NUMERICAL COMPUTATION OF INCOHERENT BREMSSTRAHLUNG FROM FAST ELECTRONS IN SINGLE CRYSTALS

N.F. Shul'ga[1], **V.V. Syshchenko**[2]*, **A.I. Tarnovsky**[2]
[1] *National Science Center "Kharkov Institute of Physics and Technology", 61108, Kharkov, Ukraine*
[2] *Belgorod State University, Belgorod, Russian Federation*

(Received May 15, 2009)

The incoherent bremsstrahlung of fast electrons in crystal is caused by thermal spread of atoms from their equilibrium positions in the lattice. Its intensity manifests substantial orientation dependence under angles of incidence close to critical angle of planar or axial channeling. The simulation procedure for the incoherent radiation is developed. The results of simulation are in a good agreement with the experimental data.

PACS: 02.70.-c, 41.60.-m, 61.85.+p

1. INTRODUCTION

Under motion of fast charged particles in a crystal along one of crystallographic axes or planes the channeling phenomenon is possible, when the particles move in channels formed by atomic strings or planes in the crystal (see, e.g., [1-4]). The redistribution of the particle flux in the crystal takes place under the channeling. Due to this fact both increase and decrease of yields of the processes connected with small impact parameters are possible. This is connected to the fact that positively charged channeling particles couldn't come to small distances to the positively charged atomic nuclei in the lattice, so such particles would collide with the atomic nuclei in the crystal more rare than under absence of the channeling. For negatively charged particles the inverse effect takes place.

So, in the case of disorientation of the crystal by the angles of order of the critical channeling angle substantial orientation dependence of yields of the processes connected to small impact parameters must take place. Such orientation dependencies have been observed earlier for the nuclear reactions yields, *delta*-electron yield, and other processes (see, e.g., [2, 3, 5, 6]).

The present paper is devoted to the analysis of orientation dependence of the yield of incoherent radiation of relativistic electrons in the crystal. The simulation procedure for this process based on the semiclassical theory of bremsstrahlung was proposed in [7]. In the this article we use our procedure for interpretation of early [6] and recent [8] experimental results.

2. SIMULATION OF THE INCOHERENT RADIATION

Radiation of relativistic electron in matter develops in a large spatial region along the particle's momentum called as the coherence length l_{coh} [3, 9]. If the electron collides with a large number of crystal atoms on the coherence length, the effective constant of the interaction of the electron with the lattice atoms may be large in comparison with the unit, so we could use the semiclassical description of the radiation process. In the dipole approximation the spectral density of bremsstrahlung is described by the formula [3]

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

where $q = \frac{\varepsilon}{\varepsilon'}(\omega - \mathbf{kv})$, $\mathbf{k}$ is the wave vector of the radiated photon, ε is the energy of the initial electron, $\mathbf{v}$ is its velocity, $\varepsilon' = \varepsilon - \hbar\omega$, $\mathbf{W}_q = \int\limits_{-\infty}^{\infty}\dot{\mathbf{v}}_{\perp}(t)e^{icqt}dt$ is the Fourier component of the electron acceleration in the direction orthogonal to $\mathbf{v}$, $\delta = m^2c^3\omega/2\varepsilon\varepsilon' \sim l_{coh}^{-1}$. Particularly, for the case of radiation of the electron in the field of single atom (using the screened Coulomb potential $U(r) = (Ze/r)\exp(-r/R)$, as the potential of the atom, where Z is the atomic number, R is Thomas-Fermi radius) we have:

$$\mathbf{W}_q^{(1)}(\boldsymbol{\rho}_0) = \quad (2)$$

$$= \frac{2Ze^2c}{\varepsilon}\sqrt{q^2+R^{-2}}K_1\left(\rho_0\sqrt{q^2+R^{-2}}\right)\frac{\boldsymbol{\rho}_0}{\rho_0},$$

where $K_1(x)$ is the modified Bessel function of the third kind, $\boldsymbol{\rho}_0$ is the impact parameter. Since the

