Simulation of Incoherent Radiation of Fast Particles in an Oriented Crystal

V. V. Syshchenko[a], A. I. Tarnovskii[a], and N. F. Shul'ga[b]

[a] *Belgorod State University, Belgorod, 308015 Russia; e-mail: syshch@bsu.edu.ru*
[b] *Akhiezer Institute for Theoretical Physics, National Science Center, Kharkov Institute of Physics and Technology, Kharkov, 61108 Ukraine*

Abstract—Incoherent bremsstrahlung of high-energy electrons in a crystal is due to the thermal spread of atoms with respect to their equilibrium positions in the lattice. In this paper, an incoherent-radiation simulation procedure based on semiclassical formulas of bremsstrahlung theory is developed. A significant orientation dependence of the intensity of hard incoherent radiation is demonstrated for angles of electron incidence on a densely packed crystallographic axis (plane) that are close to the critical axial (plane) channeling angle. The simulation results are in good agreement with the experimental data.

INTRODUCTION

The channeling phenomenon can occur in crystals in the case of motion of fast charged particles along a crystallographic axis (or a plane) where the particles move in channels formed by atomic strings or crystal planes [1–3]. There is a certain redistribution of a particle stream in a crystal during the channeling process. As a result, the yields of the processes related to the small impact parameters can be either increased or decreased. This is connected to the fact that positively charged particles in the channeling regime cannot very closely approach the atomic nuclei in the lattice; therefore, such particles collide with nuclei more rarely than in the absence of channeling. The inverse effect occurs for negatively charged particles.

If the crystal is disoriented by a small angle with respect to the stream, then the particles involved in above-barrier motion with respect to atomic strings and crystal planes appear in addition to channeled particles [3–5]. For the above-barrier particles, there is also some redistribution of the stream density of particles in the crystal, and this redistribution essentially differs from the redistribution of the stream density of channeled particles. In the case of above-barrier motion near the atomic planes, positively charged particles hover in the region of the atomic nucleus localization in crystallographic planes for a sufficiently long time, while negatively charged particles traverse this region faster than positively charged ones. And if the crystal disorientation angle significantly exceeds the critical channeling angle, then there is no effect of redistribution of the particle stream in the crystal [3].

Thus, the orientation dependence of the yields of the processes related to the small impact parameters must exist in the case of crystal disorientation by angles on the order of the critical channeling angle. This orientation dependence was observed previously for the yields of nuclear reactions, delta electrons, and some other processes [2, 3, 6, 7].

This paper deals with an analysis of the orientation dependence of the intensity of the incoherent radiation of relativistic electrons and positrons for particles moving near a densely packed crystallographic axis and a plane in the crystal. The simulation procedure for this process is based on the semiclassical bremsstrahlung theory and numerical simulation of particle motion in a crystal regarded as a set of parallel atomic strings. In this case, the incoherent scattering by thermal vibrations of lattice atoms is taken into account together with the coherent scattering of particles by continuous potentials of atomic strings. Thus, using the developed procedure, one can take the particle dechanneling and rechanneling effects into account, which makes this procedure applicable for targets of arbitrary thicknesses. The simulation results are compared to the experimental data on the orientation dependence of the photon yield in the range of energies close to the emitting electron energy [7]; these data were obtained previously at the Kharkov Institute of Physics and Technology.

