Theory of axial channeling of electrons

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In the approximation of a two-dimensional Wigner-Seitz cell per atomic string in a crystal, we consider the problem of evolution of the population of the levels of transverse motion of an electron with thickness of the crystal. With increase of the electron energy from values ~ 1 MeV to ultrarelativistic energies the nature of the transverse motion changes qualitatively—from a substantially quantum motion to a classical motion. In the ultrarelativistic limit the greatest fraction of channeled electrons is obtained for angles of incidence much less than the critical channeling angle. At any angles of incidence only a part of the possible bound states distinguished by values of transverse angular momentum and energy are filled. In the low-energy region the model of localized states gives a simple and comparatively accurate quantitative description of the existing experimental data on the spectrum and population of bound states. The problem of inelastic nuclear scattering of channeled electrons reduces to solution of the differential-difference equation for the diagonal elements of the density matrix, which in the quasiclassical limit goes over to the Fokker-Planck equation. The corresponding kinetic coefficients of the equation are expressed in terms of the angular spread averaged over the classical trajectory. It is shown that at distances to an atomic string of the order of or less than the screening constant the angular spread has a Gaussian shape. At large distances the result goes over to the well known result of the Lindhard theory. Estimates of the dechanneling length made on the basis of the calculated kinetic coefficients turn out to be much less than the known values. In the quantum limit the calculated values of the dechanneling length are in good agreement with those obtained from the widths of γ transitions.

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1. INTRODUCTION

Interest in the channeling of electrons has increased significantly at the present time as the result of the experimentally observed phenomena of radiation of channeled particles[1-3] and bending of particle beams by curved crystals.[4] As in the case of positively charged particles, the collective nature of the interaction of electrons with close-packed atomic strings or planes of a crystal leads to the formation of bound and quasifree states of the transverse motion of the beam. The formation of these states plays a dominant role both in formation of the hard part of the radiation spectrum of the particles[5] and in the efficiency of use of curved crystals as deflecting systems.

The transverse-motion-states population initially produced at the surface of the crystal changes with thickness of the crystal as the result of multiple scattering by nuclei and electrons. In the formulation of this problem there is a qualitative distinction between the cases of incidence of positive and negative particles, whereas the channeling effect itself is manifested in particles of different signs identically, as the scattering in a potential well of finite depth in the transverse plane. Thus, the main mechanism of dechanneling for positive particles in metals is scattering by conduction electrons, which are distributed nearly uniformly over the cross section of the channel. Channeled electrons, on the other hand, are concentrated in the region of increased nuclear density—which is substantially nonuniform, since the characteristic size of the amplitude of the transverse motion, which is about equal to the screening constant a, is comparable with the amplitude u of the thermal vibrations of the lattice atoms. It must be added that the nature of the transverse motion of electrons changes qualitatively with energy: from classical at the ultrarelativistic limit to substantially quantum at $E \sim 1$ MeV.

The density matrix formalism[6,7] gives the possibility of describing from a unified point of view the entire set of phenomena in the angular and spatial distributions of channeled particles. In a previous article of the present author[8] this formalism was developed for nonrelativistic protons localized in a single channel. For the dechanneling problem this approximation is completely justified, since the band broadening of the discrete levels and the formation of sub-barrier forbidden bands for electrons with $E > 1$ MeV, which was taken into account in the work of Kagan and Kononets,[6,7] is important only in a narrow region of transverse energies near zero. In addition, the use of localized wave functions of the atomic type permits comparatively simple calculation of the spectrum, the initial population of the channeled particles (Sec. 2), and also its evolution with thickness of the crystal as the result of inelastic collisions. The problem of inelastic scattering of channeled particles, which is considered in Secs. 3 and 4, reduces to solution of a differential-difference equation which in the classical limit goes over to the Fokker-Planck equation, and the kinetic coefficients which determine the average increase and the diffusion of the transverse energy of the particles coincide with their classical limits.

The entire discussion is limited to the case of greatest practical interest of incidence of a beam of electrons along closepacked directions in the lattice, in which all of the phenomena associated with channeling are most pronounced.

2. INITIAL POPULATION OF STATES OF CHANNELED ELECTRONS

The correlated nature of the collisions of fast particles with an atomic string leads to the result that the

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motion of a particle can be considered as occurring in a continuous two-dimensional potential of the atomic string,[9] averaged over the transverse thermal vibrations of the atoms[6,10]:

$$U_{th}=-\frac{Ze^2}{d}\langle f(r)\rangle=-U_0F_s(r),\quad F_s(0)=1. \tag{1}$$

Here Ze is the charge of the atom, d is the lattice constant, f is the screening function, and $\langle\ldots\rangle$ indicates averaging over the thermal vibrations:

$$\langle f(r')\rangle=\frac{\alpha}{\pi}\int d\mathbf{u} f(r')e^{-\alpha u^2}$$
$$\alpha=a^2/2\overline{u^2},\quad r'=|\mathbf{r}-\mathbf{u}|, \tag{2}$$

where $\overline{u^2}$ is the mean square thermal displacement of an atom and a is the screening constant.