*Corresponding author E-mail address: syshch@bsu.edu.ru

characteristic values of q making the main contribution to the integral (1) are $q \sim \delta \ll R^{-1}$ we can take $q = 0$ in (2):

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

Integrating over q, and after that over the impact parameter, we obtain with logarithmic accuracy the Bethe-Heitler result for radiation efficiency by the unit particle flux in the field of the atom:

$$\hbar\omega\frac{d\sigma_{BH}}{d\omega} = \int \frac{dE}{d\omega}d^2\rho_0 = \quad (4)$$

$$= \frac{16}{3}\frac{Z^2e^6}{m^2c^5}\frac{\varepsilon'}{\varepsilon}\left(1 + \frac{3}{4}\frac{(\hbar\omega)^2}{\varepsilon\varepsilon'}\right)\ln\left(\frac{mRc}{\hbar}\right).$$

Note that the integral over the impact parameter diverges at small values of ρ_0. The divergence results from the use of the dipole approximation, which is valid at $\rho_0 \geq \hbar/mc$. We take this constraint into account by introducing the lower limit of integration ($\rho_{min} = \hbar/mc$ that is the Compton wavelength of the electron), so this result is obtained with logarithmic accuracy.

Consider now the radiation of the electron interacting with the crystal that is the system of atoms periodically arranged in space. The case of our interest is the electron incidence onto the crystal under small angle ψ to one of its crystallographic axes (the z axis). It is known [3] that averaging of the equation for the $|\mathbf{W}_q|^2$ over the thermal vibrations of atoms in the lattice leads to the split of this value (and so the radiation intensity) into the sum of two terms describing coherent and incoherent effects in radiation:

$$\overline{|\mathbf{W}_q|^2} = \quad (5)$$

$$= \sum_{n,m} e^{iqc(t_n - t_m)}\ \overline{\mathbf{W}_q^{(1)}(\boldsymbol{\rho}_n + \mathbf{u}_n)}\ \overline{\mathbf{W}_q^{(1)}(\boldsymbol{\rho}_m + \mathbf{u}_m)} +$$

$$+ \sum_n \left\{\overline{\left(\mathbf{W}_q^{(1)}(\boldsymbol{\rho}_n + \mathbf{u}_n)\right)^2} - \left(\overline{\mathbf{W}_q^{(1)}(\boldsymbol{\rho}_n + \mathbf{u}_n)}\right)^2\right\},$$

where the indexes n and m numerate the atoms under collisions, t_n is the time moment when the electron collides with the n-th atom, $\boldsymbol{\rho}_n = \boldsymbol{\rho}(t_n) - \boldsymbol{\rho}_{\boldsymbol{n}}^{\mathbf{0}}$ is the impact parameter of the collision with the n-th atom in its equilibrium position $\boldsymbol{\rho}_n^0$, $\boldsymbol{\rho}(t)$ is the trajectory of the electron in the plane orthogonal to the z axis, and $\mathbf{u}_n$ is the thermal shift of the n-th atom from the position of equilibrium. Like in the case of the radiation on the single atom, we take $q = 0$ and then, substituting the formula for $\mathbf{W}^{(1)}$ from (3), we find the following expression for the incoherent part of the quantity of interest:

$$|\mathbf{W}_{incoh}|^2 = \frac{4Z^2e^4c^2}{\varepsilon^2R^2}\sum_n F(\rho_n), \quad (6)$$

where

$$F(\rho) = \quad (7)$$

$$= \overline{\left(K_1\left(\frac{|\boldsymbol{\rho} + \mathbf{u}|}{R}\right)\right)^2} - \left(\overline{\frac{\boldsymbol{\rho} + \mathbf{u}}{|\boldsymbol{\rho} + \mathbf{u}|}K_1\left(\frac{|\boldsymbol{\rho} + \mathbf{u}|}{R}\right)}\right)^2.$$

It is easy to demonstrate that the function F depends only on the absolute value of $\boldsymbol{\rho}$. Numerically computed plots of the function F for silicon and diamond crystals under room temperature are presented on Fig.1.

