Induced and spontaneous transitions between discrete levels of electrons channeled in crystals

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The spectrum of quasicharacteristic radiation of channeled particles is studied as a function of the crystal parameters and the energy and directivity of the beam. A theory of dechanneling which takes into account elastic scattering of the channeled electrons by nuclei is developed. It is shown that the dependence of the dechanneling length on the form of the wave function has a strong effect on the ratio of the intensities of individual spectral lines in thick crystals. A scheme for creation of population inversion between levels of the transverse motion is proposed. The band structure of the superbarrier levels of a channeled electron is investigated. The pulsations of the width of the allowed and forbidden superbarrier bands on variation of the beam energy or the crystal parameters is calculated. The values of the matrix elements of transitions between super-barrier and sub-barrier levels are compared.

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The use of relativistic electron fluxes moving in external electromagnetic fields to obtain radiation has increased in interest in recent years in connection with the problem of creating sources of short-wave radiation. Particularly promising in this connection is the recently predicted and observed radiation of relativistic leptons channeled in single crystals (see the review by Wedell). In a number of experiments devoted to study of the radiation of channeled particles, in the background of an extended spectrum one clearly distinguishes peaks corresponding to transitions between discrete energy levels of the transverse motion. This circumstance provides an analogy between channeled particles and a relativistic beam of excited atoms. Here the questions which have become traditional in laser physics naturally arise. What are the probabilities of spontaneous and induced transitions in a system of channeled particles? What information on the medium (the crystal) can be obtained from analysis of the radiation spectrum? And finally, is it possible to create a short-wave laser based on channeled particles?

The last question is especially interesting for possible applications. However, for an answer to these questions sufficient experimental and theoretical bases do not yet exist. Therefore the study of questions related to the thorough elucidation of the fundamentals of radiation during channeling (such as determination of the transition matrix elements, creation of population inversion, estimates of level widths, and so forth) is extremely important.

The present article is devoted to investigation of the influence of the parameters of the channeled-particle + crystal system on the spectrum of quasicharacteristic radiation. In the first section we determine the rate of redistribution of the population of the levels of the transverse motion of a channeled particle under the influence of elastic scattering of the particle by the atoms of the crystal lattice. The interest in such investigations is due to the fact that these processes lead both to a broadening of the radiation line and to a change of the ratio of intensities of individual spectral lines in crystals of various thicknesses. In the second section we show that the dependence of the dechanneling length on the form of the "transverse" wave function can be used to invert the levels population. Calculations carried out have shown that in production of radiation it is more efficient to use levels in a nonunimodal (i.e., multihumped) interplanar potential, since in this case the maxima of the probability density of the electron coordinates at the upper working level are reached in the interplanar space, thereby increasing the partial dechanneling length decreasing the level width, and consequently lowering the threshold for production of radiation. The third section is devoted to calculation of the spectra of the quasicharacteristic radiation. The values of the dipole moments of transitions between sub-barrier levels calculated for various forms of potential are compared. For the first time an accurate calculation is made of the band structure of the superbarrier levels for an interplanar potential other than the Kronig-Penney potential. Values of matrix elements are estimated for transitions between superbarrier levels and from them to sub-barrier levels.

1. INFLUENCE OF THE DISCRETENESS OF AN ATOMIC PLANE ON THE POPULATION OF THE LEVELS OF THE TRANSVERSE MOTION

The radiation spectrum of a channeled particle is quite well described in the framework of the model of an averaged potential of the planes of the form

\[ V(x) = \sum_{x_n,0} V_n \exp \left( \frac{iKx_n^2}{2} \right), \]

\[ V_n = \frac{1}{\Omega} \int V(r) \exp(-iKx) dr, \tag{1} \]

