Angular Distributions of DCR from Axially Channeled Electrons in \( \langle 110 \rangle \) LiF Crystal

K B Korotchenko, E I Fiks, Yu L Pivovarov and T A Tukhfatullin
Tomsk Polytechnic University, Tomsk, 634050 Russia
korotchenko@tpu.ru

Abstract. The formulae and new computation method for calculation of angular distributions of diffracted channeling radiation (DCR) from relativistic electrons axially channeled in a crystal are presented. Numerical results are obtained for \( \gamma = 20 \) electrons channeled in \( \langle 110 \rangle \) LiF crystal.

1. Introduction
Parametric X–radiation (PXR) from relativistic electrons is explained in detail in the framework of kinematic and dynamics theories [1]. More detailed theory was proposed in Ref.[2] which takes into account both the channeling of electrons and diffraction of emitted photons. The new combined effect in X-radiation was called in [2] Diffracted Channeling Radiation (DCR). Later, the theory was extended to take into account the band structure of transverse energy levels and initial population of levels (states) for planar channeled electrons in Refs.[3–4]. In Ref.[3] calculations of DCR angular distributions were performed for electrons with relativistic factor \( \gamma = 18,20, 25, 50, 75, \) and \( 100 \) channeled along \( \langle 110 \rangle \) and \( \langle 111 \rangle \) Si planes , while in Ref.[4] for \( \gamma = 107 \) and \( \langle 111 \rangle \) LiF planes.

Here, we present new method of calculations and obtained results for DCR angular distributions from axially channeled electrons. This problem is more complicated compared to the case of DCR from planar channeled electrons [2–4], since one needs:

• to calculate 2D periodic potential for axial channeling;
• to solve 2D eigenvalue problem instead of 1D in order to determine transverse energy band structure and eigenfunctions \( \Psi(r_z,k_z) \) for the Schrödinger equation with relativistic mass of electron \( \gamma m_e \);
• to define initial populations of states and dipole matrix elements using determined 2D eigenfunctions;
• to modify a formula for DCR angular distribution derived in [2–4] for planar channeling to the case of axial channeling.

2. Electron axial channeling in a crystal: a theoretical background
As is well known [5], the wave function \( \Psi(r,t) \) of electron with an energy \( E > 1 \) MeV, channeled along the crystal axis may be written as

\[
\Psi(r,t) = \exp(-i(p_z z - E t) / h) \phi(r_z) . \tag{1}
\]
Here, $\mathbf{r}_\perp$ is the radius vector perpendicular to the channeling axes, $p_\parallel$ is the longitudinal momentum. For the stationary states of the transverse motion along XY–plane the wave function of electron is the solution of the Klein–Gordon equation, which transforms into Schrödinger equation with relativistic mass $m_r$ [5] when $2E_i >> (E_\perp - U(\mathbf{r}_\perp))$, with $E_i = \sqrt{(cp_i)^2 + m_r^2c^4}$ and $E_\perp$ is the energy of electron transverse motion. In a periodic potential $U(\mathbf{r}_\perp)$ which is the case of axial channeling, the wave function $\phi(\mathbf{r}_\perp)$ and energy of transverse motion of electron $E_\perp$ are continuous functions of electron wave vector $\mathbf{k}_\perp$, which lies in the first Brillouin zone (e.g., see[6]). That is:

$$\phi'(\mathbf{r}_\perp, \mathbf{k}_\perp) = \sum_m C'(\mathbf{g}_{\perp m}, \mathbf{k}_\perp) \exp[i(\mathbf{k}_\perp + \mathbf{g}_{\perp m})\mathbf{r}_\perp], \quad (2)$$

Using the Fourier expansion of periodic function $U(\mathbf{r}_\perp) = \sum_m U(\mathbf{g}_{\perp m}) \exp[i(\mathbf{k}_\perp + \mathbf{g}_{\perp m})\mathbf{r}_\perp]$, we obtain the eigensystem problem [5], [7–8]:

$$\sum_m A_{mn} C'(\mathbf{g}_{\perp m}, \mathbf{k}_\perp) = E'(\mathbf{k}_\perp) C'(\mathbf{g}_{\perp m}, \mathbf{k}_\perp), \quad A_{mn} = U_{mn} + \delta(\mathbf{g}_{\perp m}, \mathbf{g}_{\perp n})(\hbar^2 |\mathbf{g}_{\perp m} + \mathbf{k}_\perp|^2 / 2m_r\gamma). \quad (3)$$

