Kumakhov radiation by low-energy axially channeled electrons

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We have developed a method for calculating the band structure and the band population for electrons with energy 1–5 MeV in axial channeling in crystals. We have calculated the band structure for the ⟨111⟩ channel in silicon and diamond crystals. We have investigated the band population as a function of the angle of incidence of the electrons on the crystal. Within the critical channeling angle, in addition to sub-barrier bands, higher, superbarrier bands are also efficiently populated. We show that it is possible to obtain a population inversion of the bands. We have studied Kumakhov radiation in the x-ray region. The radiation in transitions between low-lying sub-barrier states is the most intense. A comparison with experimental data indicates satisfactory agreement of the results.

1. INTRODUCTION

During the last twenty years the channeling of charged particles in crystals has been studied both experimentally and theoretically (see for example the review by Gemmel[1]). The basic physical ideas of channeling were set forth in the fundamental paper by Lindhard.[2] Up to 1975 the greater part of the studies in this area were devoted mainly to channeling of heavy particles (protons, α particles, and so forth).

Beginning in 1976 the channeling of relativistic electrons and positrons has also been studied. This is due in considerable measure to the work of Kumakhov,[3] who predicted the effect of intense spontaneous radiation. In his articles the basis of the classical and quantum theory of this effect was developed, and also it was shown that spontaneous radiation in channeling has a high spectral and spectral-angular density, is polarized, and is spatially monochromatic. These properties of the radiation have attracted the attention of experimenters in the large nuclear centers where electron accelerators are located. Experiments carried out at SLAC,[4] Serpukhov,[5] Saclay,[6] Khar'kov,[7] Tomsk,[8] SUNY,[9] Aarhus,[10] and elsewhere have confirmed the main results of the theory.

At the present time there are already a number of reviews devoted to this problem.[11–13] The spontaneous radiation accompanying channeling of relativistic electrons and positrons has been called in the literature "channeling radiation" or "Kumakhov radiation" (see for example the reviews[11–13]).

At high channeled-particle energies (above 100 MeV a quantum approach is necessary. In the low-energy region (1–10 MeV) the influence of neighboring atomic planes and strings on the motion of the particle turns out to be important, i.e., it is necessary to consider the motion of the electron in the periodic potential of the planes and axes of the crystal.

As a result the energy spectrum of the particle has a band structure. The problem of finding the band structure for electrons in planar channeling was solved in Refs. 14–16. At low electron energies Kumakhov radiation has been investigated by Tulupov.[17]

The present work is devoted to Kumakhov radiation emitted by low-energy electrons moving in an axial channel of a crystal.

2. RADIATION IN AXIAL CHANNELING OF ELECTRONS. THEORY

At relativistic particle energies the potential of interaction of the particle with the crystal is considerably smaller than the total energy of the particle, and the motion of the particle can be described by the Dirac equation with accuracy to terms of order $V^2(\mathbf{r})/E^2$:

$$(-c^2\hbar^2\Delta+m_0^2c^4+2EV(\mathbf{r}))\psi(\mathbf{r})=E^2\psi(\mathbf{r}). \tag{1}$$

We shall consider the thermal vibrations of the crystal atoms to be isotropic and to have a Gaussian distribution in each coordinate. We shall average the potential $V(\mathbf{r})$ over the thermal vibrations:

$$V_t(\mathbf{r})=\int d\mathbf{r}'V(\mathbf{r}-\mathbf{r}')f(\mathbf{r}'), \tag{2}$$

$$f(\mathbf{r}')=\frac{1}{(2\pi u_1^2)^{3/2}}\exp(-\mathbf{r}'^2/2u_1^2), \tag{3}$$

where u_1^2 is the mean square of the one-dimensional amplitude of the vibrations of the atoms.

We shall introduce the continuous potential of an atomic string[2]:

$$U_t(\mathbf{R})=\frac{1}{d}\int dzV_t(\mathbf{r}), \tag{4}$$

where d is the distance between atoms in the string, z is the coordinate directed along the string, and $\mathbf{R}=\{x,y\}$ is the coordinate in the plane transverse to the channel axis. Then the electron wave function can be represented in the form of the product of the wave function of the free motion along the z axis and the wave function of the transverse motion $\psi(\mathbf{R})$ which satisfies the Schrödinger equation with the relativistic mass of the particle:

$$\left[-\frac{\hbar^2}{2m}\nabla_{\mathbf{R}}^2+U_t(\mathbf{R})\right]\psi(\mathbf{R})=E_\perp\psi(\mathbf{R}), \tag{5}$$

where $E_\perp$ is the transverse energy of the particle.