PROCEDURE

The process of relativistic electron radiation in some material evolves in a large spatial region along the particle momentum; this region is called the *coherence length* [3, 8]. If the electron collides with a large number of crystal atoms in this region, then the effective

constant of its interaction with lattice atoms can be large as compared to unity and one can use a semiclassical approximation to describe electron radiation in a crystal. In this case, in the dipole approximation, the bremsstrahling spectral density can be described by the formula [3, 9]

$$\frac{d\mathrm{E}}{d\omega} = \frac{e^2\omega}{2\pi c^4}\int_{\delta}^{\infty}\frac{dq}{q^2}\left[1+\frac{(\hbar\omega)^2}{2\varepsilon\varepsilon'}-2\frac{\delta}{q}\left(1-\frac{\delta}{q}\right)\right]|\mathbf{W}_q|^2, \quad (1)$$

where $q = \frac{\varepsilon}{\varepsilon'}(\omega - \mathbf{kv})$; $\mathbf{k}$ is the wave vector of the emitted photon, $|\mathbf{k}| = \omega/c$; ε and $\mathbf{v}$ are the respective energy and velocity of the initial electron, $\varepsilon' = \varepsilon - \hbar\omega$; $\mathbf{W}_q = \int_{-\infty}^{\infty}\dot{\mathbf{v}}_{\perp}(t)e^{icqt}dt$ is the Fourier component of the electron acceleration in the direction orthogonal to $\mathbf{v}$, and $\delta = m^2c^3\omega/2\varepsilon\varepsilon'$. In particular, for the radiation of the electron in an isolated-atom field (we represent the atomic potential in the form of a screened Coulomb potential $U(r) = (Ze/r)\exp(-r/R)$, where Z is the atomic number and R is the Thomas–Fermi radius), we have

$$\mathbf{W}_q^{(1)}(\boldsymbol{\rho}_0) = \frac{2Ze^2c}{\varepsilon}\sqrt{q^2+R^{-2}}K_1(\rho_0\sqrt{q^2+R^{-2}})\frac{\boldsymbol{\rho}_0}{\rho_0}. \quad (2)$$

Here, $K_1(x)$ is the modified Bessel function of the third kind (the Macdonald function) and $\boldsymbol{\rho}_0$ is the impact parameter. Because the characteristic values of q giving the largest contribution to the integral in (1) are $q \sim \delta \ll R^{-1}$, we can set $q = 0$ in (2) and obtain

$$\mathbf{W}^{(1)}(\boldsymbol{\rho}_0) = \frac{2Ze^2c}{\varepsilon R}K_1\left(\frac{\rho_0}{R}\right)\frac{\boldsymbol{\rho}_0}{\rho_0}. \quad (3)$$

Integrating over q and then over the impact parameter, we obtain, with logarithmic accuracy, the Bethe–Heitler result for the radiation efficiency of the unit-density particle beam incident on the atom:

$$\hbar\omega\frac{d\sigma_{\mathrm{BH}}}{d\omega} = \int\frac{d\mathrm{E}}{d\omega}d^2\rho_0 = \frac{16}{3}\frac{Z^2e^6}{m^2c^2}\left(1+\frac{3}{4}\frac{(\hbar\omega)^2}{\varepsilon\varepsilon'}\right)\ln\left(\frac{mRc}{\hbar}\right). \quad (4)$$

We note that the integral over the impact parameter diverges for small ρ_0. This divergence is related to the dipole approximation valid for $\rho_0 \geq \hbar/mc$. We take this restriction into account by introducing a cut-off in the lower integration limit ($\rho_{\min} = \hbar/mc$ is the electron Compton wavelength); the logarithmic accuracy of the result is due to this fact.

We now consider the emission of an electron interacting with a crystal, which is a system of atoms periodically located in the space. We study the case of an electron incident on the crystal at a small angle ψ to one (the z axis) of the densely packed crystallographic axes. It is well known [3] that the averaging of the expression $|\mathbf{W}_q|^2$ over the thermal vibrations of atoms in a crystal results in the decomposition of this quantity (and of the radiation intensity) into two terms describing the coherent and incoherent effects in the radiation:

