Monte-Carlo Simulations of Electron Channelling a Bent (110) Channel in Silicon

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Abstract
Results obtained with a new Monte-Carlo code for the channelling of 855 MeV electrons along the crystallographic plane (110) in a bent Silicon crystal are presented. The definitions of the dechannelling length and the asymptotic acceptance of the channel are given in a form that is suitable for the Monte-Carlo procedure. The dependence of these quantities on the crystal bending is studied.

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1. Introduction
In this article we study the channelling of ultrarelativistic electrons in a bent planar channel using a new Monte-Carlo code.

Channelling takes place if charged particles enter a single crystal at small angle with respect to a major crystallographic direction: a plane or an axes \cite{1}. The particles get confined by the electrostatic potential of the crystal and move preferably along the corresponding crystallographic planes or axes following their shape. This phenomenon has been intensively studied since the Sixties of the last century. Recently, practical applications of channelling have been inducing growing interest in the scientific community.

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In particular, the crystals with bent crystallographic planes are used to steer high-energy charged particle beams replacing huge dipole magnets. Since its appearance \[2\] and first experimental verification \[3\] this idea has been attracting a lot of interest worldwide. Bent crystals have been routinely used for beam extraction and deflection in the Institute for High Energy Physics, Russia \[4\]. A series of experiments on the bent crystal deflection of proton and heavy ion beams were performed \[5, 6, 7, 8, 9\]. The bent crystal method has been proposed to extract particles from the beam halo at CERN’s Large Hadron Collider \[10\]. The possibility of deflecting positron \[11\] and electron \[9, 12, 13\] beams has been studied as well.

Another very promising application of the channelling phenomenon is the crystalline undulator, — 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 was demonstrated theoretically a decade ago \[14, 15\] (further developments as well as historical references are reviewed in \[16\]). The advantage of the crystalline undulator is the 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 of a crystalline undulator very short (up to several microns) and, therefore, the wavelength of the produced radiation can reach the (sub)picometer range, where conventional sources with comparable intensity are unavailable \[17\].

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 then 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 \[18, 19\]. 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 dechanneling 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 easier 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.

To develop a comprehensive theory of the crystalline undulator, one has to understand the behaviour of the electron in a bent crystal channel. To study this problem, we have developed a new Monte-Carlo code that allows us to simulate the particle channelling and analyse their trajectories. In contrast to other channelling codes [20, 21, 22], 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 the present paper, we restrict our analysis to channels with constant curvature. Our 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. Additionally, the results can be useful to developers of crystalline devices for extraction, bending and collimation of electron beams.

We study the channelling of 855 MeV electrons in a straight and bent single crystal of Silicon along the plane (110). This plane is chosen for the analysis because it can be deformed by growing of Si$_{1-x}$Ge$_x$ crystals [23] with a periodically varying Ge content $x$ [24, 25]. The electron energy corresponds to the conditions of the channelling experiments at Mainz Microtron (Germany) [26].

2. The Physical Model and the Simulation Algorithm

In this section we review the basic ideas of the physical model and the algorithm implemented in our Monte Carlo code. A more detailed description can be found in [27].

The model is intended for studying the interaction of ultrarelativistic projectiles with single crystals. Due to the high speed of the projectile, its interaction time with a crystal atom is very short. The motion of the atomic electrons as well as the thermal motion of the atomic nuclei during the interaction time can be neglected. Therefore, the crystal is represented as a collection of static charges. 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 is approximated by a three dimensional normal distribution with the variance equal to the squared
amplitude of thermal vibrations of the crystal atoms $a(T)$. We used the value $a(T) = 0.075 \, \text{Å}$ in our calculations, which corresponds to the room temperature \[28\]. The probability distributions of the electrons, given by squared absolute value of the wave function of the atom. Instead of the exact wavefunction, we use a spherical symmetric distribution that on average reproduces the electrostatic potential of the atom in Molière’s approximation \[29\].