Here, $\mathbf{g}_{\perp m}$ are the transverse reciprocal lattice vectors, which lie in a plane perpendicular to channeling axes, $C'(\mathbf{g}_{\perp m}, \mathbf{k}_\perp)$ are the Fourier components of electron wave function $\phi'(\mathbf{r}_\perp, \mathbf{k}_\perp)$, $U_{mn} = U(\mathbf{g}_{\perp m} - \mathbf{g}_{\perp n})$, $\delta(a,b)$ is the Kronecker delta.

3. The solution of eigensystem problem for the case of axial channeling

The numerical methods of solving an eigenvalue problem (3) are well known [7–8]. Unfortunately, the result of the solution of the Eq. (3) is very sensitive to even small variation of potential function $U(\mathbf{r}_\perp)$. That’s why at first we build up the potential $U(\mathbf{r}_\perp)$, and then numerically find its Fourier components.

The experience of using this method for solving the problem (3) with the help of the Mathematica© [3–4] let us develop sufficiently simple and high-performance algorithm. For simulating of potential $U(\mathbf{r}_\perp)$ we use the formula obtained by Doyle and Turner [9] for the potential due to a single atom

$$U_{at}(\mathbf{r}) = -(2\hbar^2 / \sqrt{\pi m_r}) \sum_j a_j c_j^{-3/2} \exp(-r^2 / c_j), \quad (4)$$

where $a_j$ and $b_j = 4\pi^2 c_j$ are the coefficients, obtained by fitting of the electron scattering form factor, $r^2 = z^2 + r_\perp^2$.

Further, we choose Z–axis as channeling axis and integrate formula (4) along this axis. Next we may calculate the Fourier components of the potential using embedded Mathematica© package, but for required accuracy this is a time-consuming operation. It is easy to obtain the following equation for the Fourier components $U_{mn} = U(\mathbf{g}_{\perp m} - \mathbf{g}_{\perp n})$ in the Cartesian coordinates (for {110} LiF crystal):

$$U_{mn} = \left[1 + \exp(-im\pi)\exp(-in\pi)\right] \sum_j F_{x\perp j} F_{y\perp j} + \left[\exp(im\pi) + \exp(-in\pi)\right] \sum_j L_{x\perp j} L_{y\perp j}, \quad (5)$$

where $F_{x\perp j}$ and $F_{y\perp j}$ (the symbols $F$ and $L$ denote the values characterizing fluorine and lithium atoms respectively) are:

$$F_{x\perp j} = \frac{\sqrt{A_j m_r b_{r\perp j}}}{2a} \exp\left(-\frac{m_r^2 \pi^2}{a^2 b_{r\perp j}}\right) \left[-\text{Erfi}\left(\frac{2m_r - ia^2 b_{r\perp j}}{2a \sqrt{b_{r\perp j}}}\right) + \text{Erfi}\left(\frac{2m_r + ia^2 b_{r\perp j}}{2a \sqrt{b_{r\perp j}}}\right)\right].$$
\[ F_{jy} = \frac{\sqrt{A_j a y_j}}{\sqrt{2a}} \exp \left( \frac{2n^2\pi^2}{a^2 b_{Foj}} \right) \left[ -Erfi \left( \frac{4n\pi - ia^2 b_{Foj}}{2\sqrt{2a} b_{Foj}} \right) \right] + \left[ Erfi \left( \frac{4n\pi + ia^2 b_{Foj}}{2\sqrt{2a} b_{Foj}} \right) \right], \] (6)

Here, \( Erfi(x) \) is imaginary error function; \( m \) and \( n \) are integers, that determine the numbers of the components \( U_{mn} \), \( A_j = 2 \times 27.2116a^2d^{-1} \), \( d \) is the distance between atoms the axis, \( a \) is a lattice constant, \( a_o \) is the Bohr radius, \( 4\pi^2b_{Foj} = b_j + 8\pi^2\rho_{1F}^2 \), where \( \rho_{1F} \) is the amplitude of thermal vibrations of fluorine atoms. The formulas for lithium, i.e. \( L_{amj} \) and \( L_{amj} \), are similar to (6).