$$\langle|\mathbf{W}_q|^2\rangle = \sum_{n,m}\exp(iqc(t_n-t_m))\langle\mathbf{W}_q^{(1)}(\boldsymbol{\rho}_n+\mathbf{u}_n)\rangle \times\langle\mathbf{W}_q^{(1)}(\boldsymbol{\rho}_m+\mathbf{u}_m)\rangle + \sum_n\{\langle(\mathbf{W}_q^{(1)}(\boldsymbol{\rho}_n+\mathbf{u}_n))^2\rangle - \langle\mathbf{W}_q^{(1)}(\boldsymbol{\rho}_n+\mathbf{u}_n)^2\rangle\}, \quad (5)$$

where the indices n and m number the atoms participating in collisions with incident electrons, t_n is the instant at which an incoming electron collides with the nth atom, $\boldsymbol{\rho}_n = \boldsymbol{\rho}(t_n) - \boldsymbol{\rho}_n^0$ is the impact parameter for the collision with the nth atom in its equilibrium state $\boldsymbol{\rho}_n^0$, $\boldsymbol{\rho}(t)$ is the electron trajectory in the plane orthogonal to the z axis, and $\mathbf{u}_n$ is the thermal displacement of the nth atom relative to its equilibrium position.

In the frequency range

$$\omega \gg 2\varepsilon\varepsilon'\psi/m^2c^3a, \quad (6)$$

where a is the distance between two nearest parallel atomic strings, the term describing incoherent effects contributes mainly to the radiation intensity [3]. As in the case of radiation on the separate atom, we assume $q = 0$, substitute the expression for $\mathbf{W}^{(1)}$ in (3), and obtain the following expression for the incoherent fraction:

$$|\mathbf{W}_{\mathrm{incoh}}|^2 = \frac{4Z^2e^4c^2}{\varepsilon^2R^2}\sum_n\left\{\left\langle\left(K_1\left(\frac{|\boldsymbol{\rho}_n+\mathbf{u}_n|}{R}\right)\right)^2\right\rangle - \left\langle\frac{\boldsymbol{\rho}_n+\mathbf{u}_n}{|\boldsymbol{\rho}_n+\mathbf{u}_n|}K_1\left(\frac{|\boldsymbol{\rho}_n+\mathbf{u}_n|}{R}\right)\right\rangle^2\right\}. \quad (7)$$

It is convenient to compare the efficiency of the coherent radiation in a crystal to that of radiation in an amorphous medium (for the same number of collisions with atoms). It is easy to see that the ratio of these two quantities is given by

$$N_\gamma = \frac{\int d^2\rho_0\left(\frac{d\mathrm{E}}{d\omega}\right)_{\mathrm{incoh}}}{N\hbar\omega\frac{d\sigma_{\mathrm{BH}}}{d\omega}} = \frac{\int d^2\rho_0\sum_n F(\boldsymbol{\rho}_n)}{2\pi NR^2\ln\left(\frac{mRc}{\hbar}\right)}. \quad (8)$$

where

$$F(\boldsymbol{\rho}) = \left\langle\left(K_1\left(\frac{|\boldsymbol{\rho}+\mathbf{u}|}{R}\right)\right)^2\right\rangle - \left\langle\frac{\boldsymbol{\rho}+\mathbf{u}}{|\boldsymbol{\rho}+\mathbf{u}|}K_1\left(\frac{|\boldsymbol{\rho}+\mathbf{u}|}{R}\right)\right\rangle^2, \quad (9)$$

N is the total number of atoms with which the electron moving in the crystal collides and integration over $d^2\rho_0$

means integration over all possible entrance points (located in one unit cell in the xy plane) for electrons entering the crystal.

Calculating $F(\boldsymbol{\rho})$, one must introduce a cut-off at small distances as in the case of one separate atom; i.e., one must put $\rho < \rho_{min}$ for $\rho = \rho_{min}$. The averaging over thermal vibrations is performed by integration with a Gaussian distribution. Such integration can be performed only numerically; therefore, the values of the function $F(\boldsymbol{\rho})$ in (8) are determined by interpolating results of the numerical integration for the finite set of the values of $\boldsymbol{\rho}$. The integration over $d^2\rho_0$ can be performed by the Monte-Carlo method. The impact parameters $\boldsymbol{\rho}_n$ for collisions with atoms are determined by using the electron trajectory in the crystal obtained by numerical simulation.