In the transverse plane the potential (4) is a periodic function

$$U_t(\mathbf{R})=U_t(\mathbf{R}+\mathbf{a}), \tag{6}$$

where $\mathbf{a}$ is the two-dimensional lattice constant (in the transverse plane). In view of the Bloch theorem the wave function

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of the particle in the periodic potential (6) is subject to the condition

$$\psi(\mathbf{R}+\mathbf{a})=\exp(i\mathbf{k}_\perp a)\psi(\mathbf{R}), \tag{7}$$

where $k_\perp$ is the two-dimensional quasimomentum of the particle. We shall expand the continuous potential of the string and the wave function in the reciprocal lattice vectors **G** and **H** ($\mathbf{G}=k\mathbf{g}_1+l\mathbf{g}_2$, $\mathbf{H}=m\mathbf{g}_1+n\mathbf{g}_2$):

$$U_t(\mathbf{R})=\sum_{\mathbf{H}} U_{\mathbf{H}}\exp(i\mathbf{H}\mathbf{R}),$$

$$\psi(\mathbf{R})=\exp(i\mathbf{k}_\perp\mathbf{R})\sum_{\mathbf{G}} C_{\mathbf{G}}\exp(i\mathbf{G}\mathbf{R}). \tag{8}$$

It is easy to see that this expansion satisfies the Bloch condition (7).

Let us substitute the expression (8) into the Schrödinger equation (5). We obtain a system of algebraic equations from which we can determine the coefficients of the expansion of the wave function $c_{\mathbf{G}}$ and the particle energy spectrum:

$$\left[\frac{\hbar^2}{2m}(\mathbf{k}_\perp+\mathbf{G})^2-E_\perp\right]C_{\mathbf{G}}-\sum_{\mathbf{H}} U_{\mathbf{H}}C_{\mathbf{G}-\mathbf{H}}=0. \tag{9}$$

The system of equations (10) has an infinite number of terms, and for specific calculations it can be cut off as follows. The Fourier coefficients in the expansion for the potential fall off rapidly with increase of **H**, and therefore the expansion can be terminated when $U_{\mathbf{H}}/U_{0,0}\ll 1$. Furthermore, with increase of the transverse momentum of the electron, i.e., with increase of the transverse energy, the particle energy spectrum goes over to a continuous spectrum and the effect of the continuous potential of the atomic strings on the wave function of the transverse motion become unimportant. Hence it follows that **G** must be sufficiently large to satisfy the condition

$$\hbar^2\mathbf{G}^2/2m\gg U_{0,0}. \tag{10}$$

The expansion coefficients of the wave function $C_{\mathbf{G}}$ determine the populations of the levels in the bands and the dipole matrix element of the transition. If we match the electron wave function and its first derivative in free space at the crystal boundary with the functions inside the crystal, we find that the probability of population of a level in a band with number j is given by the formula

$$P_j=|C^j_{k,l}\delta_{k_x,k_{\perp x}+kg_x}\delta_{k_y,k_{\perp y}+lg_y}|^2, \tag{11}$$

where k_x,k_y–x, and y are the components of the electron momentum outside the crystal. Since

$$k_x=p\varphi\cos\xi/\hbar, \quad k_y=p\varphi\sin\xi/\hbar,$$

where p is the electron momentum and ξ is the polar angle, we have the possibility of investigating the population of the bands as a function of the angle of incidence φ of the particles with respect to an atomic string.