It should be noted that formulas (5–6) are the exact expressions for Fourier components of 2D–periodic potential \( U(r_j) \). The evaluation of formulas (5–6) using Mathematica© takes only several minutes. The solving of the problem (3) using the formulae (5–6) is performed further using a special procedure in Mathematica© for solution of the linear algebraic eigenvalue problem. Though the very large size of the matrix \( A_{mn} \), the calculation of its values takes about one minute.

### Figure 1a. Schematics of subbarrier energy levels (with number \( n \)) of electron transverse motion.

### Figure 1b. The structure of subbarrier energy levels (with numbers \( n = 1–16 \)) of electron transverse motion (\( \gamma = 20 \)) along \( \{110\} \) LiF.

The results of eigenvalues \( E^i \) calculation for electrons channeled along the \( \{110\} \) LiF axes are presented in Fig.1a and Fig.1b. In fact, every level in Fig.1a is energy band. Red and blue lines on Fig.1b are the odd and even numbers of quantum states corresponding to every energy band. In Fig.1b we denoted every energy level as \( n-\{i_1,i_2\} \), where \( n \) is the number of the level, \( i_1, i_2 \) are the numbers of corresponding quantum states. That is all the levels are double degenerated.

Fig.2 presents the results of calculation of \( |\Psi_i(r,t)|^2 = S^{-1} \phi^*_i(r, k_z) \phi_i(r, k_z) \) for the subbarrier quantum states (with numbers \( i = 0–31 \)) of electrons with relativistic factor \( \gamma = 20 \) (energy 10.22 MeV) channeled along the axis \( \{110\} \) LiF (\( S \) is the part of elementary cell cross–section per one axis [5], i.e. is different for \( L \) and \( F \) atoms). One can see that \( |\Psi_i(r,t)|^2 \) for the initial 22 quantum states (with numbers 0–21) coincide in pairs. For last 10 quantum states (with numbers 22–31) \( |\Psi_i(r,t)|^2 \) are differend – i.e. \( |\Psi_i(r,t)|^2 \) for quantum states of last 5 bands are varying within band.

### 4. DCR from the axially channeled electrons
The axial channeling of relativistic particles is accompanied by spontaneous radiation due to transitions between the energy levels $E'(\mathbf{k}_i)$ and $E'(\mathbf{k}_f)$ of the transverse motion. In the case of axial channeling, one can accept that photons arising under transitions can undergo diffraction on the crystallographic planes (diffraction planes) crossing the channeling axes (Fig. 3).

Fig. 2. $|\Psi_i(r,t)|^2$ for subbarrier quantum states with numbers $i = 0–31$ of electron transverse motion.

Fig. 3 shows the geometry of formation of axial diffracted channeling radiation (DCR). The momentum is conserved only in the direction parallel to the $Z$–axis, than the energy of the emitted photon can be written in the form

$$\hbar \omega = \hbar (\mathbf{gv} + \Omega_g) (1 - \sqrt{\chi_0} \cos(2\theta_B)/c)^{-1},$$

where $\hbar \Omega_g = E'(\mathbf{k}_f) - E'(\mathbf{k}_i)$, $\varepsilon_0 = 1 + \chi_0$ is the dielectric constant and $\chi_0$ is electric susceptibility, $\theta_B = \arcsin(|\mathbf{vg}|/|v_0|)$ is Bragg angle and $\mathbf{g}$ is the reciprocal lattice vector corresponding to the diffraction planes, $v_0$ is the velocity of electron along $Z$–axis.

Fig. 3. Formation of axial DCR from axially channeled electrons.