Let us consider the electron motion in a crystal at a small angle ψ to one of the densely packed crystallographic axes. This motion is such that the approximation of the atomic-string continuous potential is valid. In this case, the problem of electron motion in a crystal can be reduced to the two-dimensional problem of motion in the xy plane perpendicular to the string axes. The electron trajectory $\boldsymbol{\rho}(t)$ can be determined from the equation of motion [1–3]

$$\ddot{\boldsymbol{\rho}} = -\frac{c^2}{\varepsilon}\frac{\partial}{\partial \boldsymbol{\rho}}\sum_s U_R(\boldsymbol{\rho} - \boldsymbol{\rho}_s^0), \qquad (10)$$

where $U_R(\boldsymbol{\rho} - \boldsymbol{\rho}_s^0)$ is the potential energy of interaction of the electron with the continuous potential of the atomic string parallel to the z axis and $\boldsymbol{\rho}_s^0$ is the position of the string in the xy plane.

However, the thermal spread of the atomic positions relative to their equilibrium positions in the crystal leads to the appearance of incoherent scattering by atomic thermal vibrations together with coherent electron scattering [3].

The scattering angle of an electron in the field of a separate atom can be found from the equation of motion and described by the formula differing from expression (3) for $\mathbf{W}^{(1)}$ only by the coefficient c:

$$\boldsymbol{\vartheta}^{(1)}(\boldsymbol{\rho}_0) = \frac{2Ze^2}{\varepsilon R} K_1\left(\frac{\rho_0}{R}\right)\frac{\boldsymbol{\rho}_0}{\rho_0}.$$

Summing the angles of scattering by all atoms contained in the atomic string in the crystal and averaging the squared absolute value of this quantity over the atomic thermal vibrations, we obtain an expression similar to (5) and find that the average value of the squared incoherent scattering angle $\langle \vartheta^2 \rangle_{incoh}$ can be described by a formula coinciding with (7) within an accuracy of the coefficient c^2:

$$\langle \vartheta^2 \rangle_{incoh} = \frac{4Z^2e^4}{\varepsilon^2 R^2}\sum_n F(\boldsymbol{\rho}_n). \qquad (11)$$

Thus, simulating the electron trajectory in the crystal, one can take incoherent scattering from atomic thermal vibrations into account by adding a random quantity obeying the Gaussian distribution with variance equal to $(2Z^2e^4c^2/\varepsilon^2R^2)F(\boldsymbol{\rho}_n)$ to each of the components of the electron velocity in the xy plane at the instant of collision with the nth atom.

RESULTS AND DISCUSSION

The specific examples of simulation were chosen according to the experimental conditions described in [7]. In one of these examples, the authors recorded the radiation of 800-keV electrons incident on a Si crystal ($Z = 14$, $R = 0.194$ Å) at a small angle ψ to the $\langle 111 \rangle$ axis in the hard radiation spectral region ($\hbar\omega = 700$ MeV), where the incoherent mechanism of bremsstrahlung gives the main contribution. Figure 1 shows the experimental data (Fig. 1b in [7]) and the result of the simulation taking into account the coherent scattering of electrons by continuous potentials of atomic strings, incoherent scattering by atomic thermal vibrations, and the divergence of the electron beam on the order of 5×10^{-4} in the experiment under discussion.