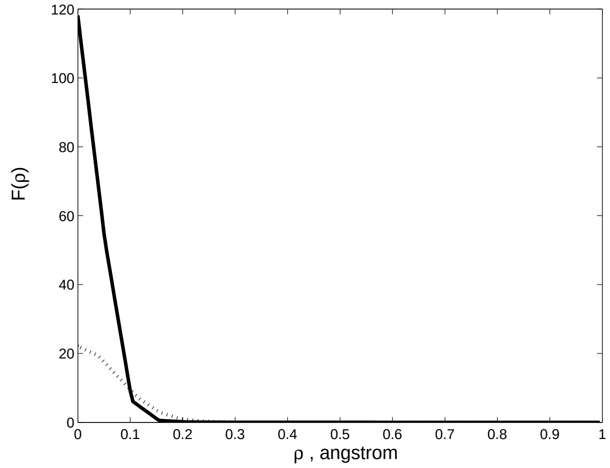

Fig.1. *Plots of the function $F(\rho)$ for diamond (solid line) and silicon (dotted line) crystals under room temperature*

It is convenient to compare the efficiency of the incoherent radiation in the crystal with the radiation efficiency in amorphous medium (with equal numbers of collisions with atoms in both cases). The ratio of these two values is equal to

$$N_\gamma = \frac{\int d^2\rho_0 \left(\frac{dE}{d\omega}\right)_{incoh}}{N\hbar\omega\frac{d\sigma_{BH}}{d\omega}} = \frac{\int d^2\rho_0 \sum_n F(\rho_n)}{2\pi NR^2 \ln\left(\frac{mRc}{\hbar}\right)}, \quad (8)$$

where N is the whole number of atoms with which the electron collides under motion through the crystal, integration over $d^2\rho_0$ means the integration over all possible points of incidence of the beam onto the crystal surface. This integration can be effectively reduced to the integration over one elementary cell in the plane (x, y) and carried out using Monte-Carlo techniques.

The impact parameters of the collisions with atoms $\boldsymbol{\rho}_n$ are determined using the simulated trajectory of the electron in the crystal. For this goal we apply the approximation of uniform potentials of the atomic strings forming the crystal. Note that thermal spread of the atoms from their positions of equilibrium in crystal leads to arising the incoherent scattering of the electrons on the thermal vibrations of atoms together with the coherent scattering on the uniform potentials of the atomic strings (see, e.g., [3], § 57). It is easy to demonstrate that the mean squared value of the incoherent scattering angle $\langle\boldsymbol{\vartheta}^2\rangle_{incoh}$ is described by the formula coinciding to (7) with additional factor c^{-2}. In the simulation procedure for the electron's trajectory the incoherent scattering is taken into account by addition the random value with Gaussian distribution with the dispersion equal to $(2Z^2e^4c^2/\varepsilon^2R^2)F(\rho_n)$ to each component of the electron's velocity in the (x, y) plane.

3. INCOHERENT RADIATION IN CRYSTAL: PLANAR CASE

In experiments [6] carried out in KIPT at the end of 1980th hard photons emitted by electrons of energy ~ 1 GeV had registered. In that range of photon energies the incoherent contribution to bremsstrahlung efficiency is predominant.

In one of that experiments the electrons of energy $\varepsilon = 1.2$ GeV had been incident on the silicon crystal under small angle θ to the plane (110) (the (x, z) plane). The angle of electron incidence to $\langle 001 \rangle$ axis (the z axis) had chosen large enough to ensure the absence of axial channeling:

$$\psi \sim 100\psi_c,$$

where the critical angle of the axial channeling

$$\psi_c = \sqrt{4Ze^2/\varepsilon a_z} \approx 3.5 \cdot 10^{-4} \text{ rad}$$

in this case. The experimental data and the results of simulation are presented on Fig. 2. We see a good agreement between them.

