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Planar channeling of electrons: Numerical analysis and theory

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Summary. — Monte Carlo results on electron channeling in silicon are presented. The simulation has been done with a new computer code that takes into account the detailed atomic structure of the crystal. The dechanneling lengths for (100), (110) and (111) crystallographic planes are estimated. The calculated dependence of the intensity of the channeling radiation on the crystal length demonstrats a good agreement with recent experimental data.

PACS 61.85.+p – Channeling phenomena (blocking, energy loss, etc.).
PACS 02.70.Uu – Applications of Monte Carlo methods.

1. – Introduction

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

Channeling phenomenon [1] finds growing application in experimental high energy physics. 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 crystal have been routinely used for beam extraction in the Institute for High Energy Physics, Russia [4]. Series of experiment on the bent crystal deflection of proton and heavy ion beams were performed at different accelerators [5-9] throughout the world. The bent crystal method has been proposed to extract particles from the beam halo at CERN Large Hadron Collider [10]. The possibility to deflect positron [11] and electron [9, 12, 13] beams has been studied as well.

Another very promising application of the channeling phenomenon is a novel source of hard electromagnetic radiation. A single crystal with periodically bent crystallographic planes can force channeling particles to move along nearly sinusoidal trajectories and radiate in hard–X- and gamma-ray frequency range. The feasibility of such a device, known

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as the "crystalline undulator", was demonstrated theoretically a decade ago [14, 15] (further developments as well as historical references are reviewed in [16]).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 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 to make the period λ_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 $\lambda \sim \lambda_u/(2\gamma^2)$ ($\gamma \sim 10^3$–10^4 being the Lorentz factor of the particle) 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 channeling regime.

More recently, an electron based crystalline undulator has been proposed [18]. On the 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 channeling. 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.

There is another reason why electron channeling needs a thorough analysis. This is the disagreement between theory and experimental data. For example, the Baier-Katkov-Strakhovenko formula for the dechanneling length (equation (10.1) in [19]), L_d, predicts $L_d = 23\,\mu$m for 1.2 GeV electrons in Si (110) planar channel, while the measured value is $L_d = 28\,\mu$m [20].

For lower energies, the discrepancy is much more dramatic: $L_d = 6.7\,\mu$m calculated *vs.* $L_d = 31\,\mu$m measured [21] and $L_d \approx 1\,\mu$m calculated *vs.* $L_d = 36\,\mu$m measured [22] for electron energies 350 MeV and 54 MeV, respectively.

Clearly, further theoretical and experimental investigations of the electron channeling are necessary (see also [23]).

We developed a new Monte Carlo code that allows to simulate the particle channeling and calculate the emitted radiation. In contrast to other channeling codes [24-26], 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 channeling of 855 MeV electrons in a straight single crystal of silicon along three different crystallographic planes: (100), (110) and (111). The parameters of the simulation correspond to the conditions of the channeling experiments at Mainz Microtron (Germany) [27]. To verify our results, we calculated the dependence of the intensity of the channeling radiation on the crystal dimension along the beam direction and compared to the experimental data.

2. – The underlying physical model

Our model is intended for studying the interaction of ultrarelativistic projectiles with single crystals. Due to a high speed of the projectile, its interaction time with a crystal atom is much smaller than a typical atomic time, so that the motion of the atomic electrons during the interaction can be neglected. As a result, the projectile "sees" a "snapshot" of the atom: the atomic electrons are seen as point-like charges at fixed positions.

The probability density to find the atomic electrons at positions $\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_Z$ (Z is the atomic number) is given by squared absolute value of the wave function of the atom, $w(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_Z) = |\psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_Z)|^2$. In the code we approximate w by a spherical symmetric probability distribution which on average reproduces the electrostatic potential of the atom within Molière's approximation [28].

The interaction of a projectile with electric charge q_p with an atomic constituent is considered as a classical scattering of q_p in the Coulomb field of a static point-like charge q_t. In the course of the collision the projectile, which initially moves with velocity $\mathbf{v}$ along the z-axis, acquires a transverse momentum $\Delta\mathbf{p}_\perp$ equal to

$$\Delta\mathbf{p}_\perp = -\frac{q_\mathrm{p} q_\mathrm{t}}{v}\,\frac{\mathbf{r}_\perp}{r_\perp^2}\,, \tag{1}$$

where $\mathbf{r}_\perp$ is the projection of the vector connecting q_t and q_p onto the (xy)-plane.