Because there is satisfactory agreement between the simulation results and the experiment, we can explain the significant increase in the radiation intensity at small ψ (as compared to the radiation intensity in an amorphous medium) by axial electron channeling. Indeed, for the incidence angles $\psi \ll \psi_c$, where the critical axial channeling angle [1–3]

$$\psi_c = \sqrt{2U_R(0)/\varepsilon} \approx \sqrt{4Ze^2/\varepsilon a_z}$$

is 5.1×10^{-4} rad in this case, axial channeling occurs for the majority of particle entrance points in the crystal. For the motion in the channeling regime, the electron (a negatively charged particle) moves near the atomic string, experiencing collisions with atoms with small impact parameters, which leads to the maximum efficiency of incoherent radiation. At the same time, the positron (a positively charged particle) in the axial channeling regime moves far from atomic strings, which results in the minimum radiation efficiency. For clarity, we neglected the beam divergence and incoherent scattering by atomic thermal vibrations in Fig. 2. As ψ is increased, the number of channeled particles decreases; then the different impact parameters for the collisions with atoms become equiprobable as in an amorphous medium, and the incoherent radiation efficiency becomes equal to the radiation efficiency in an amorphous medium (with an accuracy of the Debye–Walter factor).

We now consider the effect of atomic planes in the crystal on the incoherent radiation intensity. Let an electron beam be incident on a crystal at a small angle θ to one of the densely packed crystallographic axes. We assume that the angle ψ (being small and such that the approximation of the continuous potential of the

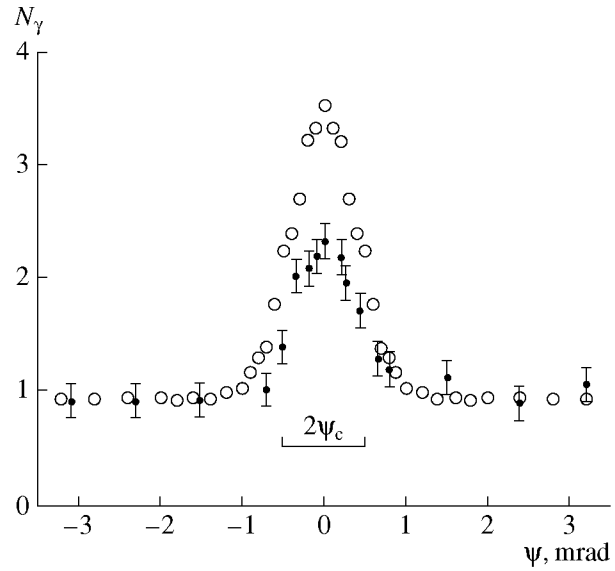

Fig. 1. Yield of 700-MeV photons depending on the incidence angle of 800-Mev electrons to the ⟨111⟩ axis of a Si single crystal of thickness of 30 μm [7] (experimental points) and the relative efficiency of incoherent electron radiation obtained by using the simulation results based on formula (8) taking into account incoherent electron scattering by thermal vibrations of lattice atoms and electron beam divergence (circles).

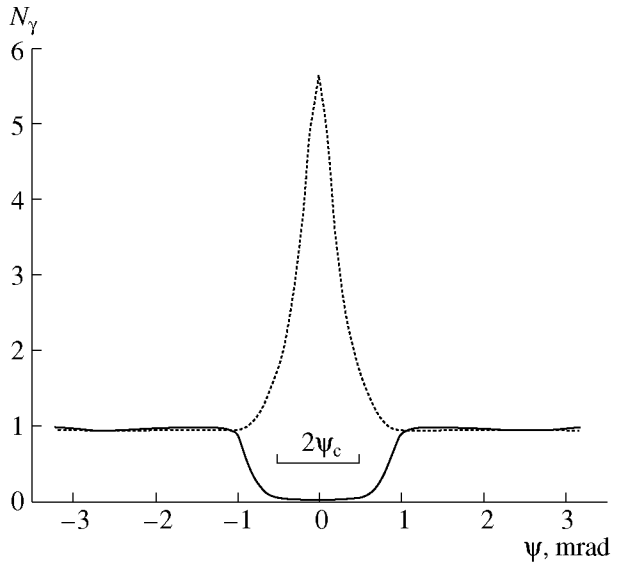

Fig. 2. Relative efficiency of incoherent crystal positron (solid line) and electron (dashed line) radiation obtained by using the simulation results under the conditions of Fig. 1 without considering incoherent particle scattering by atomic thermal vibrations and electron beam divergence.