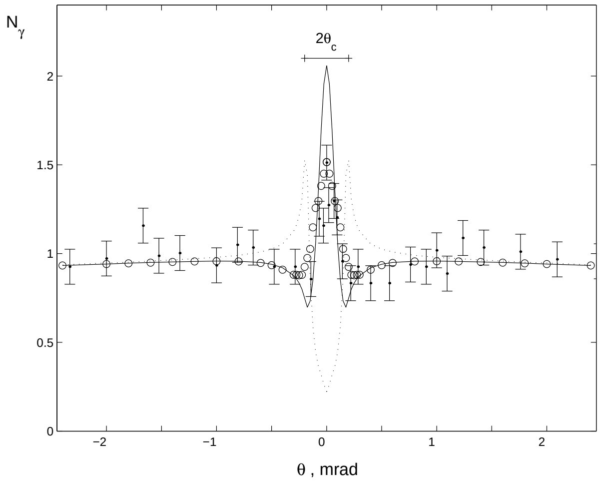

Fig.2. *Photon yields with the energy 1.1 GeV vs the incidence angle of electrons with the energy 1.2 GeV to the (110) plane of a 30 μm thick silicon crystal [6] (error bars) and the efficiency of incoherent radiation of electrons as a result of the simulation with (circles) and without (solid line) account of the incoherent scattering of the electrons on the thermal vibrations of the lattice atoms. Dotted line corresponds to the radiation from positrons under the same conditions (without account of the incoherent scattering)*

The character of the orientation dependence of the incoherent radiation is determined by the specialties of the particle's dynamics in the crystal. This fact could be illustrated under comparison of the orientation dependencies of the incoherent radiation by electrons and positrons under the same conditions (solid and dotted lines on Fig. 2). For the θ values close to zero the planar channeling takes place for the most part of points of incidence of the particle onto the crystal. The electron (negatively charged particle) under planar channeling spends the most part of the time of its motion through the crystal in close vicinity to atomic plane, with small impact parameters of collisions with atoms that leads to the maximum in the efficiency of incoherent radiation. On the other side, the positron under planar channeling spends the most part of the time far from atomic planes that leads to the minimum in the incoherent radiation intensity.

In the case of θ values close to the critical angle of planar channeling θ_c the above-barrier positrons spend the most part of the time in close vicinity to atomic planes that leads to maxima in the incoherent radiation efficiency. Oppositely, the above-barrier electrons rapidly move through atomic planes that leads to minima in the incoherent radiation intensity.

Under $\theta \gg \theta_c$ the energy of transverse motion of the particle $\varepsilon_\perp = \varepsilon\theta^2/2$ [3] exceeds by far the height of the potential barrier formed by uniform potential of the atomic plane in the crystal. In this case the trajectory of the particle is almost rectilinear. For such trajectory all possible impact parameters of collisions with atoms are almost equiprobable, like in amorphous medium, and the incoherent radiation efficiency become equal to that in amorphous medium (in accuracy to Debye-Waller factor) and independent on the crystal orientation.

The electron scattering on the thermal oscillations of the lattice atoms could lead to the dechanneling of the electron, when the motion in the planar channel changes to the above-barrier motion. Therefore, the maxima and minima described above become less sharp.

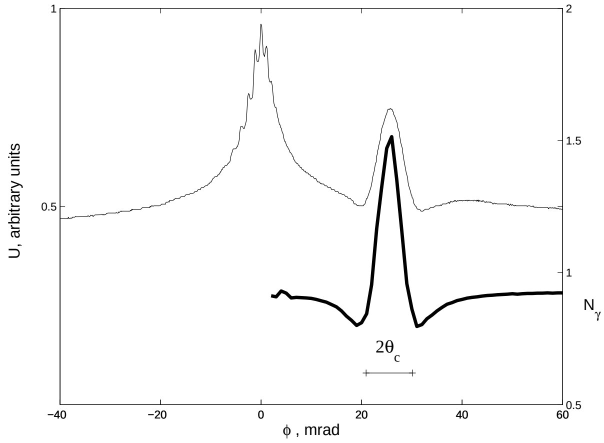

Fig.3. *Integral radiation intensity (thin line) in the experiment ([8], Fig. 14 (b)) and the incoherent contribution as a result of simulation (thick line)*