In calculation of the spectra of Kumakhov radiation by electrons with energy in the MeV range it is possible to use the dipole approximation.[18] In the very interesting case of radiation along the path of the particle (the energy of the quanta lies in the x-ray range) the number of quanta emitted by an electron per unit pathlength is given by the expression[19]

$$\frac{d^2N}{dz\,d\Omega}=\frac{e^2\omega_{j,j'}|p_{\perp j,j'}|^2}{\pi\hbar(m_0c^2)^2}, \tag{12}$$

where

$$\omega_{j,j'}=\Omega_{j,j'}/(1-\beta_\parallel), \quad \Omega_{j,j'}=(E_{\perp j}-E_{\perp j'})/\hbar,$$

$d\Omega$ is the element of solid angle, and $p_{\perp j,j'}$ is the dipole matrix element of the transition, which is determined by direct calculation,

$$p_{\perp j,j'}=-\hbar\sum_{k,l,k',l'} C^j_{k,l}C^{j'}_{k',l'}(kg_x+lg_y)\,\delta_{k_\perp+kg_x+lg_y,\,k_\perp'+k'g_x+l'g_y}. \tag{13}$$

It follows from (12) that in the dipole approximation the quasimomentum of the electron is conserved during the radiation.

The continuous potential $U_t(\mathbf{R})$ can be obtained from analytic approximation of the atomic scattering amplitudes calculated by Doyle and Turner[20] in the Hartree-Fock approximation. After averaging over the thermal vibrations and along the atomic string we obtain

$$U_t(R)=\sum_{i=1}^{4}\frac{2\hbar^2}{m_0d}\frac{a_i}{b_i/(2\pi)^2+2u_1^2}\exp(-R^2/(b_i/(2\pi)^2+2u_1^2)). \tag{14}$$

Another possibility is use of the Moliere potential. In this case the continuous potential of the string has the following form[21]:

$$U(R)=\frac{2z_1z_2e^2}{d}\sum_{i=1}^{3}c_iK_0(b_iR/a_{\mathrm{TF}}), \tag{15}$$

where $K_0(y)$ is a modified Bessel function of the second king of zero order. Averaging (15) over the thermal vibrations requires an additional numerical integration. The influence of thermal vibrations can be taken into account in a somewhat different way. The value of $U_t(0)$ is determined analytically[21]:

$$U_t(0)=\frac{z_1z_2e^2}{d}\sum_{i=1}c_i\exp(b_i^2u_1^2/2a_{\mathrm{TF}}^2)E_1(b_i^2u_1^2/2a_{\mathrm{TF}}^2), \tag{16}$$

where $E_1(y)$ is the exponential integral function. For $0\leqslant R\leqslant\sqrt{2}u_1$ the potential of the string is approximated by a parabola, the location of the vertex of which is given by the expression (16), and at $R=\sqrt{2}u_1$ the parabola is matched to the potential (15), while for $R>\sqrt{2}u_1$ the continuous potential is used in the form (15). Below we shall present the results of a calculation with the two approximations considered for the potential.

3. RESULTS OF THE CALCULATION

The results of calculation of the energy band structure for silicon and diamond crystals as a function of electron energy are shown in Fig. 1. From this figure it can be seen that with increase of the energy the number of bands in the potential well increases. The lower levels have practically no band broadening, and at $E\sim 5$ MeV only the upper sub-bar-

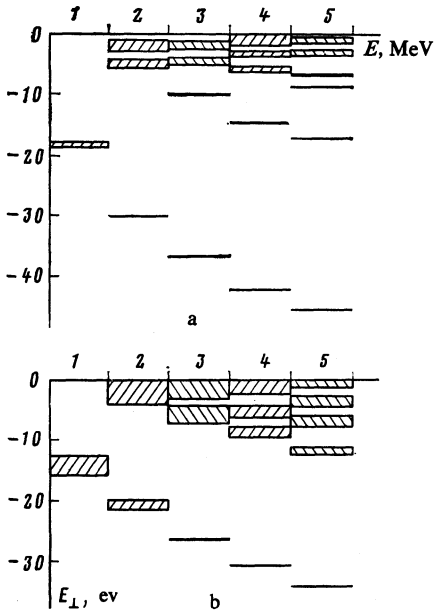

FIG. 1. Band structure for electrons in axial channeling in crystals of silicon (a) and diamond (b) as functions of the energy. The axis is ⟨111⟩, and the allowed bands are hatched.

rier levels are broadened. For a diamond crystal the bands turn out to be broader, since the potential well is shallower (less than z_2) and the strings are more closely spaced, i.e., the mutual influence of neighboring potential wells is greater.