The total transverse momentum acquired by the projectile in collision with the atom is a vector sum of (1) over all atomic charges q_t. 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. Such an assumption is applicable to high energy electrons and positrons whose ionization energy losses in matter are much smaller than the radiative losses (see, for example, Figure 27.10 in [29]).

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.

3. – Simulations

The calculations were performed for $E = 855\,\mathrm{MeV}$ electron channeling in Si crystal along the (100), (110) and (111) crystallographic planes.

At the crystal entrance 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 using uniform distribution along the channel width. The trajectory of the particle was simulated using the "snapshot" model described in the previous section. The simulation of a trajectory was carried out over the whole length of the crystal, *i.e.* for $0 \le z \le L_\mathrm{cr}$, unless the deviation of the projectile from its initial direction became too large: $p_\perp/p > 100/\gamma$.

Each simulated trajectory was analyzed to determine the segments corresponding to the channeling and dechanneling regime. The particle was considered to be in the

channeling regime if it changed the direction of the y component of its velocity two or more times without crossing the channel boundaries, *i.e.* if it made at least one complete channeling oscillation. After crossing the boundary of the channel, the particle was considered to be dechanneled until it performed another full channeling oscillation or until terminating the simulation of the trajectory.

The number of trajectories simulated for the analysis of the dechanneling process was 40000, 30000 and 28000 for planar channels (111), (110) and (100), respectively. The chosen crystal length $L_{\rm cr} = 270.4\,\mu$m is equal to the maximum length used in recent channeling experiments [27].

Channeling radiation was calculated for the plane (110) and for the "amorphous" orientation (*i.e.* for a crystal oriented randomly avoiding major crystal directions) and for seven different values of $L_{\rm cr}$ ranging from $7.9\,\mu$m to $270.4\,\mu$m. In each case 50000 trajectories were simulated.

4. – Dechanneling length within the Monte Carlo approach

To make a quantitative assessment of the dechanneling process one needs a proper definition of the dechanneling length consistent with the Monte Carlo approach.

Let $z_{\rm d1}$ be the point where the projectile particle dechannels for the first time. Let us define the function $N_{\rm ch0}(z)$ as the number of particles for which $z_{\rm d1} > z$. In other words, $N_{\rm ch0}(z)$ is the number of particles which move up to the point z in the channeling regime and dechannel in some further point. Then, the average distance $L(z)$ from the point z to the first dechanneling point can be defined as follows:

$$L(z) = \frac{\sum_{k=1}^{N_{\rm ch0}(z)} \left(z_{\rm d1}^{(k)} - z\right)}{N_{\rm ch0}(z)}\,. \tag{2}$$

The sum is carried out over the particles with $z_{\rm d1} > z$.

Generally speaking, $L(z)$ depends not only on z, but also on the angular distribution of the particles at the crystal entrance. Nonetheless, as will be shown below, the kinetic theory of channeling 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, *e.g.*, eq. (1.38) in [30]) one can obtain the following expression for $N_{\rm ch0}(z)$:

$$N_{\rm ch0}(z) = N_0 \sum_{j=1}^{\infty} a_j \exp[-z/L_j]. \tag{3}$$

Here only coefficients a_j depend on the initial 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 $L_{\rm d}$ is defined as the largest of the parameters L_j in (3). The corresponding term dominates the asymptotic behaviour as $z \gtrsim L_{\rm d}$:

$$N_{\rm ch0}(z) \asymp N_0 a_d \exp[-z/L_{\rm d}]. \tag{4}$$

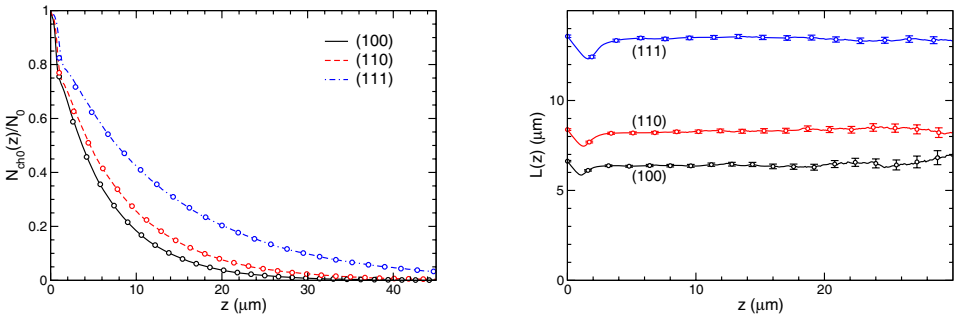

Fig. 1. – Left panel: fraction $N_{\rm ch0}(z)/N_0$ of the particles staying in the same channel as the one at the entrance into the crystal calculated for three planar channels as a function of the penetration depth z. Lines: the results of Monte Carlo simulations. Open circles: the asymptotes $\propto \exp[-z/L_{\rm d}]$ with the $L_{\rm d}$ values listed in table I. Right panel: the function $L(z)$ (see eq. (2)) which becomes equal to the dechanneling length at large penetration depths z. Open circles with error bars mark the statistical errors.

Expression (2) for $L(z)$ has the following counterpart in the kinetic theory:

$$L(z) = -\frac{1}{N_{\rm ch0}(z)} \int_z^\infty {\rm d}z_{\rm d1}(z_{\rm d1} - z) \frac{N_{\rm ch0}}{{\rm d}z_{\rm d1}}. \tag{5}$$

The substitution of (4) into (5) demonstrates that, indeed, the coefficient a_d cancels out and $L(z)$ becomes equal to $L_{\rm d}$ in the asymptotic region.

Although in [30] the diffusion equation was solved for a positively charged projectile and in the harmonic potential approximation, the exponential asymptotic behaviour of $N_{\rm ch0}(z)$, and, consequently, a constant asymptotic value of $L(z)$ is a more general result. As will be shown in the next section, our simulations demonstrate that it is also valid for projectile electrons.

Hence, within the Monte Carlo procedure the dechanneling length $L_{\rm d}$ is defined as the asymptotic value of $L(z)$ in the region where it is independent of z.

5. – Results of simulation and their analysis

The ratio $N_{\rm ch0}(z)/N_0$ as a function of z is shown in fig. 1 (left panel) for three different Si crystal channels. This ratio decreases rather fast and, as was expected, has an exponential asymptotic behaviour.

The function $L(z)$ (see (2)) calculated for the same channels is plotted in fig. 1 (right panel). As mentioned, $L(z)$ becomes constant (within statistical errors) at large z corresponding to exponential behaviour of the curves shown in left panel of fig. 1. The asymptotic values, $L_{\rm d}$, are listed in table I.

To calculate the dependences presented in fig. 1 only those particles were accounted for which remained in the channeling regime from the entrance to the crystal. The fraction of these particles rapidly decreases with z.

In contrast, the fraction $N_{\rm ich}(z)/N_0$ of the particles which are in the channeling regime at the point z regardless of their previous channeling status decreases rather slowly

TABLE I. – *Monte Carlo results for the dechanneling length L_d for three different crystal channels.*

Crystal plane	Dechanneling length (μm)
(111)	13.57 ± 0.12
(110)	8.26 ± 0.08
(100)	6.38 ± 0.07

(see the left panel of fig. 2). This is due to the rechanneling process. Random collisions with the crystal constituents can reduce the transverse energy. As a result, a dechanneled particle can return to the channeling regime.

The asymptotic behaviour of the curves in the left panel of fig. 2 can be explained using the following arguments. At sufficiently large z, the distribution of the dechanneled 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:

$$w(p_y) = \frac{1}{\sqrt{2\pi}\sigma(z)} \exp\left[-\frac{p_y^2}{2\sigma^2(z)}\right] \tag{6}$$

with the variance proportional to z: $\sigma^2(z) \propto z$. The rechanneling is dominated by the phase space density in the vicinity of $p_y = 0$. The density is $1/\sigma(z) \propto 1/\sqrt{z}$ and governs the asymptotic behaviour of the fraction of the channeling particles shown in fig. 2 (left panel).