Fig.3 presents the results of recent experiment at Mainz Microtron MAMI [8] where the integral radiation intensity (with the photon energy higher than 15 MeV) emitted by 855 MeV electrons on the silicon crystal had been registered. Under scanning the goniometric angle ϕ both ψ and θ angles are changed, and in the case under consideration $\psi \approx \phi$. Left maximum on the figure is determined by the coherent radiation on many crystallographic planes with common $\langle 100 \rangle$ axis. Right maximum is caused by the incoherent radiation on the $(0\bar{1}1)$ according to the mechanism described above.

4. INCOHERENT RADIATION IN CRYSTAL: AXIAL CASE

Analogous orientation dependence of the incoherent radiation efficiency takes the place in the case of incidence of the electron beam under small angle ψ to any crystallographic axis densely packed with atoms (see Figs.4 and 5).

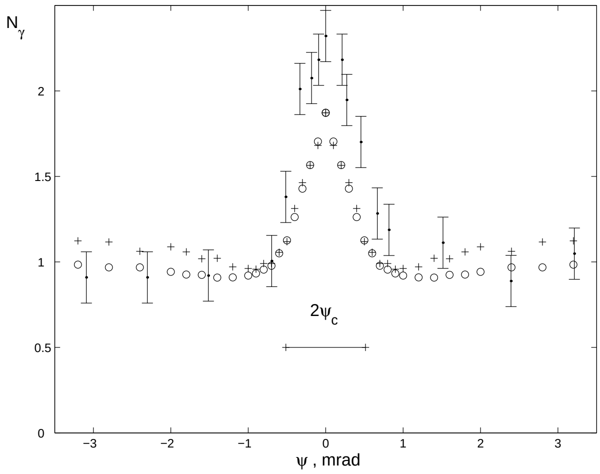

Fig.4. *Yields of photons with the energy 700 MeV emitted by 800 MeV electrons vs the incidence angle of the electrons to $\langle 111 \rangle$ axis of silicon crystal of 30 μm thickness [6] (experimental bars) and the relative efficiency of the incoherent radiation as a result of simulation, when the beam axis is parallel to $(22\bar{1})$ plane (circles) and $(\bar{1}10)$ plane (crosses)*

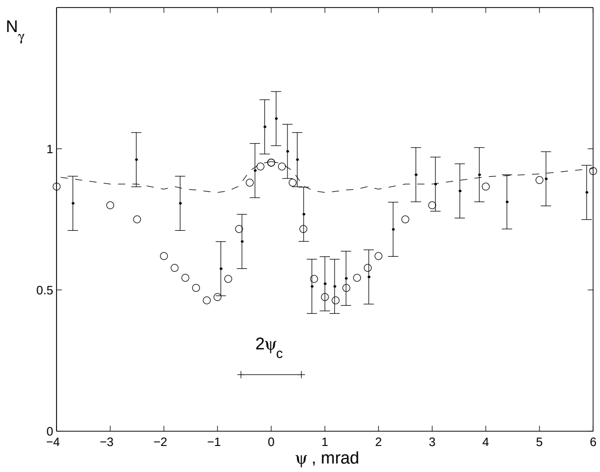

Fig.5. *Photon yields vs the incidence angle of electrons to $\langle 110 \rangle$ axis of diamond crystal of 300 μm thickness [6] (experimental bars) and the relative efficiency of the incoherent radiation as a result of simulation with (circles) and without (dashed line) the collimation of radiation*

In the case of thick crystal the account of collimation of radiation in the experiment also becomes important. In the experiment [6] the registered photons were collimated with the angle $\theta_{coll} = 2mc^2/\varepsilon$. Since the characteristic bremsstrahlung angles for relativistic particles have namely that value, the use of (1) for the radiation intensity integrated over all possible radiation angles is valid. However, the particle passing through the thick crystal could deflect from its initial direction of motion for large angle because of multiple scattering in the lattice. The radiation produced on the corresponding parts of the electron's trajectory would not contribute into the photon yield registered in the experiment. As a result, we obtain deep (about 50%) gap in registered radiation efficiency under $\psi \sim \psi_c$ (see Fig. 5).