atomic string is valid) much exceeds the critical axial channeling angle, $\psi \gg \psi_c$. For such large angles ψ, the simulation procedure for the particle trajectory in the crystal can be simplified significantly (and the required computer time can be decreased) as compared to the method based on the numerical integration of equation of motion (10). Indeed, because the atomic string potential decreases rapidly with distance, the electron trajectory is bent mainly at a small region located at the least distance from the string axis. For this reason, we approximate the actual particle trajectory by a broken line; the angles between the portions of this line in the *xy* plane are equal to the azimuthal angles of the particle scattering (deflection) in the field of the corresponding strings:

$$\Delta\varphi(b) = \pi - 2b \int_{\rho_{\min}}^{\infty} \frac{d\rho/\rho^2}{\sqrt{1 - \dfrac{U_R(\rho)}{\varepsilon_\perp} - \dfrac{b^2}{\rho^2}}}. \qquad (12)$$

where b is the impact parameter for the collision with the string, $\varepsilon_\perp = \varepsilon\psi^2/2$ and $\rho_{\min}$ is the distance of the closest approach of the electron to the atomic string axis [3, 4]. The successive passage from one collision with the string to another is performed in the simulation process. At each step, the coordinates of the atomic string with which the atom will collide and the impact parameter for this next collision are determined by using the known parameters of the current rectilinear portion of the trajectory. The details of this procedure are described in [9].

Incoherent scattering is taken into account by adding, to the azimuthal incoherent scattering angle (12), a random quantity obeying a Gaussian distribution with the dispersion $\langle\vartheta^2\rangle_{\text{incoh}}/2\psi^2$ (see (11), where the summation is over all atoms of this string, with which the particle experiences sufficiently close collisions). Using such a model, which is more realistic than that in [9], one can take into account the dechanneling phenomenon in which the particles moving in channels formed by crystal atomic planes can leave these channels because of the scattering by atomic thermal vibrations.

Hard radiation of 1.2 GeV electrons incident on a Si crystal at a small angle θ to the (110) plane was recorded in the experiment whose results (Fig. 2 in [7]) are reproduced in Fig. 3. In this case, the electron incidence angle to the ⟨001⟩ axis (the z axis) was chosen to be sufficiently large in order to guarantee the absence of axial channeling:

$$\psi \sim 100\psi_c .$$

(the critical axial channeling angle is 3.5×10^{-4} rad in this case). Fig. 3 shows the simulation results for incoherent radiation depending on the incidence angle θ taking and not taking into account the incoherent electron scattering by atomic thermal vibrations in the crystal. In the former case, we observe sufficiently good agreement of the simulation results with the experimental data. The electron beam divergence under the exper-

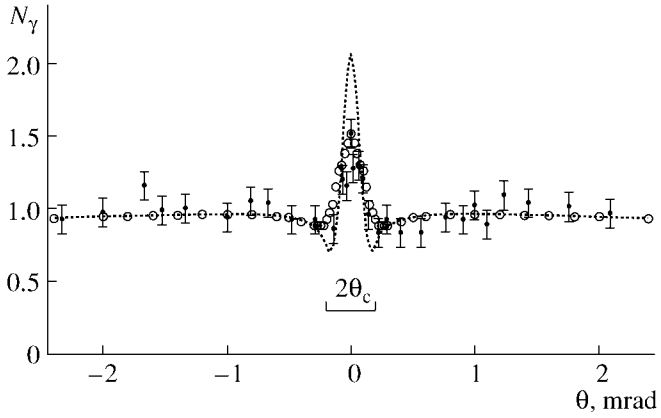

Fig. 3. Yield of 1.1-GeV photons depending on the 1.2-GeV electron incidence angle to the (110) plane of a Si single crystal of thickness of 30 μm [7] (experimental points) and the incoherent electron radiation efficiency obtained by using the simulation results taking (circles) and not taking (dashed line) into account incoherent electron scattering by thermal vibrations of lattice atoms.

