotted. The crystallographic planes are shown by the solid horizontal lines, and the dashed lines show the boundaries between the channels (the maxima of the interplanar potential). Four of five trajectories demonstrate rechannelling. One of the particles rechannels twice.
The probability of rechanneling is; therefore, the longer the crystal is along the beam direction, the larger the point. The thick dashed lines show the corresponding exponential channels as a function of the distance vicinity of the point rechanneling is dominated by the phase space density in the vicinity of the point.

Note that times.

Figure 8. The ratio \( N_{ch}(\tilde{z})/N_0 \) (see the text) for different planar channels as a function of the distance \( \tilde{z} \) from the rechanneling point. The thick dashed lines show the statistical errors. Note that the asymptotic values of \( L(\tilde{z}) \) are the same as for \( L(z) \) (cf figure 5).

\[
\sigma^2(z) \propto z. \quad \text{The rechanneling is dominated by the phase space density in the vicinity of the point } p_y = 0. \quad \text{It decreases as } 1/\sigma(z) \propto 1/\sqrt{z} \quad \text{and governs the asymptotic behaviour of the fraction of the channelling particles shown in figure 6.}
\]

For the analysis of the rechanneled particles, one can consider the quantity \( N_{ch}(\tilde{z}) \), which is the number of particles that rechannelled at least \( n \) times and travelled at least the distance \( \tilde{z} \) from the \( n \)th rechanneling point \( z_{nr} \) in the channelling regime, i.e. this is the number of particles for which

\[
z_{d(n+1)} - z_{rn} > \tilde{z}, \quad (32)
\]

where \( z_{d(n+1)} \) is the point of \((n+1)\)th dechannelling. Note that the longer the crystal is along the beam direction, the larger the probability of rechanneling is; therefore, \( N_{ch}(\tilde{z}) \) for \( n > 0 \) depend on \( L_{ch} \), in contrast to \( N_{ch0} \).

It is reasonable to expect that the particle ‘forgets’ the value of its initial transverse momentum by the point of its first rechanneling or even earlier. Therefore, all the rechannellings (first, second, and so on) are expected to be statistically identical and it makes sense to analyse them together. We introduce the quantity

\[
N_{rch}(\tilde{z}) = N_{ch1}(\tilde{z}) + N_{ch2}(\tilde{z}) + N_{ch3}(\tilde{z}) + \cdots, \quad (33)
\]

Note that \( N_{rch} \) may be larger than the total number of particles \( N_0 \), because each particle may rechannel several times.

The ratio \( N_{rch}(\tilde{z})/N_0 \) for \( L_{ch} = 270.4 \mu m \) for three crystal channels is plotted in figure 8. Similar to \( N_{ch0}(z) \), this quantity decreases fast with \( \tilde{z} \) and has an exponential asymptote.

It is possible to introduce the quantity \( L(\tilde{z}) \), which is a counterpart of (26) for rechanneled particles:

\[
L(\tilde{z}) = \frac{\sum_{n} \sum_{k} \left( z_{d(n+1)}^{(k)} - z_{rn}^{(k)} - \tilde{z} \right)}{N_{rch}(\tilde{z})}. \quad (34)
\]

The first sum in the numerator runs over all particles that rechannelled at least once. The second sum runs over all rechannellings of each particle.

The quantity \( L(\tilde{z}) \) is plotted in figure 9. The behaviour of \( L(\tilde{z}) \) and \( L(z) \) (see figure 5) at small values of \( \tilde{z} \) and \( z \) is different, because the transverse momentum distribution of the rechannelled particles is quite different from that of the ideally parallel initial beam. But asymptotic behaviour of both quantities is essentially the same: they both reach a constant value, which is, by definition, the dechannelling length \( L_d \).

In table 1, the values of \( L_d \) obtained from the analysis of rechanneled particles are compared to those obtained for the initial beam. They coincide within the statistical errors. This confirms that the dechannelling length calculated according to our definition does not depend on the initial transverse momentum distribution of the projectiles.

7. Comparison to experiment

The dechannelling length cannot be measured directly in an experiment because it is not possible to separate the particles that were in the channelling regime from the entrance point and the rechannelled particles. Only signals related to the total number of channelling particles can be measured. Extracting the dechannelling length from these data involves a model-dependent procedure. Therefore, comparing the values of \( L_d \) obtained by Monte Carlo simulations to estimations found in the experimental publications would be a comparison of two theoretical models rather than an experimental verification of the code.

A correct way to check a physical model and the corresponding computer code is to use it for calculation of those quantities that can be directly measured in an experiment. Then these results should be compared to the experimental data.

In the experiment at Mainz Microtron [24] the intensity of the channelling radiation was measured for crystal samples
of different dimensions $L_d$ along the beam axis. To make a comparison with these data, we modelled the Mainz experiment with our code.