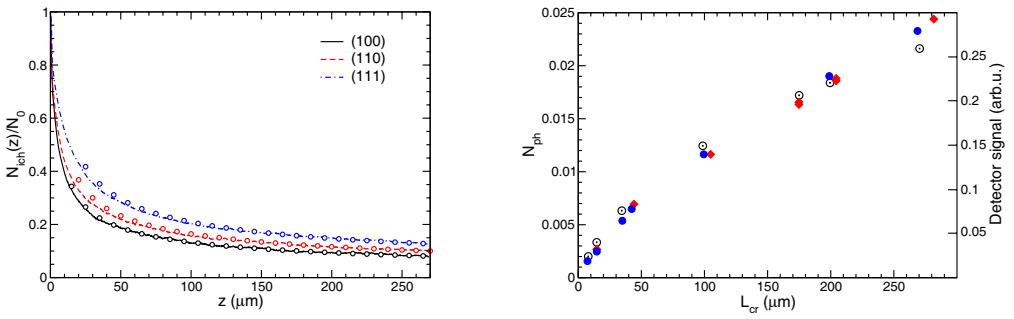

Fig. 2. – Left panel: the fraction of channeling particles as a function of penetration depth z for the indicated crystal channels. Lines: the results of Monte Carlo simulations. Open circles: the corresponding asymptotes $\propto z^{-1/2}$. Right panel: channeling radiation as a function of crystal length. The filled symbols are experimental data [27], the open cycles are results of our calculations. The left vertical axis shows the number of emitted photons per projectile within the energy interval $0.4\,\text{MeV} < \hbar\omega < 9.0\,\text{MeV}$. The right vertical axis is calibrated in arbitrary units used in the experimental paper.

6. – Comparison with the experiment

Experimentally, the dechanneling length cannot be measured directly since it is not possible to distinguish between the particles which move in channeling regime all the way from the entrance point from the rechanneled particles. Only the signals related to the total number of channeling particles can be measured. Extracting the dechanneling length from these data involves a model-dependent procedure. Therefore, comparing the L_{d} values obtained in Monte Carlo simulations to the estimations found in the experimental papers 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 the calculation of the quantities which can be directly measured in an experiment. This will allow one a direct comparison with the experimental data.

In the recent experiment at Mainz Microtron [27] the intensity of channeling radiation was measured for several crystal samples of different length L_{cr} along the beam. To make a comparison with these data, we modeled the Mainz experiment with our code.

The average number of photons in the energy interval $0.4\,\mathrm{MeV} < \hbar\omega < 9.0\,\mathrm{MeV}$ was calculated for a 855 MeV electron moving through a Si crystal with the plane (110) oriented along the electron beam. Then, the background was subtracted, *i.e.* the same quantity but calculated for a randomly oriented Si crystal. The photons were taken emitted within the cone with the angle $\theta \leq 1.31\,\mathrm{mrad}$ with respect to the beam direction. This value corresponds to the aperture of the gamma spectrometer used in the experimental setup. The calculations were performed for different values of L_{cr}.

The intensity of the channeling radiation is presented in [27] in arbitrary units. We equated 12 arbitrary unit to 1 photon per projectile to adjust the overall scale. The results are shown in fig. 2 (right panel). As is seen, our results demonstrate reasonable agreement with the experiment, which proves the reliability of the code.

7. – Conclusion and outlook

We have presented our results obtained with a new Monte Carlo code for modeling of channeling of ultrarelativistic charged particles in crystals. The calculations were performed for 855 MeV electrons channeling in single Si crystal (100), (110) and (111) crystallographic planes.

According to our simulation, if rechanneling is disregarded, the number of channeling electrons rapidly decreases with the penetration depth z and quickly approaches the exponential asymptote. Similar behaviour follows from the kinetic theory of channeling.

The definition of the dechanneling length L_{d} is formulated suitable for application within the Monte Carlo approach. The definition is consistent with that used previously in the framework of kinetic theory of channeling.

The calculated values of L_{d} for (100), (110) and (111) planar channels in Si lie in the $10\,\mu$m range.

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

To verify the code, we calculated the intensity of the channeling radiation and compared the result with the experimental data [27]. A good agreement has been observed.

This confirms that the code is a reliable tool for modeling the channeling of ultrarelativistic charged particles.

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