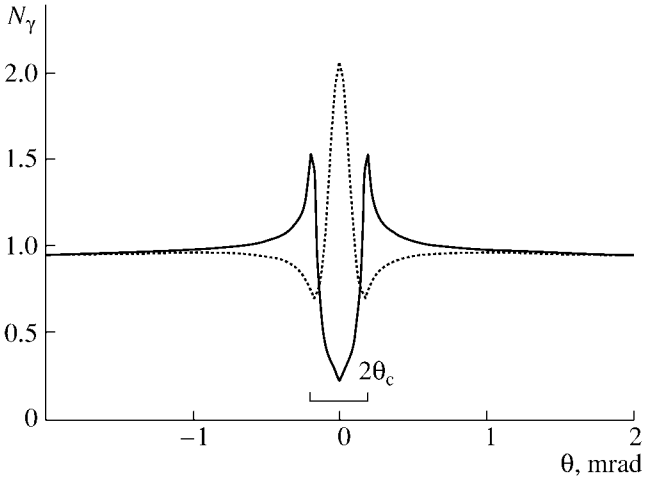

Fig. 4. Relative efficiency of incoherent crystal positron (solid line) and electron (dashed line) radiation under the conditions of Fig. 3 without considering incoherent particle scattering by atomic thermal vibrations.

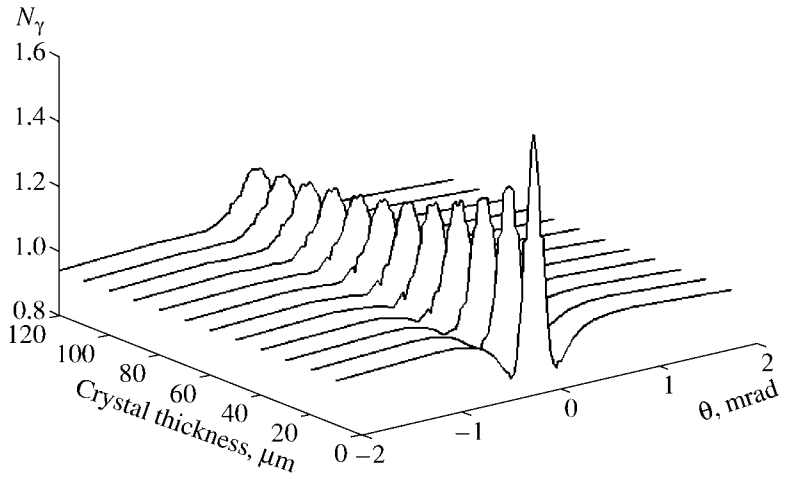

Fig. 5. Variation of the orientation dependence of the incoherent electron radiation efficiency under the condition of Fig. 3 as a function of the crystal thickness.

imental conditions is 10^{-4} rad and does not affect significantly the radiation intensity.

In this case, the character of the orientation dependence of the incoherent radiation efficiency is also due to the special features of the electron dynamics in the crystal. It can be demonstrated most clearly by a comparison of the orientation dependences of the electron and positron incoherent radiation under the same conditions (see Fig. 4, where the possibility of incoherent particle scattering by atomic thermal vibrations in the crystal is not taken into account for clarity). Plane channeling occurs for the majority of particle entrance points in the crystal for θ close to zero. In the plane-channeling regime, the electron moves mainly near the atomic plane in the crystal and the impact parameters for atomic collisions are small, which leads to the maximum incoherent radiation efficiency. On the other hand, the positron in the plane-channeling regime mainly moves far from the atomic planes, which results in the minimum radiation efficiency.