where \( V(r) \) is the static potential of the crystal lattice, \( \Omega \) is the volume of the unit cell of the crystal, and \( x \) is the rms amplitude of the thermal vibrations of the crystal atoms. The \( x \) axis is chosen perpendicular to the plane of channeling. The spectrum calculated for a number of simple approximations of the interplanar potential is actually in good agreement.
with the experimental spectrum, as has been shown in Refs. 2 and 3. The averaged potential approximates the real potential best for levels in which the probability of finding the particle near an atomic plane is small. In some low-lying sub-barrier levels this probability is rather large, and therefore a more complete description of the motion of particles which are in these levels requires inclusion in addition to the averaged potential of the Coulomb divergence of the potential near the centers of the nuclei. These perturbations of the potential produce transitions of electrons between levels of the transverse motion in the averaged potential, which leads to a dependence of the level width on its number. It is most natural to choose the perturbing potential as follows:

$$V, (r) = V(r) - V_0(r) = V_{K_{erp}}(iK - x_i^2),$$  

(2)

From the Dirac equation it is possible to obtain the following equation for the spatial part of the wave function of a channeled electron with energy $E$:

$$\Delta_k + \pi^2 - U(r) = 0;$$

(3)

We shall choose a system of reference such that the $z$ axis is perpendicular to the entrance face of the crystal and lies in the channeling plane, and the $x$ axis as before is normal to the channeling plane. We shall represent the solution of Eq. (3) in the form of the following sum:

$$\psi(r) = \sum_n \psi_n(y, z) u_n(x).$$

(4)

Here we assume summation over all sub-barrier levels and integration over the allowed bands of superbarrier energies; $u_n(x)$ are the eigenfunctions of Eq. (3) with the potential $V_0(x)$. If we take as the potential of an individual atom the screened Coulomb potential

$$V_0(r) = -\frac{Ze^2}{r} \exp\left(-\frac{|r-x_i|}{b_0}\right),$$

then the average potential $V_{av}(r) = V_0(r)$ has the form

$$V_{av}(x) = \frac{-ze^2}{2} \exp\left(\frac{x^2}{2b_0^2}\right) \times \left\{ 1 - \Phi\left(\frac{x}{b_0}, \frac{x}{a_{1/2}}\right) \right\},$$

(5)

where $e^{-1}$ is the density of atoms in the channeling plane and $\Phi \{g\}$ is the probability integral. It is easy to see that $|\psi_n(y, z)|^2$ has the meaning of the density of population of the $n$th level in the channel at the point with coordinates in the channeling plane $(y, z)$.

Substituting (4) into (3) and using the orthogonality of the functions $u_n(x)$, we obtain the following equation for $\psi_n(y, z)$:

$$\Delta \psi_n + k^2 \psi_n - \sum_m M_{nm} \psi_m;$$

(6)

here

$$M_{nm}(y, z) = \int \psi_n^* (x) U_n (r) u_m (x) dx,$$

$$k^2 = \frac{\nu^2}{m^2} \Phi (gy^2 + \phi^2 h^2),$$

$$k_{nm} = k^2 + 2mE_{nm}/\hbar^2.$$
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in it by

Thus, the dechanneling length is determined by the overlap

where

Substituting into this formula the expression for

form

Taking into account the smallness of the perturbing

terms, we can rewrite Eq. (16) in the form:

where

Substituting into this formula the expression for \( U_i(\mathbf{r}) \) in the
form (2), we can easily transform it to the following form:

where

\( U_{\ell}(L) \) is a function which coincides in form with the
expression (2) and with the screening radius \( b_{\ell} \) replaced in it by

\( b_{\ell} = (\hbar k_e + K)^{-1} \).