According to [2], the matrix element of DCR probability (transition probability of electron between energy levels $i \rightarrow f$ with photon emission) is written in the form:

$$M_{gf} = e \langle \phi_f, p_f | \hat{A} \hat{P} | \phi_i, p_i \rangle / \gamma m c.$$

(9)
We had chosen $Z$–axis as channeling axis, so $\hat{p} = (\hat{p}_z, \hat{p}_i)$ is the momentum operator ($\hat{p}_i$ is the electron longitudinal momentum after photon emission), where $\hat{p}_i = m v \gamma$, $A = (A_z, A_i)$ is the photon field that is given in a form of the Bloch wave:

$$A = \sum_{\alpha} A_{\alpha} \exp(i \vec{k}_{\alpha} \cdot \vec{r}) + c.c. = \sum_{\alpha} \sum_{\alpha'} A_{\alpha \alpha'} \vec{e}_{\alpha \alpha'} \exp(i \vec{k}_{\alpha} \cdot \vec{r}) + c.c.,$$  \hspace{1cm} (10)

where $\vec{h} \in (0, \vec{g}, \ldots)$. If we set that the momentum of channeled electron along $Z$–axis is conserved, we can assign arising virtual photon both wave vector $\vec{k}_{\alpha}$ and the polarization vector $\vec{e}_{\alpha \alpha'}$ where $\sigma = \perp$ is the polarization state.

Using Eq. (10), the matrix element $M_{\sigma}'$ (for the $\sigma$–polarized photon) in two–wave approximation ($h = 0, g$) may be decomposed into two parts:

$$M_{\sigma}' = - \frac{e}{\gamma m c} \left\langle \hat{p}_y, \hat{p}_i \right| A_{\alpha 0} \vec{e}_{\alpha 0} \exp(-i \vec{k}_{\alpha} \cdot \vec{r}) \left| \hat{p}_y, \hat{p}_i \right\rangle + \left\langle \hat{p}_y, \hat{p}_i \right| A_{\alpha 0}^* \exp(-i \vec{k}_{\alpha} \cdot \vec{r}) \vec{e}_{\alpha 0} \left| \hat{p}_y, \hat{p}_i \right\rangle. \hspace{1cm} (11)$$

According to [2], the first term in Eq (11) represents or the Čerenkov radiation (when $i = f$), or CR (when $i \neq f$), under the channeling condition. The second term in Eq. (11), according to [2], represents the emission of diffracted photon. When $i = f$ (the transition of the channeled electron is intraband) this term gives PXR under channeling conditions (PXRC). When $i \neq f$, this term describes the emission of diffracted photon due to the interband transition of electron between the transverse states – DCR.

According to Ref. [2], in two wave approximation ($h = 0, g$) may be decomposed into two parts:

$$A_{\alpha g} = A_{\alpha 0}/2 \sqrt{1 + W_{\alpha}^2}, \quad W_{\alpha} = \left( R - \left( \chi_{g} |P_{\sigma}\rangle \langle P_{\sigma}| \right)/R \right)/2 |\chi_{g}| |P_{\sigma}|,$$  \hspace{1cm} (12)

where $W_{\alpha}$ is “resonance error” and

$$R = \left( \theta_{x} - \cot \theta_{y} \Omega_{g}/\omega_{\beta} \right)^2 + \theta_{y}^2 + \theta_{z}^2 + 2 \Omega_{g}/\omega_{g}, \quad P_{\sigma} = \vec{e}_{\alpha 0} \vec{e}_{\alpha \perp}, \quad \theta_{z} = \gamma^{-1} + |\chi_{g}|,$$  \hspace{1cm} (13)

$\omega_{\beta} = c \frac{|g|/2 \sin \theta_{y}}{\Omega_{g}}$ is the Bragg frequency, $\chi_{g}$ is the Fourier component of the electric susceptibility. Then, using the dipole approximation and relation $\langle f |\hat{p}_y, \hat{p}_i |i \rangle = -i \gamma m \Omega_{g} \langle f \hat{r}, |i \rangle \rangle$ one can rewrite the second term of Eq. (11) in the following form:

$$2c \sqrt{1 + W_{\alpha}^2} M_{\sigma \perp} = \text{i} e A_{\alpha 0} \left\langle \hat{p}_y, \hat{p}_i \right| \beta \epsilon_{\alpha g} \hat{k}_{\perp} \cdot \left( \hat{x} \vec{e}_{\perp y} + \hat{y} \vec{e}_{\perp x} \right) + \Omega_{g} \vec{e}_{\perp} \cdot \left( \hat{x} \vec{e}_{\perp y} + \hat{y} \vec{e}_{\perp x} \right) \left| \hat{p}_y, \hat{p}_i \right\rangle. \hspace{1cm} (14)$$