In Fig. 2 we have shown the first Brillouin zone for a two-dimensional lattice, and also the dependence of the transverse energy of the electron on the quasimomentum as it varies from zero to the band edge (the point k_1). We can see from Fig. 2 that for the first band the dependence of the

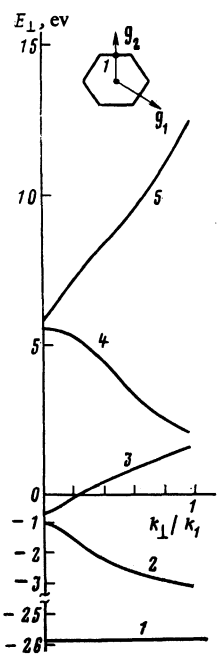

FIG. 2. Transverse energy as a function of quasimomentum for electrons with $E_{kin} = 1$ MeV moving in a ⟨111⟩ channel of a silicon crystal.

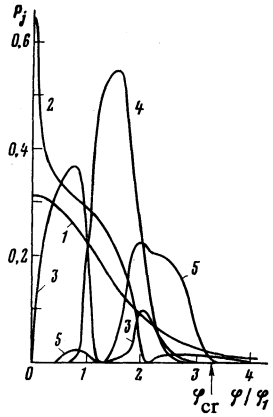

FIG. 3. Probability of population of bands as a function of the angle of incidence of the electron beam for the ⟨111⟩ axis of a silicon crystal; $E_{kin} = 1$ MeV. The numbers of the curves coincide with the numbers of the bands.

transverse energy of the particle on the quasimomentum can be neglected, whereas the second band has a width ~2 eV. With increase of the transverse energy this dependence becomes stronger and stronger and approaches a parabolic dependence.

In Fig. 3 we have shown the results of calculation of the probabilities of population of bands as a function of the angle of incidence of electrons with $E_{kin} = 1$ MeV with respect to the ⟨111⟩ axis of a silicon crystal. The angle φ_1 corresponds to the point 1 in Fig. 2 ($\varphi_1 = 2\pi\sqrt{2}\hbar/pa$, where a is the lattice constant, and for $E_{kin} = 1$ MeV we have $\varphi_1 = 2.27 \cdot 10^{-3}$ rad). The arrow shows the Lindhard critical channeling angle. Within the critical angle not only sub-barrier bands, but also the superbarrier bands 4 and 5 are efficiently populated. Only for angles $\varphi \lesssim \varphi_1$ are practically all particles captured inside the potential well. However, as will be shown below, the radiation in transitions from superbarrier bands turns out to be less intense than in transitions inside the potential well.

By choice of the angle of incidence it is possible to achieve an inverted population of the bands: for example, the difference of the populations of the second and first bands can reach about 10%. It must also be taken into account that the particles which populate the first band will be scattered significantly faster than in the second band, which will lead to an increase of the inversion.

As in the case of planar channeling, in axial channeling it is possible to distinguish three types of transitions for radiation during channeling and under conditions close to channeling[17]:

1. Transitions between bands inside the potential well (Kumakhov radiation).

2. Transitions from superbarrier bands into the potential well.

3. Transitions between superbarrier bands (radiation during quasichanneling).

The number of quanta radiated by an electron per micron of path for all three types of transitions was calculated as a function of the angle of incidence onto the crystal for the ⟨111⟩ axis in silicon (Fig. 4). The transition 2–1 (the first

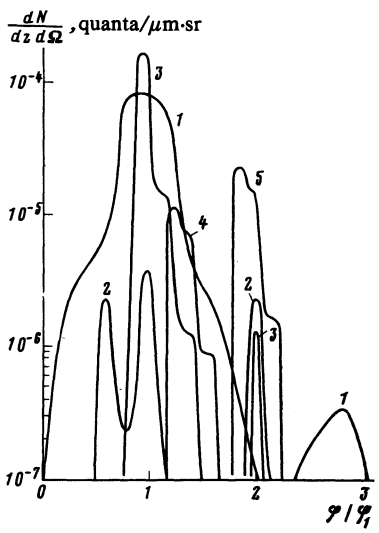

FIG. 4. Number of quanta radiated per unit pathlength along the motion of the particle, as a function of the angle of incidence of the electrons on a silicon crystal; the axis is ⟨111⟩ and $E_{kin} = 1$ MeV. The transitions are as follows: (1) 2–1, (2) 3–1, (3) 4–1, (4) 4–2, (5) 4–3.