Taking into account the smallness of the perturbing terms, we can rewrite Eq. (16) in the form:

\[
P_{\ell}(L) = P_{\ell}(0) \exp \left( - \frac{L}{L_{\ell}^*} \right),
\]

where the partial dechanneling length \( L_{\ell}^* \) is determined by the following expression:

\[
(L_{\ell}^*)^{-1} = \int \frac{d^2q}{4\pi^2} |\mathbf{K}(\mathbf{r}, K)| \int \frac{d^2q}{4\pi^2} |\mathbf{K}(\mathbf{r}, K)|
\]

Thus, the dechanneling length is determined by the overlap of the square of the modulus of the wave function of the transverse motion of the channelled electron and the function \( G(x) \). The function \( G(x) \) is a sum of averaged potentials \( U_{\ell}(\mathbf{r}, K) \), i.e., of bellshaped functions with maxima in the atomic plane and screening radii \( b_{\ell} \) smaller than \( b_0 \). The contribution of each component \( K \), is determined by the Gaussian factor. Therefore as \( u \to 0 \) the half-width of the function \( G(x) \) will approach zero, and for finite \( u \) it can be estimated as

\[
h_{\ell} = \hbar k_e (b_0^2 + u^2)^{-1/2}.
\]

The integral over \( q \) in the expression for \( G(x) \) leads to unimportant phase factors. For example, if the beam incident on the crystal is approximated by a spherical wave with a divergence \( \Delta q \) and a direction of the wave vector \( \mathbf{k}_0 = (0, q_0, 0) \), determined by the geometry of the experiment, then for \( \Delta k \leq k_0 \) this integral will have the following form:

\[
\Delta x = \int dq \exp \left( \frac{-q_0^2}{4\Delta k} \right) \frac{1}{2\Delta k} e^{i(k_0 - q_0) x}
\]

where \( \Delta x \) is the distance between the target and the source.

Thus, according to Eqs. (18)-(20) the partial dechanneling length will depend on the form of the wave function of the given level, on the radius of the distribution of electronic charge of the atom, and, through the amplitude of the thermal vibrations, on the temperature of the crystal. Using these dependences, we can control the value of the population of distinguished levels in the crystal volume. \(^1\)

2. INVERSION IN NONUNIMODAL POTENTIAL WELLS

It follows from the investigations presented above that the particles which are dechannelled most rapidly are those in levels in which the wave function reaches a maximum in the atomic plane. In unimodal symmetric interplanar potentials, such levels will be levels with even numbers, which gives the possibility of obtaining by choice of the sample thickness an inversion of the population between even and odd levels. \(^2\) A deficiency of this scheme is the relative smallness of the dechanneling lengths of the particles in the two selected levels. This is due to the fact that in a unimodal well the maxima of the wave functions of the first few levels, for which the inversion mechanism indicated is most effective, are reached at distances comparable with the amplitude of thermal vibrations of the atoms. Optimization of the process of creating a population inversion, as we shall see below, is possible if we form the channel using atomic planes in which the interplanar potential is nonunimodal, such as the (111) plane in a diamond-like lattice (Fig. 1). In nonunimodal wells we can introduce the concept of levels of molecular and atomic types. In levels of the atomic type the electron moves in a potential determined mainly by the distribution of the charge of one of the crystal planes. In levels of the molecular type the potential is a superposition of the potentials of two nearest neighbor planes. In Fig. 1 the levels of the molecular type lie above the "hump" of the potential, i.e., they have energies \( E_m < U(0) \).

To produce an inversion, as was noted in Ref. 6, it is
necessary to take a crystal of thickness $L$ such that $L_1 < L < L_2$, where $L_1$ and $L_2$ are the partial dechanneling lengths of electrons in the lower and upper working levels.

Since the width of the line produced is inversely proportional to the dechanneling length of the lower working level, it is desirable that the upper of the levels of the atomic type be odd. In Fig. 2 as an illustration we have shown the pattern of the distribution of probabilities for the coordinates of electrons in the levels of the transverse motion in channeling in the (111) plane of silicon for a beam energy $E = 10$ MeV.

An idea of the magnitude of the population of levels of the molecular type is given in Fig. 3, in which we have shown the transformation of a plane electron wave incident on crystal from outside as it propagates in the crystal. It is evident from the figure that the probability of population of level 3 in this case is rather high, since just this level makes the maximum contribution to the region $x = 0$.

