Radiation Spectra of Channeled Electrons in Thick Si (111) Crystals

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Abstract. Dechanneling processes for electrons in a (111) Si crystal based on the solution of Fokker-Planck equation have been studied. The dynamics of particle distribution density has been investigated in dependence on both energy and initial scattering distribution of electron beams. The influence of dechanneling process on spectral intensity of channeling radiation for electrons in a crystal is investigated.

1. Introduction
Studies on relativistic electron/positron 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 both monochromaticity and intensity; moreover, such sources are tunable within broad energy spectrum. Due to the principal difference in interaction potentials at channeling for electrons and positrons, the radiation sources based on positron channeling might be much powerful for positrons because of the large dechanneling length in comparison with the beams of electrons. However, till now there is an uncertainty in calculations of dechanneling processes for moderate energies [1].

General features of electron/positron channeling radiation at moderate energies have been recently analyzed without the details of beam dechanneling [2]. As known at the energies higher then 100–150 MeV the description of electron/positron channeling in most of the crystals (or crystallographic directions) can be done within the classical approximation (Some details of the analysis for classical and quantum approximations at electron channeling for a specific crystal are presented in [3]), the motion is characterized by the particle trajectories, which the projectiles form within the continuous potentials of crystal planes or axes at either planar 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 beam both transverse-spatial and energy distributions 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 describing the kinetics of the beam evolution down the crystal can be reduced in well-known Fokker-Planck equation [3, 4].

Another solution approach to this problem based on the binary collisions method of simulations for the trajectories of channeled electrons in a crystal [5].

In our work we have studied the dechanneling processes for electrons in a (111) Si crystal, based on the solution of Fokker-Planck equation [6, 7]. The dynamics of particle distribution density has...
been investigated in dependence on energy as well as initial scattering distributions of electron beams. This method, combined with the theory developed in [8, 9], was used to calculate the radiation spectra at planar channeling of relativistic electrons and positrons in thick crystals.

2. Basics of the channeling motion

The electron motion in the channeling regime in a crystal is determined by the average potential of planes/axes that can be modeled within various well-known approximations [10, 11]. The potential energy for interaction of electrons with (100), (110) and (111) crystal planes in the transverse direction are given in figure 1. Herewith, the longitudinal motion of charged particles (down the crystal) is considered to be free.

![Figure 1. Potential energy of electron in the planes (100), (110), (111) Si crystals.](image)

At Si (100) and (110) electron channeling the motion of projectile can be distinguished as either under-barrier or above-barrier (for details, see in [11, 12]). However, for the case of Si (111) channeling, the motion becomes more complex, and we can define three various types of the electron motion [8]. The analysis below is done for this specific case, which is presently less studied.

The equation of transverse motion for a relativistic electron in the potential \( U(x) \) (averaged planar potentials of the main Si crystallographic directions are shown in figure 1) is described by classical equations

\[
\gamma m \ddot{x} = F = -\frac{\partial U(x)}{\partial x}, \quad \gamma = \frac{1}{\sqrt{1 - v^2/c^2}}.
\]

in the assumption of nonrelativistic transverse motion \( v_\perp \ll c \); \( v_\perp / c \ll 1 / \gamma \). For the initial conditions: the inlet point into the crystal \( x(0) = x_0 \), the transverse momentum of electron \( p_\perp(0) = p_\perp \theta_0 \), where \( \theta_0 \) is the incidence angle of an electron momentum with respect to the channeling planes, the transverse projectile energy in a crystal can be defined as follows

\[
\varepsilon_\perp = U(x) + \frac{p_\perp^2(0)}{2m} = U(x_0) + \frac{p_\perp^2 \theta_0^2}{2m},
\]

\[
p(0) = p_\perp(0) + p_\parallel(0)
\]

Depending on the ratio between \( \theta_0 \) and critical channeling angle \( \theta_c = \sqrt{2U_0/\varepsilon} \), as well as on the height of internal potential barrier \( \Delta U = U_0 - U_1 \) (figure 1), three solution types of Equation (1) could be resolved. As seen from figure 1 two solutions describing electron channeling in neighbor potential wells are of under-barrier origin, and the third solution describes electron quasichanneling for over-barrier motion.

