On Moderate Energy Electron Dechanneling in Thick Si Crystals

O.V. Bogdanov\textsuperscript{1}, and S.B. Dabagov\textsuperscript{2,3}

\textsuperscript{1}Tomsk Polytechnic University, Lenin Ave. 30, Tomsk, 634050 Russia
\textsuperscript{2}INFN Laboratori Nazionali di Frascati, Via E. Fermi 40, I-00044 Frascati (RM), Italy
\textsuperscript{3}PN Lebedev Physical Institute, Leninsky pr. 53, 119991 Moscow, Russia

Abstract

A model of planar channeling of 400 MeV electrons taking into account the dechanneling processes in a crystal is developed. The dynamics of the initial angular distribution of relativistic electrons as a function of standard deviation has been studied. The simulation results for the density function of channeled projectiles distribution in a thick Si (111) crystal are presented.

PACS: 61.85.+p
1 INTRODUCTION

Studies on electron interaction in solids under the channeling conditions is of continuous interests due to its ability to produce electromagnetic radiation well-known as channeling radiation. This type of radiation is characterized by high monochromaticity and intensity; moreover, such sources are tunable within broad energy spectrum. The radiation sources based on positron channeling might be very powerful because of the large dechanneling length for positrons in comparison with the beams of electrons. However, till now there is uncertainty in calculations of channeling processes for moderate energies [1].

General features of electron/positron channeling radiation at moderate energies have been recently analyzed without details of the beam dechanneling [2]. As known at the energies higher then 100-150 MeV the description of electron/positron channeling in crystals can be done within the classical approximation; the motion is characterized by the particle trajectories, which the projectiles form within the continuous potentials of crystal planes or axes at either planar channeling or axial channeling, respectively. However, the motion under the channeling regime is rather unstable due to the strong scattering processes caused by various interactions in a crystal (the perturbations by thermal atomic vibrations, electron subsystem, etc.). That is why in order to calculate the radiation intensity we have to know the transverse particle distribution in the field of continuous potential, in other words, we have to solve the diffusion equation for the beam. For light relativistic projectiles the typical diffusion equation is reduced in well-known Fokker-Planck equation [3].

In our work we have studied the dechanneling processes for electrons in a (111) Si crystal, based on the solution of Fokker-Planck equation [4, 5]. The dynamics of particle distribution density has been investigated in dependence on both energy and initial scattering distribution of electron beams. This method, combined with the theory developed in [6, 7], was used for calculating the radiation spectra for planar channeling of relativistic electrons and positrons in thick crystals.

2 POTENTIAL ENERGY OF ELECTRONS IN A SYSTEM OF SI (111) PLANES

In the case of (100) and (110) planar channeling in a diamond-like lattice, there are two types of solutions of the equation of motion. On the contrary, in the case of (111) planar channeling along double planes, there are three types of solutions for the transverse displacement and velocity, which depend on the relation between the angle of incidence into a crystal \( \theta_0 \) and the critical channeling angle \( \theta_c = \sqrt{2U_0/e} \), and on the height (or depth) of the internal potential barrier \( \Delta U = U_1 - U_0 \) (see, Fig. 1).

![Figure 1. Potential energy of electron in the system of double planes (111) in a Si crystal.](image)
Two of these solutions describe the motion of channeled (under-barrier) electrons, while the third one describes the motion of quasi-channeled (above-barrier) electrons.

Below we used the following classification for various types of the motion (Table 1): cd denotes the under-barrier motion along one of the two planes forming (111) continuous potential; cu denotes the under-barrier motion along two planes forming (111) planar channel; nc denotes the above-barrier motion in the one-dimensional periodic potential formed by periodic sequence of the potential shown in Fig. 1.

Table 1. Classification of trajectories type for planar electron channeling.

<table>
<thead>
<tr>
<th>Type of trajectory</th>
<th>Transverse energy</th>
<th>Period of motion</th>
</tr>
</thead>
<tbody>
<tr>
<td>cd</td>
<td>$-U_o \leq \varepsilon \leq -U_1$</td>
<td>$T_{cd}$</td>
</tr>
<tr>
<td>cu</td>
<td>$-U_1 \leq \varepsilon \leq 0$</td>
<td>$T_{cu}$</td>
</tr>
<tr>
<td>nc</td>
<td>$0 \leq \varepsilon$</td>
<td>$T_{nc}$</td>
</tr>
</tbody>
</table>

In accordance with three types of motion, we can define three groups of the periods of motion: cd and cu – for channeled (under-barrier) electrons, i.e. $T_{cd}$, and $T_{cu}$, and nc – for above-barrier electrons, $T_{nc}$ [6].