In addition to the increase of the partial dechanneling lengths corresponding to levels of the molecular type, the half-width of the wave functions of these levels also increases appreciably, and consequently the matrix elements of radiative transitions from them also increase. In Table I we have given values of the matrix elements in the potential of the (111) plane of silicon for $y = 10, 16, 24$ (compare with Table II).

Using these data, we can easily evaluate the threshold density of the electron current at which the gain due to induced radiation exceeds the loss. For a single hump potential, corresponding estimates were made by us in Ref. 6 (see

| Transition | $|\gamma_{max}| \cdot A$ | $|\gamma_{max}| \cdot A$ |
|------------|----------------|----------------|
| $y=10$     | $y=16$ | $y=24$ |
| 1-0        | 0.347 | 0.570 | 0.329 |
| 2-1        | 0.356 | 0.338 | 0.223 |
| 3-2        | -     | 0.177 | 0.392 |
| 4-3        | -     | 0.045 | 0.058 |
| 5-4        | -     | 0.029 | 0.430 |
| 6-5        | -     | 0.018 | 0.005 |

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also Ref. 7. Using the values given in Table I, it is easy to see that the combined action of the factors enumerated above decreases by at least an order of magnitude the threshold current density reaches the quite achievable value $j = 10^5 \text{A/cm}^2$ (compare with Ref. 6).

Similar methods can be used to create an inversion in channeling of positive particles; indeed, in channeling in the (111) plane of crystals of the NaCl type the interplanar potential for positively charged particles is nonunimodal. In this case also it is not difficult to achieve a situation in which the first of the levels of the molecular type will have a maximum of the wave function in a plane consisting of the atoms with smaller atomic number.

3. ENERGY SPECTRUM OF THE TRANSVERSE MOTION

In the energy spectrum of the transverse motion of a channelled particle it is possible to distinguish two groups of levels: sub-barrier (with transverse energy $E_L < 0$) and superbarrier with $E_L > 0$. The role of the sub-barrier levels, both in channeling and in radiation during channeling, has been studied in considerable detail in the literature. We note here only the fact that these levels are not very sensitive to the form of interplanar potential, and therefore sufficiently good approximations for the potential exist. This permits accurate calculation of the characteristics of the interaction of channelled particles with electromagnetic radiation.

As an illustration we compare below a modified Moliere potential and a Pöschl-Teller potential.

In Fig. 4 we have given the potential of the (110) plane of silicon obtained by averaging over the channeling plane the Moliere potential of an individual atom (the modified Moliere potential), and its approximation by a Pöschl-Teller potential:

$$U(x) = U_{\text{mp}}/\sqrt{x}$$

and by a potential of the form

$$U(x) = U_{\text{pt}}/\sqrt{2x}.$$

We note that the latter potential is convenient for calculation of radiation spectra by computer.

In Table II we have given values of the matrix elements of transitions between levels with numbers which coincide with the numbers of the columns and rows at the intersection of which the given element appears. Above the diagonal of the table are elements calculated by computer for a modified Moliere potential, and below the diagonal are elements calculated analytically for the Pöschl-Teller potential.

Calculations were carried out for channeling of 56-MeV electrons in the (110) plane of silicon. It can be seen from the table that rather good agreement is observed between the two calculations.

A question which has been little investigated in channeling theory is that of the form of the energy spectrum of superbarrier levels. The studies which have been carried out up to this time apply to the case of a Kronig-Penney rectangular potential. In the present section we shall discuss the question of the shape of the spectrum of superbarrier levels and its dependence on the parameters of the crystal and beam for the case of a potential which is closer to the real interplanar potential than is the potential mentioned above, namely, for a periodic sequence of Pöschl-Teller potentials

$$U(x) = U \sum_{n=-\infty}^{\infty} \{\text{ch} \alpha(x-n)\}^{-1},$$

where $d$ is the interplanar distance.