The code performs 3D simulation of the projectile motion in the crystal. The coordinate frame is defined in such a way that the axis $z$ coincides with the beam direction. The plane (110) of the crystal is parallel to the coordinate plane $(xz)$ and, consequently, it is orthogonal to the axis $y$. The interaction of the projectile with a crystal constituents is considered as a classical scattering in a Coulomb field of a static point-like charge. The trajectory of the projectile is modelled using the following algorithm. The particle moves along straight line segments between the points where its projection on the axis $z$ coincides with the $z$ coordinate of a crystal constituent: an electron or a nucleus. At this point the transverse momentum of the projectile is changed by the quantity

$$
\Delta p_\perp = -q_p q_t \frac{\vec{r}_\perp}{v r_\perp^2}.
$$

Here $q_p$ and $q_t$ are electric charges of the projectile and the target constituent, respectively, $\vec{r}_\perp$ is the vector connecting the projectile and the target constituent (it is parallel to the axis $(xy)$), $v \approx c$ is the projectile speed. Then the projectile is propagated further along a straight line segment until its $z$ coordinates coincides with that of the next crystal constituent and a new modification of the momentum is performed. The ionization losses of high energy electrons or positrons in matter are very small \[30\]. The radiation losses become noticeable starting from the projectile energies of several tens GeV. In our calculations they are also neglected. Therefore, the absolute value of the projectile momentum remains unchanged during the simulation.

A crystal constituent is taken into account if it belongs to the lattice node located within a cylinder of the radius $40a_{TF}$ around the particle ($a_{TF}$ is the Thomas-Fermi radius of the atom). 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 $\Delta z_c$ is approximately $200 \, \text{Å}$. 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 result, the cylinders form a ‘pipe’ filled by the crystal lattice and the particle channels inside it.

In the case of a bent crystal with channel shape defined by the function \( y_B(z) \), the above procedure is modified in the following way. If \((x_p, y_p, z_p)\) are the coordinates of the projectile, and \((x_c, y_c, z_c)\) is the endpoint of the cylinder axis: \( z_c = z_p + \Delta z_c, x_c = x_p + \Delta z_c p_x/p_z, \) and \( y_c = y_p + \Delta z_c p_y/p_z \). First, an undistorted lattice is built around the straight line segment connecting the points \((x_p, y_p - y_B(z_p), z_p)\) and \((x_c, y_c - y_B(z_c), z_c)\). Then each lattice node is shifted according to the bending profile: \((x_n, y_n, z_n) \rightarrow (x_n, y_n + y_B(z_n), z_n)\). As a result, the trajectory becomes surrounded by a ‘pipe’ filled by the bent crystal lattice.

It is convenient to characterise the curvature of the bent crystal by the centrifugal parameter \( C \). Let \( U(\nu) \) be the potential energy of the projectile in the field of crystal constituents averaged over the surface \( y = \nu + y_B(z) \). Then the centrifugal parameter is defined as

\[
C = \frac{F_{c.f.}}{U'_{\text{max}}}.
\] (2)

Here \( F_{c.f.} \) is the centrifugal force acting on the projectile in the bent channel and \( U'_{\text{max}} \) is the maximum derivative of the average potential energy with respect to \( \nu \), i.e. the maximum force acting on the projectile in the average potential. The value \( C = 0 \) corresponds to the straight crystal and \( C = 1 \) is the critical value at which the potential barriers between the crystal channels disappears.

The centrifugal force is related to the projectile energy \( E \) and to the bending radius \( R_C \) via \( F_{c.f.} = E/R_C \). Therefore, expression (2) can be rewritten as

\[
C = \frac{E}{R_C U'_{\text{max}}}.
\] (3)

In the case of a channel with a constant bending radius, the shape is defined by the equation

\[
y_B(z) = R_C - \sqrt{R_C^2 - z^2}.
\] (4)

The channel boundaries for a straight crystal are defined as the planes satisfying the equation \( y = y_{\text{top}}^{(n)} \), where \( y_{\text{top}}^{(n)} \) is the coordinate of the potential
energy maximum between the \(n\)-th and \((n + 1)\)-st channel. For \(C \neq 0\) these planes become bent surfaces following the shape of the channel:

\[
y = y_{\text{top}}^{(n)} + y_B(z).
\]  

(5)

In this case, the channel boundaries do not coincide with the maxima of the potential energy which is modified by centrifugal effects (see figure 1).

3. Simulations

The calculations were performed for \(E=855\) MeV electrons channelling along the plane (110) for twelve different values of \(C\) in the range from 0 to 1.

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. The simulation of the trajectory was terminated if the particle went through the crystal, \(z > L_{\text{cr}}\) (\(L_{\text{cr}}\) is the crystal dimensions along the beam direction), or if the deviation of the projectile from its initial direction became too large: \(|\vec{p}_\perp|/p_z > 100/\gamma\) (here \(p_\perp\) and \(p\) are respectively the transverse and the longitudinal momenta and \(\gamma\) is the Lorentz factor of the projectile.)