3. Beam kinetics at channeling

Let assume that the initial angular distribution of relativistic electrons in the beam satisfies the normal law (known also as the Gaussian distribution):

\[
\frac{1}{\sqrt{2\pi \sigma^2}} e^{-x^2/2\sigma^2}
\]
Here, $\sigma_y$ is the standard deviation.

The relation for transverse energy of a particle with energy $E_0$: $E_{\perp}(x) = \frac{E_0 \theta^2}{2} + U(x)$ defines, as known, the angular dependence of the projectiles at channeling

$$\theta(E_{\perp}) = \sqrt{\frac{2(E_{\perp} - U(x))}{E_0}},$$

(4)

Hence, the projectile density distribution function will be given by the following integral

$$F_{0}(E_{\perp}) = \frac{1}{\sqrt{2\pi\sigma_{E_{\perp}}^2}} \exp\left[-\frac{\theta(E_{\perp})^2}{2\sigma_{E_{\perp}}^2}\right] \exp\left[-\frac{-\theta(E_{\perp}) - \theta_0)^2}{2\sigma_{\theta}^2}\right] dx.$$  

(5)

The points $x_d, x_u$ correspond to the solutions of equation $E_{\perp} = U(x)$ for $E_{\perp}/E_0 < 1$, and $x_u = d_p/2, x_d = -d_p/2$ for the $E_{\perp}/E_0 \geq 1$ case.

Figure 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 particles undergoes the above-barrier motion even at $\theta_0 = 0$ (unlike a model with equal probability of the particles distribution over transverse energy where all particles get to the channel [8, 14]).

![Figure 2](image)

**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: $\sigma_y = 1/2\theta_C, \sigma_y = \theta_C, \sigma_y = 1.5\theta_C$.

The kinetic description of the channeling phenomenon was first suggested by Lindhard using the equation of motion of the diffusion type (see [3]). Successfully, Kitagawa and Ohtsuki have first reduced the diffusion at channeling to the solution of the Fokker-Planck equation in phase space of transverse coordinates and velocities [4]. General expression of the Fokker-Planck equation can be written in the following from

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

(6)

$$\frac{\partial F(z,0)}{\partial E_{\perp}} = 0, \quad \frac{\partial F(z,E_{\perp},c)}{\partial E_{\perp}} = 0,$$
in which the drift coefficient $D_{e}^{(1)}(E_{\perp}) = \frac{\Delta E_{\perp}}{\Delta z}$ is responsible for the mean transverse energy increase, while the term $D_{e}^{(2)}(E_{\perp}) = \frac{1}{2} \left( \frac{\Delta E_{\perp}^2}{\Delta z} \right)$ is the diffusion coefficient. The coefficients are averaged by the period of motion in a channel (The period of motion may vary in dependence of the motion type, above-barrier or under-barrier, with the difference factor of 2.).

Both drift and diffusion coefficients have been calculated within the Kitagava-Ohtsuki approximation [3] evaluating the integrals

$$D_{e}^{(1)}(E_{\perp}) \equiv \int_{x_{d}}^{x_{a}} \exp \left( -x^2/2u_{i}^2 \right) \frac{d}{\theta(E_{\perp}, x)} \, dx \quad (7)$$

and

$$D_{e}^{(2)}(E_{\perp}) \equiv \int_{x_{d}}^{x_{a}} \frac{d}{\theta(E_{\perp}, x)} \exp \left( -x^2/2u_{i}^2 \right) \, dx \quad (8)$$

where $N = \frac{E_{i}^2}{2E_{i}X_{0}} \frac{d_{p}}{T(E_{\perp}) \sqrt{2\pi}u_{i}}$ is the function defined by the projectile as well as crystal parameters, with $E_{i}$ is the total electron energy, $u_{i} = 0.076 \, \text{Å}$ is the thermal vibration amplitude, the coordinates $x_{d}, x_{a}$ 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 $U_{0} = 21.2 \, \text{eV}$ and $d_{p} = 1.92 \, \text{Å}$, respectively. The time parameter can be reduced from the solution of motion equation:

$$T(E_{\perp}) = \sqrt{\frac{E}{2c^2}} \int_{-x_{0}}^{x_{0}} \frac{dx}{\sqrt{E_{\perp} - U(x)}} \quad (9)$$

where $x_{0}$ is defined by $E_{\perp} = U(x_{0})$ at $E_{\perp}/U_{0} < 1$; and $x_{0} = d_{p}/2$ - at the case of $E_{\perp}/U_{0} \geq 1$.