We calculated the average number of photons in the energy interval $0.4 \text{ MeV} < \hbar \omega < 9.0 \text{ MeV}$ emitted by a 855 MeV electron moving through a silicon crystal with plane $(1 \ 1 \ 0)$ parallel to the beam direction. Then we subtracted the background, i.e. the same quantity but calculated in the case of a randomly oriented silicon crystal. The photons were taken into account if the angle $\theta$ between their wave vector and the beam direction does not exceed 1.31 mrad, which corresponds to the aperture of the gamma spectrometer in the experimental setup of the Mainz experiment. The calculation was performed for different values of $L_d$.

The intensity of the channelling radiation is presented in [24] in arbitrary units. We equated 12 au to 1 photon per projectile to adjust the overall scale. The results are shown in figure 10. As is seen, our results demonstrate reasonable agreement with the experiment, which proves the reliability of the code.

8. Conclusion and discussion

We first presented the result obtained with a new Monte Carlo code for modelling of the channelling of ultrarelativistic charged particles in a crystal. The calculation was performed for 855 MeV electrons channelling in a single crystal of silicon along $(1 \ 0 \ 0)$, $(1 \ 1 \ 0)$ and $(1 \ 1 \ 1)$ crystallographic planes.

According to our simulation, if rechannelling is disregarded, the number of channelling electrons decreases fast with the penetration depth $z$ and quickly approaches an exponential asymptote. A similar behaviour was previously seen in the kinetic theory of channelling in the case of a positively charged projectile.

We formulated a definition of the $1/e$ dechannelling length $L_d$ that is suitable for application within the Monte Carlo approach. Our definition is consistent with the one previously used in the kinetic theory of channelling. Applying this definition to the initial beam and to rechanneled particles gives essentially the same result. This demonstrates that $L_d$ is a universal quantity and does not depend on the initial transverse momentum distribution of projectiles.

We calculated the dechannelling length for the studied planar channels. It appeared to be in the 10 $\mu$m range.

Our simulations show that the rechannelling of electrons is a notable phenomenon. It dominates the number of channelling particles already at the penetration depth of a few tens of microns. Due to rechannelling, the total number of channelling particles, included the rechanneled fraction, decreases slowly following the $\propto 1/\sqrt{z}$ asymptote.

To verify our code, we calculated the intensity of the channelling radiation and compared it with the experimental data obtained at Mainz Microtron [24]. A good agreement was observed. This confirms that our code is a reliable tool for modelling the electron channelling if the projectile energy is around 1 GeV.

There is no obstacle for successful application of the code also to positrons of the same energy range or to electrons and positrons of higher energy up to several tens of GeV. Extending the applicability domain of the code to much lower or to much higher projectile energies requires further improvements of the underlying physical model and the computation algorithm.

At low projectile energies (around 100 MeV or lower) the splitting of the transverse energy levels of a channelling electron or positron can be as large as a few electron-volts, which is comparable with the depth of the potential well. Because only discrete transverse energy levels are allowed, scattering from the crystal constituents will lead to an increase of the transverse energy only when the energy transfer in the collision is equal to the splitting. Hence, only collisions with large scattering angles can contribute to the increase of transverse energy. Due to a smaller probability of such collisions, the dechannelling length may become noticeably larger than predicted by classical calculations. For these reasons, a study of low-energy electron and positron channelling would require quantum properties of the projectile to be taken into account.

At high electron or positron energies (hundreds of GeV or higher), the radiation energy losses become essential and cannot be ignored. Therefore, our model has to be further developed to take these into account.

In the case of heavy projectiles, the radiation energy losses are much less important. Therefore, in principle, our model can be applied to heavy projectiles of TeV energy range or even higher. However, calculations of heavy projectile channelling may involve very long crystals because of a large dechannelling length. This could require a prohibitive amount of computer time. Therefore, further refinement and optimization of the algorithm may be necessary in this case.

---

4 There is, however, a discrepancy in the dechannelling length: the value for the $(1 \ 0 \ 0)$ channel estimated by the Mainz group $L_d = 18 \ \mu$m [24] is a factor of more than 2 larger than our result $L_d = 8.26 \ \mu$m. It has to be pointed out that a model-dependent procedure was used in [24] to estimate the $L_d$. Therefore, the discrepancy in the dechannelling length does not mean that there is disagreement of our results with the experiment. The reasons for the discrepancy are still to be clarified. Preliminary, we attribute it to different definitions of the dechannelling length.
Acknowledgments

We are grateful to Hartmuth Backe, Werner Lauth and Dirk Krambrich for fruitful discussions. Our work was supported by the Deutsche Forschungsgemeinschaft (DFG).