Then the simulated trajectories were analysed and the segments corresponding to channelling and dechannelling mode were determined. At the entrance point of the crystal, the projectile was assumed to be in the channelling mode. Regardless of the value of its transverse energy, the particle was considered to be channelling until it crossed the channel boundary (5).

The crystal dimensions along the beam direction was \(L_{\text{cr}} = 120\ \mu\text{m}\) for a straight channel. For nonzero \(C\), \(L_{\text{cr}}\) was chosen so that very few or no particle remain in the channelling mode at the exit from the crystal. The number of the simulated trajectories was 100000 for the straight channel and 25000 for each nonzero value of \(C\).

4. Definition of the Dechannelling Length and the Asymptotic Acceptance of the Channel

To make a quantitative assessment of the particle dechannelling process, one needs a definition of the dechannelling length that would be suitable for the Monte Carlo approach.
Figure 1: The average potential energy of the projectile in the field of the crystal planes modified by the centrifugal effects. The centrifugal parameter $C$ is defined by equation (2).
Let $z_{d1}$ be the point of the first the channel boundary by the projectile. We define the quantity $N_{\text{ch0}}(z)$ as the number of trajectories 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 dechanneling point:

$$L(z) = \frac{\sum_{k=1}^{N_{\text{ch0}}(z)} (z_{d1}^{(k)} - z)}{N_{\text{ch0}}(z)}.$$  \hspace{1cm} (6)

The sum in the numerator of 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 the 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 [31]), one can obtain the following expression for $N_{\text{ch0}}(z)$

$$N_{\text{ch0}}(z) = N_0 \sum_{j=1}^{\infty} A_j \exp \left( -z/L_j \right).$$  \hspace{1cm} (7)

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 dechanneling length $L_d$ is defined as the largest of the parameters $L_j$ in (7). The corresponding term dominates the asymptotic behaviour at $z \gtrsim L_d$:

$$N_{\text{ch0}}(z) \approx N_0 A_d \exp \left( -z/L_d \right).$$  \hspace{1cm} (8)

The expression (6) for $L(z)$ has the following counterpart in the kinetic theory

$$L(z) = \frac{1}{N_{\text{ch0}}(z)} \int_z^\infty dz_{d1} (z_{d1} - z) \frac{N_{\text{ch0}}(z_{d1})}{dz_{d1}}.$$  \hspace{1cm} (9)

Substituting (5) into (9) 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 [31] for positively charged projectile in harmonic potential approximation, the exponential asymptotic behaviour of $N_{\text{ch0}}(z)$, and, consequently, a constant asymptotic value of $L(z)$
is a more general result. As it will be shown in the next section, our simula-
tions demonstrate that it is also valid for electrons.

Hence, in our Monte Carlo procedure the dechannelling length \( L_d \) is de-
fined as the asymptotic value of \( L(z) \) \((\ref{eq:6})\) in the region where it ceases to depend on \( z \).

Due to the exponential asymptote \((\ref{eq:8})\), the quantity

\[
A(z) = \frac{N_{\text{ch}0}(z)}{N_0} \exp \left(\frac{z}{L_d}\right)
\]

should approach a constant value \( A_d \) at sufficiently large \( z \). We shall call the quantity \( A_d \) the \textit{asymptotic acceptance} of the channel. The asymptotic acceptance depends on the initial transverse momentum distribution of the particles in the beam.

5. Analysis of the Results

The ratio \( \frac{N_{\text{ch}0}(z)}{N_0} \) of the particle that never crossed the channel bound-
ary is shown in Figure 2 as function of \( z \) for several values of \( C \). This fraction

![Figure 2: Fraction \( \frac{N_{\text{ch}0}(z)}{N_0} \) of the particles that stay in the same channel from their entrance into the crystal for different values of the centrifugal parameter \( C \) as function of the penetration depth \( z \). The dashed lines show the corresponding exponential asymptotes \( \propto \exp(-z/L_d) \).](image-url)
decreases rather fast and, as it was expected, has an exponential asymptotic behaviour.

The quantity $L(z)$ for the same values of the centrifugal parameter are plotted in figure 3. Indeed, $L(z)$ becomes constant (within the statistical errors) at large $z$ corresponding to exponential behaviour of the curves of figure 2. The asymptotic value for the straight channel is $L_d(C = 0) = 8.464 \pm 0.057 \mu m$.

The dependence of the ratio $L_d(C)/L_d(C = 0)$ on the centrifugal parameter is shown in figure 4.