Figure 3 shows the dependence of time parameter on electron transverse energy.

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

Taking into account the above mentioned conditions, the dependences of both drift and diffusion coefficients on transverse energy are shown in figure 4.
Figure 4. The drift (a) and diffusion (b) coefficients of electron at planar channeling in a Si (111) crystal.

It should be underlined that at transverse energy $E_{\perp} = U_0$, for which the time parameter has a singularity, both drift and diffusion coefficients are characterized by deep minima. It takes place due to the fact that the electron density (its probability) at the potential maximum is very high. Since the nuclear density in the mid-plane between the crystallographic planes is rather low (mainly negligible), the probability of projectile scattering on nuclei becomes small. That is why, kinetic coefficients reach their minima at that plane that is in contrast to the condition $E_{\perp} = 0$, for which electron appears at a crystal plane. For $E_{\perp} = 0$ 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 $E_{\perp}$.

Figure 5. Probability of electron density at planar channeling in a Si (111) crystal.
Figure 6. Electron dechanneling function for the case of Si (111) planar channeling.

\[ J(z, E_\perp) = -\frac{\partial}{\partial E_\perp} \left[ D_2(E_\perp) F(z, E_\perp) \right] + D_1(E_\perp) F(z, E_\perp) = J_{\text{diff}}(z, E_\perp) + J_{\text{drift}}(z, E_\perp) \]  

(10)

\[ L_d(z) = \frac{f_{\alpha\beta}(z)}{J_{\text{diff}}(z, E_\perp = U_0)} \]  

(11)

* is chosen from the condition that particle flux determined by the decrease of dechanneling function \( f_{\alpha\beta}(z) = \int F(z, E_\perp) dE_\perp \) in \( e \) times (figure 6): \( \frac{f_{\alpha\beta}(0)}{f_{\alpha\beta}(z)} = e \).

This definition for dechanneling length does not depend on standard deviations in angular distribution, thus becoming the channel characteristics. For 855 MeV electrons channeling in a Si (111) crystal the dechanneling length calculated by (11) equals to 18.8 µm.

### 4. Dependence of channeling radiation on beam-crystal parameters

As known the length-normalized radiation intensity of relativistic charged particles at channeling in crystals is defined by the following expression [12, 13]

\[ I_{\text{thin}} \frac{dW}{d\omega dz} = \frac{e^2 \tilde{\omega}}{c^4 T^2} \sum_{n=1}^{\infty} \Theta \left( 1 - \frac{\omega T}{4 \pi n^2} \right) \left( 1 - \frac{T \omega}{2 \pi n^2} + \frac{1}{2} \left( \frac{T \omega}{2 \pi n^2} \right)^2 \right) \left| \mathbf{v}_T \right|^2, \]

\[ \tilde{\omega} = \frac{2 \pi n}{T}, \quad \mathbf{v}_T = \int_0^T \mathbf{v}_T(t) e^{i\tilde{\omega} t} dt \]  

(12)

where \( \mathbf{v}_T \) is the Fourier-component of transverse particle velocity. Successively, channeling radiation taking into account the particle initial angular distribution can be evaluated as

\[ I_{F_{\perp}}(h \omega, E_\perp) = I_{\text{thin}}(h \omega, E_{\perp}) \cdot F_{\perp}(z, E_\perp) \]  

(13)

However, this approach is valid only for very thin crystals. Indeed, for thick crystals we have to pay attention to the projectile dechanneling (with the crystal thickness increase the projectiles become unbound by the channel potential due to the increase of their transverse energies), which contributes to variation of the distribution function \( F(z, E_\perp) \). Hence, the expression for radiation intensity in thick crystals can be written as follows

\[ I_{\text{thick}}(h \omega, E_\perp) = \frac{1}{L} \int_0^L I_{\text{thin}}(h \omega, E_{\perp}) \cdot F(z, E_\perp) dz \]  