References

[1] Lindhard J 1965 Kong. Danske Vid. Selsk. Mat.-Fys. Medd. 34 (issue 14)
[2] Tsyganov E N 1976 TM-682, TM-684, Fermilab, Batavia
[3] Elishev A G et al 2005 Nucl. Instrum. Methods B 234 14
[4] Arduini G et al 1998 Phys. Lett. B 422 325
[5] Carrigan R A et al 2002 Phys. Rev. ST Accel. Beams 5 043501
[6] Fillier R P et al 2006 Phys. Rev. ST Accel. Beams 9 013501
[7] Strokov S et al 2007 J. Phys. Soc. Japan 76 064007
[8] Scandale W et al 2008 Phys. Rev. ST Accel. Beams 11 063501
[9] Uggerhøj E and Uggerhøj U I 2005 Nucl. Instrum. Methods B 234 31
[10] Bellucci S et al 2006 Nucl. Instrum. Methods B 252 3
[11] Strokov S et al 2006 Nucl. Instrum. Methods B 252 16
[12] Scandale W et al 2009 Phys. Rev. A 79 012903
[13] Scandale W et al 2009 Phys. Lett. B 681 233
[14] Scandale W et al 2010 Phys. Lett. B 693 545
[15] Korol A V, Solov’yov A V and Greiner W 1998 J. Phys. G: Nucl. Part. Phys. 24 L45
[16] Korol A V, Solov’yov A V and Greiner W 1999 Int. J. Mod. Phys. E 8 49
[17] Korol A V, Solov’yov A V and Greiner W 2004 Int. J. Mod. Phys. E 13 867
[18] Korol A V, Solov’yov A V and Greiner W 2005 Topics in Heavy Ion Physics—Proc. Memorial Symp. for Gerhard Soff (Frankfurt am Main, Germany, 25–28 April) ed W Greiner and J Reinhardt (Budapest: EP Systema) pp 73–86
[19] Tabrizi M, Korol A V, Solov’yov A V and Greiner W 2007 Phys. Rev. Lett. 98 164801
[20] Bellucci S et al 2006 Phys. Rev. ST Accel. Beams 9 013501
[21] Strokov S et al 2007 J. Phys. Soc. Japan 76 064007
[22] Arduini G et al 1998 Phys. Rev. ST Accel. Beams 11 063501
[23] Uggerhøj E and Uggerhøj U I 2005 Nucl. Instrum. Methods B 234 31
[24] Bellucci S et al 2006 Nucl. Instrum. Methods B 252 3
[25] Strokov S et al 2006 Nucl. Instrum. Methods B 252 16
[26] Scandale W et al 2009 Phys. Rev. A 79 012903
[27] Scandale W et al 2009 Phys. Lett. B 681 233
[28] Scandale W et al 2010 Phys. Lett. B 693 545
[29] Korol A V, Solov’yov A V and Greiner W 1998 J. Phys. G: Nucl. Part. Phys. 24 L45
[30] Korol A V, Solov’yov A V and Greiner W 1999 Int. J. Mod. Phys. E 8 49
[31] Korol A V, Solov’yov A V and Greiner W 2004 Int. J. Mod. Phys. E 13 867
[32] Korol A V, Solov’yov A V and Greiner W 2005 Topics in Heavy Ion Physics—Proc. Memorial Symp. for Gerhard Soff (Frankfurt am Main, Germany, 25–28 April) ed W Greiner and J Reinhardt (Budapest: EP Systema) pp 73–86
[33] Tabrizi M, Korol A V, Solov’yov A V and Greiner W 2007 Phys. Rev. Lett. 98 164801
[34] Bellucci S et al 2006 Phys. Rev. ST Accel. Beams 9 013501
[35] Strokov S et al 2007 J. Phys. Soc. Japan 76 064007
[36] Arduini G et al 1998 Phys. Rev. ST Accel. Beams 11 063501
[37] Uggerhøj E and Uggerhøj U I 2005 Nucl. Instrum. Methods B 234 31
[38] Bellucci S et al 2006 Nucl. Instrum. Methods B 252 3
[39] Strokov S et al 2006 Nucl. Instrum. Methods B 252 16
[40] Scandale W et al 2009 Phys. Rev. A 79 012903
[41] Scandale W et al 2009 Phys. Lett. B 681 233
[42] Scandale W et al 2010 Phys. Lett. B 693 545
[43] Korol A V, Solov’yov A V and Greiner W 1998 J. Phys. G: Nucl. Part. Phys. 24 L45
[44] Korol A V, Solov’yov A V and Greiner W 1999 Int. J. Mod. Phys. E 8 49
[45] Korol A V, Solov’yov A V and Greiner W 2004 Int. J. Mod. Phys. E 13 867
[46] Korol A V, Solov’yov A V and Greiner W 2005 Topics in Heavy Ion Physics—Proc. Memorial Symp. for Gerhard Soff (Frankfurt am Main, Germany, 25–28 April) ed W Greiner and J Reinhardt (Budapest: EP Systema) pp 73–86
[47] Tabrizi M, Korol A V, Solov’yov A V and Greiner W 2007 Phys. Rev. Lett. 98 164801
[48] Bellucci S et al 2006 Phys. Rev. ST Accel. Beams 9 013501
[49] Strokov S et al 2007 J. Phys. Soc. Japan 76 064007
[50] Arduini G et al 1998 Phys. Rev. ST Accel. Beams 11 063501
[51] Uggerhøj E and Uggerhøj U I 2005 Nucl. Instrum. Methods B 234 31