Surprisingly, the dechannelling length remains nonzero even at $C = 1$, where the potential barriers between the channels disappear and therefore the transverse motion of the particle is no more constrained by the interplanar potential. The reason of such behaviour is likely the random scattering of the particles by the crystal constituents. There is a nonzero probability that the projectiles is scattered in such a way that it trajectory remains within the channel boundaries (5). The fraction of such particles decreases exponentially. Therefore, the curve for $C = 1$ in figure 3 behaves in a similar way as the for $C < 1$ having a constant asymptote, which corresponds to a

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure3.png}
\caption{The quantity $L(z)$ that becomes equal to the dechannelling length at large penetration depth $z$. The thin lines show the statistical errors. The straight dashed lines correspond to the asymptotic values.}
\end{figure}
Figure 4: The ratio $L_d(C)/L_d(C = 0)$ of the dechannelling length in bent channels to the one in the straight channels as function of the centrifugal parameter $C$. At $C < 0.3$ the ratio can be parametrised by the function $(1 - C)^{2.9}$ (shown by the solid line). For comparison, the behaviour $(1 - C)^2$ obtained in the diffusion theory in the parabolic potential approximation is shown by the dashed line.
nonzero dechannelling length.

It is seen from figure 4 that the ratio \(L_d(C)/L_d(C = 0)\) follows the law \((1 - C)^{2.9}\) for \(C < 0.3\). At \(C > 0.3\), it decreases less steeply. This can be interpreted as the effect of the random scattering that becomes comparable to the guiding effect of the interplanar potential at \(C \approx 0.3\).

The quantity \(A(z)\) defined by (10) is plotted in figure 5. This quantity indeed approaches a constant value in the same region of \(z\) where the quantity \(L(z)\) does. This value is by definition the asymptotic acceptance \(A_d\) of the channel for an ideally parallel beam. For a straight channel, the value \(A_d(C = 0) = 0.95 \pm 0.01\) is obtained.

![Figure 5: The quantity A(z) that becomes equal to the asymptotic acceptance of the channel at large penetration depth z. The thin lines show the statistical errors. The straight dashed lines correspond to the asymptotic values A_d.](image)

The dependence of the ratio \(A_d(C)/A_d(C = 0)\) on the centrifugal parameter is shown in figure 6. It is seen that the behaviour of the ratio is changed at \(C = 0.3\): it falls as \((1 - C)^2\) at \(0.1 < C < 0.3\) then becomes nearly constant at \(0.3 \leq C \leq 0.9\). Then it jumps up at \(C = 1\). At very small \(C\), the behaviour is close to \(1 - C\) law, which coincides with the one obtained in the diffusion approach for a parabolic potential.
Figure 6: The ratio $A_d(C)/A_d(C = 0)$ of the asymptotic acceptance of bent channels to the one in the straight channel as function of the centrifugal parameter $C$. At $0.1 < C < 0.3$ the ratio can be parametrised by the function $(1 - C)^2$ (shown by the solid line). For comparison, the behaviour $(1 - C)$ obtained in the diffusion theory in the parabolic potential approximation is shown by the dashed line.
6. Conclusion and Discussion

We presented the Monte-Carlo study of electron channelling in the (110) channel of a bent Silicon crystal. The calculation were done for the beam energy of 855 MeV for several value of the centrifugal parameter.

According to our simulation, the number of channelling electrons rapidly decreases with the penetration depth $z$ and quickly approaches an exponential asymptote. Similar behaviour was previously seen in the kinetic theory of channelling in the case of positively charged projectile.

We formulated definitions of the dechannelling length $L_d$ and the asymptotic acceptance of the channel $A_d$ that are suitable for application within the Monte Carlo approach. Our definition is consistent with the one previously used in the kinetic theory of channelling.

We calculated the dechannelling length for the set of values of the centrifugal parameter. The dechannelling length decreases as $(1 - C)^{2.9}$ at $0 < C < 0.3$. At larger $C$ the guiding effect of the channel becomes so weak that the random diffusion of the particles along the bent channel is comparable to channelling effect. This results into the change of the behaviour of $L_d(C)$. Similarly, the behaviour of the asymptotic acceptance $A_d(C)$ changes at $C = 0.3$ from $(1 - C)^2$ decreasing to nearly constant and then increasing behaviour.

The obtained result can be used for choosing the optimum bending of the crystals used for deflection and collimation of electron beams.

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