Here, $\vec{k}_{\perp} = \vec{k} - \vec{g} = \vec{k}_0 + \vec{u}$ (Fig.3), $\epsilon_{\alpha g}$ is $Z$–component of $\vec{e}_{\alpha g}$ and we have written the radius vector $\hat{r}$, through its components $\hat{r}_{\perp} = x \vec{e}_{\perp y} + y \vec{e}_{\perp x}$, where the polarization vectors are both $\vec{e}_{\perp y}$ and $\vec{e}_{\perp x}$ are lying in $XY$ plane and $\vec{e}_{\perp \alpha}$ is the polarization vector parallel to the diffraction plane, $\beta = \gamma c$. Formally, Eq. (14) coincides with the formula obtained in Ref.[2] for DCR at planar channeling if $X$–component of radius vector $\hat{r}_{\perp}$ is zero $x = 0$.

Then, taking into account the relations $P_{\parallel} = \vec{e}_{\parallel} \cdot \vec{e}_{\perp 0}$, $P_{\perp} = \vec{e}_{\perp} \cdot \vec{e}_{\perp 0}$, and definition of coordinates [1] $\theta_{x, y} = c (\vec{k} - \vec{k}_{\alpha})_{x, y}$, $\omega_{\beta} = c u_{\alpha, y} \omega_{\beta}^{\alpha}$, $\vec{k}_{\perp} = \vec{k}_{\perp} + \vec{g}$ (Fig.3), one can obtain the radiation probability for DCR

$$w_{g} \propto |M_{\sigma \perp}^r|^2 = |M_{\sigma \perp}^r|^2 = |M_{\sigma \perp}^r|^2 = |M_{\sigma \perp}^r|^2 + |M_{\sigma \perp}^r|^2.$$  \hspace{1cm} (15)

Then number of photons emitted into elementary solid angle per unit length of the crystal:

$$d'N_{g} /d\theta_{x} d\theta_{y} dz =$$

VIII International Symposium on Radiation from Relativistic Electrons in Periodic Structures IOP Publishing Journal of Physics: Conference Series 236 (2010) 012016 doi:10.1088/1742-6596/236/1/012016

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\[
\frac{\alpha \omega_0^2 \beta^4}{4 \pi^2 \sin^2 \theta_\beta} \left( \left( y_{\beta} \theta_{\beta} \theta_{x} + x_{\beta} \theta_{\beta} + x_{\beta} \theta_{\beta} \right) \frac{\Omega_{\beta} / \omega_{\beta} / \beta^2}{1 + W_{\beta}^2} \right)^2 + \left( x_{\beta} \theta_{\beta} + y_{\beta} \left( \theta_{\beta}^2 - P_{\beta} \Omega_{\beta} / \omega_{\beta} / \beta^2 \right) \right) \left( 1 + W_{\beta}^2 \right),
\]

(15)

where \( \alpha \) is the fine structure constant, \( x_{\beta} = \langle \phi_{\beta} \left| x \phi_{\beta} \right\rangle \) and \( y_{\beta} = \langle \phi_{\beta} \left| y \phi_{\beta} \right\rangle \). It is clear that if \( x_{\beta} = 0 \) (i.e. transverse motion exists only along \( Y \)-axis), the formula (15) coincides with the formula obtained in Ref.[2] for DCR at planar channeling.

5. Initial populations and matrix elements for axially channeled electrons
Using calculated 2D wave functions \( \phi^0 (r_x, k_x) \), we may start with analysis of axial channeling radiation and DCR.

First, it is necessary to know initial populations of transverse energy levels of channeling electrons:

\[
P_i (k_o, k_x) = \left| \left\langle \phi^0 (r_x, k_x) \left| \phi^0 (r_x, k_x) \right\rangle \phi^0 (r_x, k_x) \left| d_x, d_y \right\rangle \right|^2 = \phi^0 (r_x, k_x) = \exp(-i k_x r_x).
\]

(16)

Here \( \phi^0 (r_x, k_x) \) is the wave function for transverse motion of incident free electron with wave vector \( k = (k_x, k_x) \), where \( |k_o| \approx |k| \sin \theta \| k \| \theta \), with \( \theta \) being the angle between the \( p = \hbar k \) and channeling axis \( \left( Z \text{-axis} \right) \), \( d_x, d_y \) are the distances between the channeling axes in plane \( XY \).