We note that if the condition $1 - (\tanh (ad/2)|\xi|)$ is satisfied, the potential in each of the periods is essentially no different from that given by (21). This condition is satisfied for all cases of channeling of interest to us; for example, for the (110) plane of silicon we have $1 - \tanh (ad/2) = 0.003$.

If we take as linearly independent solutions in one interval of periodicity even and odd wave functions, then the dispersion equation is well known to have the form

$$\cos Kd = \frac{u(s)u'(s) + v(s)v'(s)}{u'^2 - v'^2},$$

where $u(s) = u - s\alpha$, $v(s) = v - s\alpha$, $\alpha = d/\lambda$, and $K$ is the quasimomentum of the transverse motion of the electron. It can be seen from Eq. (24) that the boundaries $E_L$ of the allowed energy bands are determined by the two conditions

$$u(s, \alpha) = 0.$$
(the center of the Brillouin zone, \( K = 0 \)) and
\[ u_{+} (a) = 0 \]  
(18)

(the edge of the Brillouin zone, \( K = \pm \pi/d \)).

In the Pöschl-Teller potential the even and odd wave functions for positive energy values have respectively the forms\(^{16}\)
\[ u(x) = A \cosh^{-1} (ax) F (a', b', 1/2; \cosh^2 (ax)), \quad v(x) = B \sinh (ax) F (a', b', 1/2; \cosh^2 (ax)) \]  
\[ (27) \]
where
\[ a' = (s - ia)/2, \quad b' = (s + ia)/2, \quad x = (2mE/\hbar^2) \frac{r}{d}. \]

The expressions (27) and (28) can be reduced to the following more convenient form:
\[ u(x) = A \cosh^{-1} (ax) F (a', b', 1/2; \cosh^2 (ax)), \quad v(x) = B \sinh (ax) F (a', b', 1/2; \cosh^2 (ax)) \]
\[ (27a) \quad (28a) \]
where \( P_{+}(x) \) is the spherical function of the first kind. Substituting the latter expressions into the equalities (25) and (26), it is straightforward to obtain the following equations:
\[ \cos \left[ \frac{k_0 d + \rho}{2} \right] = t, \]
\[ (29) \]
where
\[ t = \frac{\Gamma (1 + i \gamma) \Gamma (n - a)}{\Gamma (1 + i \gamma) \Gamma (n)} - \frac{\cosh (ax)}{(\sinh^2 ax + \sin^2 (nx))^n} \]
\[ \times \exp \left\{ -2 \text{arctg} \left( \frac{x}{n} \right) \right\}. \]
\[ (30) \]

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\[ (30) \]

The plus sign in Eq. (29) leads to the values of the limiting energy reached in the center of the Brillouin zone and the minus sign leads to the values at the edges of the Brillouin zone.

It follows from Eqs. (29) and (30) that the maximum width of the forbidden band is reached for \( s = n + 1/2 \), where \( n \) is an integer. In this case \( |r| = \tanh \pi n \), and therefore the width of the forbidden band increases as \( s \to 0 \). When the parameter \( s \) is equal to an integer, we have \( T = 1 \), the reflection coefficient is \( R = 1 \), and the width of the forbidden band becomes equal to zero. This is due to the fact that for integral values of \( s \) the highest of the energetic sub-barrier bands reaches the top of the barrier with its upper edge, i.e., the phase space of the potential well turns out to be completely filled.

The form of the spectrum of superbarrier bands as a function of the value of the parameter \( 2m\gamma U/\hbar^2 a' \), calculated by means of Eqs. (29) and (30), is shown in Fig. 5. The calculation was carried out for the (1 10) plane of silicon, where \( ad = 6.6 \). The dependence of the width of the forbidden bands on the value of the product \( ad \) for a parameter value \( s = 1/2 \) is shown in Fig. 6.