3 THE INITIAL ANGULAR DISTRIBUTIONS

We assume that the initial angular distribution of relativistic electrons in the beam satisfies the normal law (Gaussian distribution):

$$\Phi(\theta) = \frac{1}{\sqrt{2\pi}\sigma_y} \exp\left[-\frac{(\theta - \theta_0)^2}{2\sigma_y^2}\right]$$  \hspace{2cm} (1)

Here, $\theta_0$ is the angle of incidence of electron beam with respect to the channeling plane, $\sigma_y$ is the standard deviation.

Taking into account that for the particle of energy $E_0$ the transverse energy can be defined as

$$E_{\perp}(x) = \frac{E_0}{2} + U(x)$$ and, hence, $\theta(E_{\perp}) = \sqrt{\frac{2(E_{\perp} - U(x))}{E_0}}$,  \hspace{2cm} (2)

and that the number of particles with a given transverse energy is a positive value, the density distribution functions will be determined by the following integral

$$N_0(E_{\perp}) = \frac{1}{\sqrt{2\pi}\sigma_y}\int_{\theta(E_{\perp})}^{\theta_0} \frac{1}{\theta(E_{\perp})} \left[ \exp\left[-\frac{(\theta(E_{\perp}) - \theta_0)^2}{2\sigma_y^2}\right] + \exp\left[-\frac{(-\theta(E_{\perp}) - \theta_0)^2}{2\sigma_y^2}\right]\right] dx$$  \hspace{2cm} (3)
The points \( x_d, x_u \) correspond to the solutions of equation \( E_⊥ = U(x) \) for \( E_⊥/U_0 < 1 \), and \( x_u = d_p/2 \), \( x_d = -d_p/2 \) - for the \( E_⊥/U_0 \geq 1 \) case.

Fig. 2 shows the initial distribution at the parallel to channeling planes incidence \( \theta_0 = 0 \) for various incident beam divergences \( \sigma_y = 1/2 \theta_C \), \( \sigma_y = \theta_C \), \( \sigma_y = 1.5 \theta_C \). Obviously, due to the non-zero divergence, a part of the beam particles undergoes the above-barrier motion even \( \theta_0 = 0 \) (unlike a model with equal probability of the particles distribution over transverse energy where all particles get to the channel [6]).

![Figure 2](image-url)

**Figure 2.** The initial angular distributions of relativistic electrons channeled in Si (111) at zero incident angle \( \theta_0 = 0 \). Various curves correspond to different beam divergences: \( \sigma_y = 1/2 \theta_C \), \( \sigma_y = \theta_C \), \( \sigma_y = 1.5 \theta_C \).

## 4 FOKKER-PANCKE EQUATION FOR 400 MeV ELECTRONS CHANNELED IN Si (111)

Kinetic description of the channeling effect was first suggested by Lindhard using the equation of motion of the diffusion type (see in [3]). The Fokker-Planck equation in phase space of transverse coordinates and velocities to describe the channeling effect was first considered by Kitagava-Ohtsuki [4]. General expression of the Fokker-Planck equation is the following

\[
\frac{\partial F(z, E_⊥)}{\partial z} = \frac{\partial^2}{\partial E_⊥^2} \left[ D^{(2)}(E_⊥) F(z, E_⊥) \right] - \frac{\partial}{\partial E_⊥} \left[ D^{(1)}(E_⊥) F(z, E_⊥) \right],
\]

\[
\frac{\partial F(z, 0)}{\partial E_⊥} = 0, \quad \frac{\partial F(z, E_⊥, C)}{\partial E_⊥} = 0,
\]

in which the drift coefficient \( D^{(1)}(E_⊥) = \left\langle \frac{\Delta E_⊥}{\Delta z} \right\rangle_T \) is responsible for the mean transverse energy increase, and the term \( D^{(2)}(E_⊥) = \frac{1}{2} \left\langle \left( \frac{\Delta E_⊥}{\Delta z} \right)^2 \right\rangle_T = \left\langle 2 \frac{\Delta E_⊥}{\Delta z} (E_⊥ - U(x)) \right\rangle_T \) is the diffusion coefficient.
Drift and diffusion coefficients have been calculated within the Kitagava-Ohtsuki approximation [3] evaluating the integrals