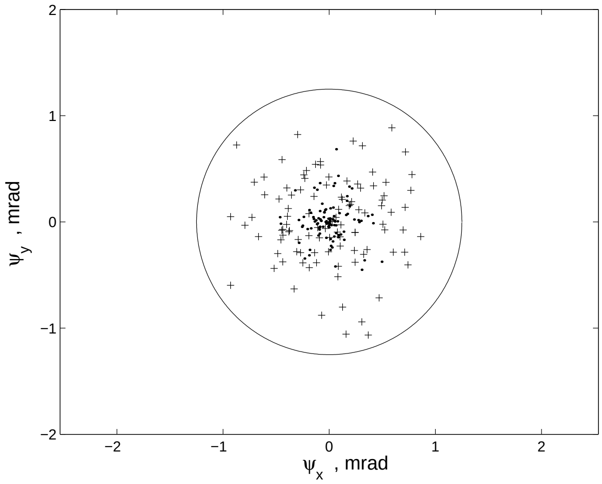

Fig.6. *Angular distributions of incoming (dots) and outgoing (crosses) electrons under conditions of Fig. 5 for the initial beam direction $\psi = 0$. The circle marcs the collimator aperture*

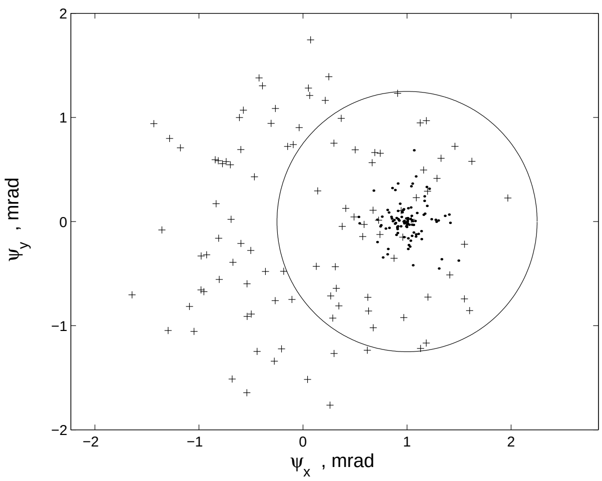

Fig.7. *The same as on Fig. 6 for the initial beam direction $\psi = 1$ mrad. The x axis corresponds to $\langle 001 \rangle$ direction*

The last effect is illustrated by Figs.6-8 where the angular distributions of the electrons outgoing from the crystal are presented. Fig. 7 demonstrates that the main effect responsible to the mentioned gap is the multiple scattering on the atomic strings with conservation of $\psi = \sqrt{\psi_x^2 + \psi_y^2}$ (the so-called "doughnut scattering" [10]), but not the incoherent scattering on thermal vibrations that changes ψ.

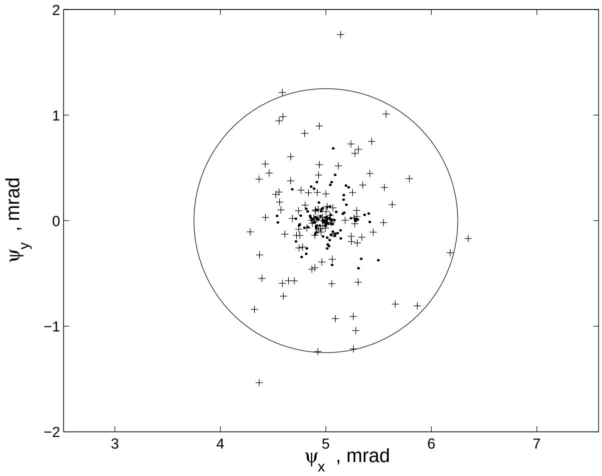

Fig.8. *The same as on Fig. 6 for the initial beam direction* $\psi = 5$ *mrad*

This work is supported in part by internal grant of Belgorod State University.