(14)

Above presented equations are used for a single particle case; moreover, they describe the features of radiation for given transverse energy \( E_\perp \). Thus, total radiation spectrum is formed by the projectiles over complete set of the transverse energies at channeling \( E_\perp \) that results in the necessity of additional averaging by transverse energy, i.e. \( \langle I_{\text{thin}} \rangle, \langle I_{F_{\perp}} \rangle, \langle I_{\text{thick}, L} \rangle \).
Figure 7. Channeling radiation spectrum for a $E = 855$ MeV electron channeled in Si (111) (a) $I_{\text{thin}}(h\omega, E_\perp)$ at homogeneous transverse energy distribution (a), and $I_{F_0}(h\omega, E_\perp)$ with initial distribution of electrons $F_0$ defined as in figure 2 (b).

Figure 8. Thickness dependence for radiation spectrum at electrons channeling in a Si (111) crystal.

Figure 8 shows the radiation spectra of channeled electrons per unit length of the crystalline target Si.

5. Conclusion

In this work we have presented a model for the dual-channeling of 855 MeV electrons in a Si (111) crystal, taking into account the effects of dechanneling. The calculations were performed for the initial angular distributions of relativistic electrons in the beam as a function of transverse energy for various angles of incidence with respect to the crystal (111) planes. Within developed model both drift and diffusion coefficients of the beam density distributions for trapped electron motion in the system of double planes (111) have been evaluated.

For 855 MeV electrons channeling in a Si (111) crystal the dechanneling length evaluated from the solution of the Fokker-Planck equation equals to 18.8 μm. Spectral characteristics of channeling radiation by electrons of moderate energies in thick crystals have been first obtained taking into account the dynamics of beam scattering at channeling as well as the initial angular distribution of channeled electrons.

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References

[1] Carrigan R. A., Negative Particle Planar and Axial Channeling and Channeling Collimation, in the book "Charged and Neutral Particles Channeling Phenomena - Channeling 2008", Dabagov S.B., and Palumbo L., Eds., World Scientific Publ. (2010) 129.

[2] Dabagov S.B., and Zhevago N.K., Nuovo Cimento 31(9) (2008) 491.

[3] Kumakhov M.A., and Shirmer G., Atomic Collisions in Crystals, Moscow: Atomizdat, 1980 (in Russian).

[4] Beloshitsky VV, Komarov FF, and Kumakhov MA, Dechanneling, flux-peaking and energy losses of fast charged particles penetrating through thick crystals, Phys. Rep. 139 (6) (1986) 293-364.

[5] Kostyuk A., Korol A., Solov'yov A.and Greiner W., J. Phys. B: At. Mol. Opt. Phys. 44 (2011) 075208.

[6] Ohtsuki Y.-H., Charged Beam Interaction with Solids, New York, 1983.

[7] Backe H.et al. Nucl. Instr. Meth. in Phys. Res. B266 (2008) 3835.

[8] Bogdanov O.V., Korotchenko K.B. and Pivovarov Yu.L., J. Phys. B: At. Mol. Opt. Phys. 41 (2008) 055004.

[9] Babaev A.A., et al., On Crystal-Assisted Processes by Means of 20–800 MeV e⁻/e⁺ LNF Beams, Preprint LNF 22 (IR) (2008) pp. 1-42.

[10] Gemmell D.S., Rev. Mod. Phys. 46 (1974) 129.

[11] Doyle P.A. and Turner P. S., Acta Crystallogr. A 24, 390 (1968).

[12] Baier V. N., V. M. Katkov and V. M. Strakhovenko 1998, Electromagnetic Processes at High Energies in Oriented Single Crystals. World Scientific, Singapore

[13] Akhiezer A.I., and Shu’lga N.F. High Energy Electrodynamics in Matter, Gordon and Breach, Luxemburg, 1996

[14] Azadegan B., and Dabagov S.B., European Physical Journal - Plus 126 (2011) 58.