type) turns out to be the most intense, and the number of quanta changes relatively little over a wide range of angles of incidence; the band broadening for this transition turns out to be small in comparison with other transitions. The transitions 4–1 and 4–3 turn out to be comparable in intensity with the 2–1 transition, but only in a narrow range of angles of incidence. On taking into account the real angular divergence of the electron beam, the number of quanta emitted in these transitions decreases greatly and they turn out to be an order of magnitude less intense than the 2–1 transition. It follows from this that for practical use the transitions between low-lying sub-barrier states turn out to be most efficient. This fact is confirmed by experiments.[9,10] Comparison of the results obtained above with those of Ref. 17 shows that radiation during axial channeling of electrons turns out to be more intense than in planar channeling at the same energy.

4. COMPARISON OF THEORETICAL AND EXPERIMENTAL RESULTS

In Fig. 5 we compare the orientation dependences observed at Aarhus[10] (circles and crosses) with the results of theoretical calculations (curves). The thickness of the silicon crystal was 1.2 μm, the electron beam energy was 4 MeV, the angular divergence of the beam was 0.05°, the solid angle of quantum detection was $0.6 \cdot 10^{-6}$ sr, and the detection efficiency was $\gtrsim 50\%$ in the range of energies 1–8 keV.[10] It follows from Fig. 5 that satisfactory agreement between theory and experiment is observed, but it is necessary to take into account that bremsstrahlung was also detected in the experiment in addition to Kumakhov radiation. In our calculations we considered only radiation during channeling. Therefore if we subtract the background from the experimental results, the difference from the theoretical curves will become more substantial.

Below we compare the theoretical and experimental[10] values for the energy of the radiated quanta in keV:

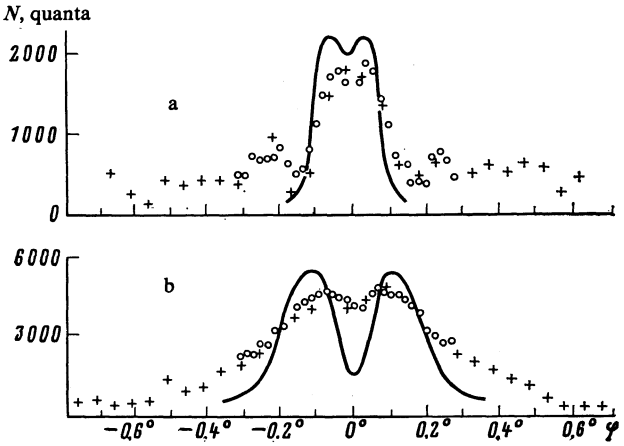

FIG. 5. Orientation dependence of the number of quanta radiated by electrons in traversing the ⟨111⟩ channel in a silicon crystal. $E = 4$ MeV. (a)—Transition 5–1, (b)—transition 2–1.

Moliere potential	6.5	4.4	2.1	1.3
Potential (14)	6.3	4.0	2.4	1.3
Experiment	6.7	4.5	2.3	1.2

These data indicate that the Moliere potential matched to a parabola gives better results than the potential (14).

Thus, our investigations show that representation of the wave function of the transverse motion of the particle in the form of a set of Bloch waves can be used effectively for calculations of the spectra of Kumakhov radiation. However, at energies above 5 MeV (and for crystals of heavier elements even at lower energies) the number of Bloch waves, which determines the number of equations in the system (9), becomes too large, and this produces definite difficulties in numerical calculations. An alternative to the approach used by us is the method of solution of the Schrödinger equation in the single-string approximation,[22] which permits calculation of the position of the energy levels of a channeled electron up to energies 100 MeV. However, in this case the position of the superbarrier bands is not determined and consequently the contribution to the radiation spectrum from transitions of types 2 and 3 is not taken into account.

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