For θ close to the critical plane-channeling angle (the value of which is $\theta_c \approx 2 \times 10^{-4}$ rad in the case under consideration), above-barrier positrons move mainly near the atomic planes in the crystal, which leads to the maximum incoherent radiation efficiency. On the contrary, above-barrier electrons pass rapidly through the atomic plane, which results in the minimum coherent radiation intensities.

For $\theta \gg \theta_c$, the energy $\varepsilon_\perp = \varepsilon\theta^2/2$ of the transverse particle motion [3] greatly exceeds the height of the potential barrier formed by the continuous potential of the atomic plane in the crystal. In this case, the particle

trajectory becomes almost rectilinear. For such a trajectory, all possible impact parameters for the atomic collisions are almost equiprobable as in an amorphous medium and the incoherent radiation efficiency becomes (with an accuracy of the Debye–Walter factor) becomes equal to that in an amorphous medium and independent of the crystal orientation.

Electron scattering from the thermal vibrations of the lattice atoms by a large angle can lead to electron dechanneling, and the electron motion becomes above-barrier instead of that in the plane channel. For this reason, the above-mentioned maxima and minima become less pronounced, as can be seen from the simulation results taking into account scattering by atomic thermal vibrations (Fig. 3) and excluding the possibility of dechanneling.

As the crystal thickness increases, the probability of electron dechanneling increases, which leads to a gradual increase in the orientation dependence of the incoherent radiation efficiency (Fig. 5).

CONCLUSIONS

The simulation results show that there is a considerable dependence of the incoherent bremsstrahlung yield on the crystal orientation with respect to the incident particle beam for incidence angles close to the critical axial and plane channeling angles. This orientation dependence is due to the special features of the dynamics of charged particles in the crystal and is significantly different for electrons and positrons. In the case of electrons, the simulation results for incoherent radiation agree well with the experimental results in [7], the authors of which measured the orientation dependence of the yield of photons with energies close to the energy of emitting electrons; in this case, the contribution of the incoherent mechanism is dominant.

ACKNOWLEDGMENTS

This work was supported by the Russian Ministry of Education and Sciences in the framework of the program "Development of the Scientific Potential of Higher Schools" (grant no. RNP.2.1.1.3263), by the Russian Federation for Basic Research (grant no. 05-02-16512), and by a Belgorod State University grant.

REFERENCES

1. J. Lindhard, Dan. Vid. Selsk. Mat. Phys. Medd **34**, 30 (1965).
2. D. S. Gemmell, Rev. Mod. Phys. **46**, 129 (1974).
3. A. I. Akhiezer and N. F. Shulga, *Electrodynamics of High Energies in v veshchestve* (Nauka, Moscow, 1993) [in Russian].
4. A. I. Akhiezer, I. A. Akhiezer, and N. F. Shulga, Zh. Eksp. Teor. Fiz. **76**, 1244 (1979) [JETP , (1979)].
5. A. I. Akhiezer, N. F. Shulga, V. I. Truten, et al., Usp. Fiz. Nauk **165** (10), 1165 () [Phys.-Usp. , ()].
6. V. F. Boldyshev, V. I. Kasilov, G. D. Kovalenko, et al., Nucl. Instrum. Methods Phys. Res. **33**, 30 (1988).
7. V. M. Sanin, V. M. Khvastunov, V. F. Boldyshev, and N. F. Shulga, Nucl. Instrum. Methods Phys. Res. B **67**, 251 (1992).
8. M. L. Ter-Mikaelyan, *Media Influence onto Electromagnetic Processes at High Energies* (Izd-vo AN Arm.SSR, Yerevan, 1969) [in Russian].
9. N. F. Shulga and V. V. Syshchenko, Izv. Akad. Nauk, Ser. Fiz. **64** (11), 2168 (2000).
10. N. F. Shulga and V. V. Syshchenko, Nucl. Instrum. Methods Phys. Res. B **227**, 125 (2005).