The influence of neighboring strings leads to the result that in the region of small transverse energies of the particle the axial symmetry of the potential profile (1) is destroyed, and the derivative along the normal to the boundary of the cell associated with one string is zero. Restricting the discussion to the transverse motion of an electron in a unit cell, we shall assume that the cell is a circle of radius R_m such that $\pi R_m^2=(nd)^{-1}$, where n is the number of atoms per cm^3, and the potential inside the cell is

$$U=-U_0(F_s(r)+F_s(r-2R_m)-2F_s(R_m))=-U_0F. \tag{3}$$

For not too small transverse energies the reckoning of the potential from zero and the zero derivative at the boundary, which have been taken into account in Eq. (3), do not affect the results, and therefore we can set $F\approx F_s$ for $r\sim a$.

The fact that $F(r)$ has a finite value at $r=0$ and drops faster than $1/r^2$ at $r>a$ has a fundamental significance for the choice of a model potential. Thus, a potential of the form $F\sim 1/r$ gives a ground-state energy which can exceed the value $F=1$ in absolute value. On the other hand, the diverging phase space at low transverse energies for $F\sim 1/r$ or $1/r^2$ (the Lindhard potential) leads to an infinite number of levels near $\varepsilon=0$. The latter difficulty can be circumvented by choosing F in the form (3) or, more simply:

$$F=-U_0[F_s(r)-F_s(R_m)].$$

In the specific calculations below we shall use as screening functions the approximations of Moliere (f_M) and Lindhard (f_L).[10] The thermal average of f_L with good accuracy (<1%) coincides with the function

$$\langle f_L\rangle=g/(1+br^2), \tag{4}$$
$$b=g/C^2,\quad C^2\approx 3,\quad g=\gamma+\ln\alpha C^2-\exp(-\alpha C^2)\,\mathrm{Ei}(-\alpha C^2), \tag{5}$$

where $\gamma=0.577$ is Euler's constant and the last term, which contains an exponential integral function at $\alpha C^2>1$, can be replaced by $1/\alpha C^2$. For example, for a single crystal of silicon at $T=300$ K, we have $b=0.98$.

The transverse motion of channeled electrons can be considered nonrelativistic[11] and obeying the Schrödinger equation with a relativistic mass m. However, when the number of bound states in the well $N\sim ma^2U_0/\hbar^2$ is large, one can use the classical description in which the radial motion of the electron occurs in a field with an effective potential which depends on the transverse angular momentum

$$\Phi_M=M^2/2r^2-F(r). \tag{6}$$

For reasons of convenience we shall go over to dimensionless values of the energy, angle, coordinate, and angular momentum expressed respectively in units of the potential well depth U_0, the critical angle $\psi_{cr}=(2U_0/E)^{1/2}$, a, and $M_0=pa\psi_{cr}$ (p and E are the longitudinal relativistic momentum and energy).

Finite motion within the cell is possible only for a limited interval of values of the transverse energy ε and the angular momentum. The energy ε corresponding to a given value of angular momentum lies in the interval between the extrema Φ_{min} and Φ_{max} of the function Φ. Numerical calculation of the potential Φ in the Moliere approximation showed that the magnitude of the centrifugal barrier does not exceed ~0.05, and therefore we can assume approximately that the bound states are limited above by the value $\varepsilon=0$. An important feature of the function Φ is the fact that there is some value of angular momentum M_{max} above which bound state states are not formed at all.[1)] This value is determined from Eq. (6) by the obvious relation $M_{max}^2=[r^3|F_r'|]_{max}$. For the ⟨111⟩ axis in Si and the function f_M this value is $M_{max}^2=2.298$. Note that in calculation of M_{max}^2 an important role is played by the zero derivative of the potential at the cell boundary (otherwise the slower falloff of F_s than F for $r>3$ will give a much larger value of M_{max}^2).

We shall now determine the population of bound and superbarrier states on the surface of the crystal. Let a beam of electrons hit the crystal at an angle θ_0 to the axial direction z. The electron at the point of entry into the crystal r_0 acquires a transverse energy $\varepsilon=\theta_0^2-F(r_0)$ and an angular momentum $\mathbf{M}=\mathbf{p}_\perp\times\mathbf{r}_0$, where $p_\perp=p\theta_0$. The initial distribution in transverse energy and angular momentum is found by integration of the microcanonical distribution over all initial coordinates r_0 in the cell:

$$\rho_0=\frac{1}{\pi R_m^2}\int d\mathbf{r}_0\delta(\varepsilon-\theta_0^2+F)\delta(M-[\mathbf{p}_\perp\mathbf{r}_0]_z). \tag{7}$$

The result of the integration is

$$\rho_0=\frac{1}{\pi R_m^2}(M_f^2-M^2)^{-1/2}|F_{R^*}'|^{-1},\quad -1+\theta_0^2<\varepsilon<\theta_0^2,\quad M^2<M_f^2 \tag{8}$$

$$\rho_0=0,\quad \varepsilon<-1+\theta_0^2,\quad \varepsilon>\theta_0^2;$$
$$M_f^2=\theta_0^2R^{*2},\quad \varepsilon-\theta_0^2+F(R^*)=0. \tag{9}$$

It is evident from this that for filled states the values of the angular momentum in modulus are bounded above by some value M_{fm} which depends on the initial angle of incidence. The maximum possible value of M_{fm}^2 for all angles θ_0, as follows from Eq. (9), is

$$M_{f\,max}^2=[\theta_0^2R^{*2}]_{max}=[F(r)r^2]_{max}. \tag{10}$$

For the ⟨111⟩ direction in Si the value of $M_{f\,max}$ at $T=300$ K calculated by means of f_M with Eq. (10) is 0.855 and is reached at $\theta_0=0.38$.