References

1. J. Lindhard. Influence of crystal lattice on motion of energetic charged particles // *K. Dansk. Vid. Selsk. Mat. Phys. Medd.* 1965, v.34, p.1-64.
2. D.S. Gemmell. Channeling and related effects in the motion of charged particles through crystal // *Rev. Mod. Phys.* 1974, v.46, p.129-228.
3. A.I. Akhiezer, N.F. Shul'ga. *High-Energy Electrodynamics in Matter.* Amsterdam: "Gordon and Breach", 1996, 388p.
4. A.I. Akhiezer, N.F. Shul'ga, V.I. Truten', A.A. Grinenko, V.V. Syshchenko. Dynamics of high-energy charged particles in straight and bent crystals // *Physics-Uspekhi.* 1995, v.38, p.1119-1145.
5. V.F. Boldyshev, V.I. Kasilov, G.D. Kovalenko, et al. // *Nucl. Instr. and Methods.* 1988 B 33, p. 30.
6. V.M. Sanin, V.M. Khvastunov, V.F. Boldyshev, N.F. Shul'ga. Orientation effects in intensity and polarization of γ-radiation emitted by 1 GeV electrons in single crystal // *Nucl. Instr. and Methods.* 1992, B67, p. 251-255.
7. N.F. Shul'ga, V.V. Syshchenko. On the incoherent radiation of relativistic electrons and positrons in crystal // *Problems of Atomic Science and Technology.* 2004, N5, p.112-116.
8. H. Backe, P. Kunz, W. Lauth, A. Rueda. Planar channeling experiments with electrons at the 855 MeV Mainz Microtron MAMI // *Nucl. Instr. and Methods.* 2008, B266, p.3835-3851.
9. M.L. Ter-Mikaelian. *High-Energy Electrodynamic Processes in Condensed Media.* New York: "Wiley Interscience", 1972, 457p.
10. J.F. Bak, J.A. Ellison, B. Marsh, *et al.* Channeling radiation from 2 to 20 GeV/c electrons and positrons (II). Axial case // *Nucl. Phys.* 1988, B302, p.525-558.

ЧИСЛЕННЫЙ РАСЧЕТ НЕКОГЕРЕНТНОГО ТОРМОЗНОГО ИЗЛУЧЕНИЯ БЫСТРЫХ ЭЛЕКТРОНОВ В МОНОКРИСТАЛЛАХ

Н.Ф. Шульга, В.В. Сыщенко, А.И. Тарновский

Некогерентное тормозное излучение быстрых электронов в кристалле обусловлено тепловым разбросом атомов относительно их равновесных положений в решетке. Его интенсивность проявляет существенную ориентационную зависимость при углах падения близких к критическому углу плоскостного или аксиального каналирования. Авторами развита процедура моделирования некогерентного излучения. Результаты моделирования находятся в хорошем согласии с данными эксперимента.

ЧИСЕЛЬНИЙ РОЗРАХУНОК НЕКОГЕРЕНТНОГО ГАЛЬМОВНОГО ВИПРОМІНЮВАННЯ ШВИДКИХ ЕЛЕКТРОНІВ У МОНОКРИСТАЛАХ

М.Ф. Шульга, В.В. Сищенко, А.І. Тарновський

Некогерентне гальмовне випромінювання швидких електронів у кристалі обумовлено термодинамічними флуктуаціями відносно рівноважних положень атомів у решітці. Його інтенсивність демонструє значну орієнтаційну залежність при кутах падіння, що близькі до критичного кута площинного або аксіального каналювання. Авторами розвинуто процедуру моделювання некогерентного випромінювання. Результати моделювання добре узгоджуються з даними експеріменту.