\[ D^{(1)}_e(E_\perp) = N \int_{x_d}^{x} \frac{\exp(-x^2/2u_1^2)}{\theta(E_\perp,x)} \, dx \]  
(5)

and

\[ D^{(2)}_e(E_\perp) = N E \int_{x_d}^{x} \theta(E_\perp,x) \exp(-x^2/2u_1^2) \, dx \]  
(6)

where \( N = \frac{E_s^2}{2E_0X_0} \frac{4}{T(E_\perp)} \frac{d_p}{\sqrt{2\pi}u_1} \) is the function defined by both projectile and crystal parameters, with \( E_s = 13.6 \) MeV, \( E \) is the total electron energy, \( u_1 = 0.076 \) Å is the thermal transverse vibration amplitude of the plane atoms, the coordinates \( x_d, x_u \) are as above defined, \( X_0 \) is the characteristic radiation length of the crystal, for the (111) crystal planes the continuum potential depth and interplanar distance are \( U_0 = 21.21\) eV and \( d_p = 1.92 \) Å, respectively; the time parameter can be reduced from the solution of the equation of transverse motion:

\[ T(E_\perp) = \frac{E}{2c^2} \int_{x_d}^{x} \frac{dx}{\sqrt{E_\perp - U(x)}} \]  
(7)

where \( x_0 \) is defined by \( E_\perp = U(x_0) \) for \( E_\perp/U_0 < 1 \); \( x_0 = d_p/2 \) for \( E_\perp/U_0 \geq 1 \) case. Fig. 3 shows the dependence of time parameter on electron transverse energy.

![Figure 3](image-url)

**Figure 3.** Time parameter for planar electron channeling in a Si (111) crystal.

Taking into account the above mentioned conditions, the dependences on both drift and diffusion coefficients of the transverse energy are shown in Figs. 4, 5, respectively.
It should be underlined, that for $E_\perp = U_0$, for which the parameter diverges, the drift and the diffusion coefficients are characterized by deep minima. It takes place due to the fact that the probability electron density at the potential maximum is very high. Since the nuclear density in middle between the crystal planes is rather low (mainly negligible), also the scattering probability becomes small. That is why the kinetic coefficients have their minima at this point, in constant to the condition $E_\perp = 0$, which corresponds to the case of electron trajectory lies in a crystal plane. Obviously, on channeling plane the transverse energy increase reaches its maximum. For $E_\perp >> U_0$ the drift coefficient approaches the constant value for amorphous matter, since the continuous potential influences only very little the trajectory of an electron, while the diffusion coefficient increases linearly as function of $E_\perp$.

---

Fig. 4. Drift coefficient for planar electron channeling in a Si (111) crystal (E = 400 MeV).

Fig. 5. Diffusion coefficient for planar electron channeling in a Si (111) crystal (E = 400 MeV).

Fig. 6. Channeled electron density distribution for a Si (111) crystal at the deviation angle $\sigma_y = 0.5\theta_C$. 

Fig. 7. Channeled electron density distribution for a Si (111) crystal at the deviation angle \( \sigma_y = 1.5 \theta_c \).

Figs. 6 and 7 show the solution of the Fokker-Planck equation for various values of the standard deviation \( (\sigma_y = 0.5 \theta_c, \sigma_y = 1.5 \theta_c) \). The increase of standard angular deviation results in the broadening of density distribution function that takes place due to the redistribution of beam particles over the channel, i.e. continuous transition of the particles from channeling to above-barrier modes of the motion in a crystal.

5 CONCLUSIONS

In this work we have presented a model for the dual-channeling (111) of electrons in the crystal, taking into account the effects of dechanneling. The calculations were performed for 400 MeV electrons channeled in Si, including:

- Investigated the initial angular distribution of relativistic electrons in the beam as a function of transverse energy for various angles of entry to (111) planes of the crystal.
- Drift and diffusion coefficients channeling of electrons in the system of double planes (111) are constructed.
- The results of numerical solution Fokker-Planck equation for (111) planar channeling of 400 MeV electrons are presented.

ACKNOWLEDGEMENTS

This work was performed within the short-term visit grant of LNF INFN. The work is partially supported by the Russian Federal Agency of Education under contract No P2596.

REFERENCES

3. M.A. Kumakhov, and G. Shirmer, Atomic Collisions in Crystals, Moscow: Atomizdat,