For integral values of \( s \) the expressions (27a) and (28a) are written in the form of a finite series. The corresponding series can be obtained, for example, from the following recurrence relations:
\[ u_{+}(x) = du_{-}(x)/dx - (s - 1) \cosh (ax) v_{-}(x) \]
\[ (31) \]
\[ v_{+}(x) = du_{-}(x) / dx - (s - 1) \cosh (ax) u_{-}(x) \]
\[ (32) \]

The plus sign in Eq. (29) leads to the values of the limiting energy reached in the center of the Brillouin zone and the minus sign leads to the values at the edges of the Brillouin zone.

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TABLE III.

<table>
<thead>
<tr>
<th>Transition</th>
<th>( s = 1 )</th>
<th>( s = 1 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( E_{F, s = 1} )</td>
<td>( \frac{2E_0}{d} ) ( \cosh (2k_0 a) )</td>
<td>( \frac{2E_0}{d} ) ( \cosh (2k_0 a) )</td>
</tr>
<tr>
<td>( E_{F, s = -1} )</td>
<td>( \frac{2E_0}{d} ) ( \cos (2k_0 a) )</td>
<td>( \frac{2E_0}{d} ) ( \cos (2k_0 a) )</td>
</tr>
</tbody>
</table>

*Here \( d_0 = a/\sqrt{2} \) is the value of the matrix element for the transition between the upper and lower sub-barrier levels in the potential (21) with \( s = 1 \).
where
\[ u(x) = -\cos kx, \quad v(x) = \sin kx. \] (33)

Let us estimate the ratio of the values of the matrix elements for transitions between superbarrier and sub-barrier bands. For simplicity we restrict the discussion to the case \( s = 1 \). The results of the corresponding calculations are given in Table III. For the calculations we used normalized wave functions (31) and (32) and the wave functions of the sub-barrier levels in the Pöschl-Teller potential. In view of the cumbersome nature of the formulas we have singled out two limiting cases \( E > E_0 \) and \( E < E_0 \), where \( E_0 = \hbar^2 a^2 / 2m \) is the energy of the lower sub-barrier level, \( E_0 \) and \( E \) are respectively the energies of the upper and lower levels of the transition.

It is evident from the table that the probability of transitions between high-lying superbarrier levels, and also of transitions from them to sub-barrier levels, is very small in comparison with the probability of a transition between sub-barrier levels.

The matrix elements of a transition from low-lying superbarrier levels are much closer to \( d_o \).

CONCLUSION
In conclusion we shall discuss the possible prospects.
1. Discrete levels of the transverse motion, as we have already mentioned, have appeared up to the present time only in spontaneous emission spectra. The analysis carried out above shows that there is a real promise of observation of induced radiation, especially in the optical range, as the result of the difference in the partial dechanneling lengths of the levels discussed. Significant interest here is presented by the situation in which the interplanar potential is nonuniform.

2. In addition we would like to call attention to another possible direction of investigation of levels of the transverse motion. We are discussing stationary and nonstationary laser spectroscopy of the transitions mentioned above. Our calculations show the possibility of use of absorption spectroscopy with the aid of a laser synchronized with the source of channeled particles. The data on the matrix elements can be used also for calculation of resonance susceptibilities.

3. From the point of view of structural studies of crystals, the spectroscopy of superbarrier levels is most promising; here the methods of nonlinear laser spectroscopy provide information inaccessible in study of spontaneous emission spectra.

In Refs. 4 and 5 the theory of dechanneling as the result of inelastic scattering was developed and it was shown (see the last article from the series in Ref. 5) that the dechanneling length is determined in this case by the overlap of the square of the modulus of the wave function of the transverse motion and a function which depends on \( u, x \), and the value of the momentum transfer [similar to Eq. (18)]. Consequently both elastic and inelastic processes will tend to lower the same levels.


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