Fig.5 presents the results of calculation of the initial populations \( P_i (k_o, k_x) \) in the case of electrons with \( \gamma = 20 \) (energy 10.22 MeV) channeled along \( \langle 110 \rangle \) axes of LiF. It is clearly seen that at axial channeling, as well as at planar channeling [3–4], the populations are strongly different for different bands, moreover the populations are nonzero for all bands. It is the effect of 2D periodicity of channeling axial problem. For example, if one considers axial channeling in one–string approximation, at \( \theta = 0 \) the quantum states with nonzero angular momentum are not populated at all.

Second, for calculation of channeling radiation probability in dipole approximation, the transition matrix elements are required:

\[
r_{ij} (k_x, k_x) = \left\langle \phi^0 (r_x, k_x) \right| \phi^0 (r_x, k_x) \left| d_x, d_y \right\rangle.
\]

(18)

However, the calculation with Mathematica© of the matrix elements \( r_{ij} (k_x, k_x) \) according Eq. (18) takes enormous amount of time. We solved this problem in the following way: in Eq. (18) we divided the summation and integration and integrals are computed with special subroutine (written in C++).
Fig. 6 shows the calculated matrix elements $|x_y(k^*_1,k^*_1)|^2$ and $|y_y(k^*_1,k^*_1)|^2$ for electrons with $\gamma = 20$ channeled along the $\langle 110 \rangle$ LiF axes. These results strongly differ from DCR at planar channeling [3-4] – the matrix elements $y_y(k^*_1,k^*_1)$ and $x_y(k^*_1,k^*_1)$ have nonzero values only for several interband transitions.

6. Angular distribution of DCR from axially channeled electrons

For calculations of the angular distribution of DCR at the Bragg angle from initial electron beam, we assume that the contribution to the DCR comes from those channeled electrons that are captured into subbarrier levels (the remaining electrons are involved in the formation of PXR), i.e.

$$d^3N_y/d\theta_x d\theta_y dz = \sum_f \left( \sum_y P_y(k_0,k_1) \right) d^3N_y / d\theta_x d\theta_y dz. \quad (19)$$

Fig. 7 shows the ratio of calculated angular distribution of DCR to the maximal value of RXR (obtained using the standard formula, see e.g. [2]), in vicinity of the Bragg angle $\theta_B \approx 0.32$ rad for the electrons with $\gamma = 20$ channeled along $\langle 110 \rangle$ axes of LiF at incident angle $\theta_0 = 0$.

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**Figure 6.** Calculated matrix elements $x_y(k^*_1,k^*_1)$ and $y_y(k^*_1,k^*_1)$ for $i \rightarrow 3$ transitions.

**Figure 7.** Left: the angular distribution of DCR versus the angle $\theta_y$ (at $\theta_x = 0$) for the electrons with $\gamma = 20$ and incident angle $\theta_0 = 0$ channeled along $\langle 110 \rangle$ LiF; the Bragg angle $\theta_B \approx 0.32$ rad. Right: contour diagram for angular distribution of DCR (only central (2) and maximal (1) peaks) and PXR. The photon energy $\hbar \omega_0 = 2.174$ keV.
Finally, Figure 8 shows 3D fragment of the central and maximal peaks of DCR presented in Fig. 6. The peaks are ring–shaped and have complex doublet structure.

![Figure 8. 3D fragments of the central (left) and maximal (right) peaks of the DCR angular distribution shown in Fig. 6.](image)

7. Conclusions
The developed numerical method of solving 2D Schrödinger equation for axial channelling of electrons allowed for the first time calculations of angular distribution of DCR from axially channelled electrons. The calculations show an appearance of narrow brilliant DCR peaks in vicinity of the Bragg angle. That means, DCR amplitude exceeds sufficiently ordinary PXR amplitude and that DCR can be observed in experiments if the crystal thickness is less than dechanneling length.

The work is partially supported by Russian Science and Innovations Federal Agency under contract No 02.740.11.0238

8. Acknowledgments
The authors are grateful to Prof. H. Nitta for useful discussions.

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