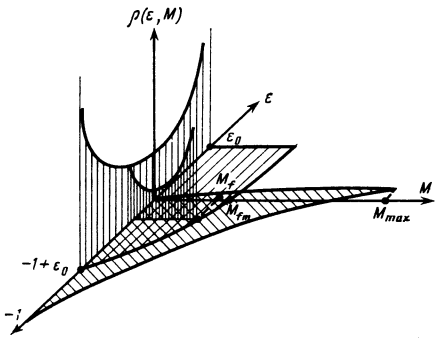

FIG. 1. Initial distribution of ultrarelativistic electrons in transverse energy and angular momentum.

Near M_f the initial distribution (8) has a square-root singularity. Another feature of the function ρ_0 follows from its inverse proportionality to the derivative of the potential, which vanishes at the points $R^*=0$ and $R^*=R_m$. Consequently, near the limiting values $-1+\theta_0^2$ and θ_0^2 the distribution of ρ_0 also has a square-root singularity.

For a nonzero angular momentum, states are filled beginning with some energy value lying above the minimum of the effective potential (6), and the interval of filled transverse energies of channeled electrons approaches zero as $M \to M_{fm}$.

The remarks above are illustrated in Fig. 1, in which we have shown the dependence of the initial distribution function on the transverse energy and angular momentum of the electron. We emphasize the main result of the foregoing analysis of ρ_0 a result of fundamental significance for the problem of electron dechanneling and qualitatively different from the planar channeling case: for any angle of incidence, only a part of the possible bound states are filled. The unpopulated states, which have large values of angular momentum and small transverse energies, as will be shown below, are the longest lived, and diffusion into these states can significantly increase the lifetime of an electron in a channel.

The total number of channeled particles calculated from Eq. (8) by means of the function f_L is

$$I_c=\frac{1}{(bR_m^2)}\left(\frac{1}{\theta_0^2+(bR_m^2)^{-1}}-1\right). \tag{11}$$

It follows from this that at $\theta_0 \sim 1$ the fraction of channeled particles is determined mainly by a geometrical factor $\sim 1/R_m^2 \sim 10^{-2}$, i.e., by the probability of landing in the region $r \lesssim a$. With decrease of the angle of incidence, I_c increases, reaching values of the order of unity at $\theta_0 \sim 1/R_m$. This is qualitatively distinct from the case of channeling of positive particles, for which $I_c \sim 1$ already at $\theta_0 \sim 1$.

Let us turn now to low energies of the electrons, for which $ma^2U_0/\hbar^2 \sim 1$. The initial population, over states distinguished by values of the orbital quantum number l and the principal quantum number n, is now determined by the diagonal elements of the density matrix in the momentum representation[6,8]

$$\rho_{nl}=\frac{2(2-\delta_{l0})}{\pi R_m^2}\left[\int_0^\infty dr r J_0(q_0 r)\Psi_{nl}(r)\right]^2. \tag{12}$$

Here q_0 is the transverse wave vector and the radial function Ψ_{nl} satisfies the Schrödinger equation

$$\Psi_{nl}''+\frac{1}{r}\Psi_{nl}'+\left(2\delta^2(\varepsilon+F)-\frac{l^2}{r^2}\right)\Psi_{nl}=0, \quad \delta^2=\frac{ma^2U_0}{\hbar^2}. \tag{13}$$

For states with $l \neq 0$ the best approximation of the potential turned out to be a function of the form

$$F_l=\beta_l\left(\frac{1}{r}-\frac{1}{R_l}\right), \tag{14}$$

where the parameters β_l and R_l were chosen from the condition of the most accurate possible agreement of the curves (6) and $\Phi_l=-F_l+l^2/2\delta^2r^2$. The potential in the form (14) permits a simple calculation of the spectrum

$$\varepsilon_{nl}=\frac{\beta_l}{R_l}-\frac{2\delta^2\beta_l^2}{(2l+2n+1)^2} \tag{15}$$

and of the populations (12). Having in mind the experimental data on the dependence $\rho_l(\theta_0)$ which were obtained from the radiation spectra,[13,14] we shall give here formulas for several well studied states:

$$\rho_{2p}=\frac{96q_0^2\lambda_{2p}^6}{R^2(\lambda_{2p}^2+q_0^2)^5}, \quad \rho_{3p}=\frac{480q_0^2\lambda_{3p}^6(\lambda_{3p}^2-q_0^2)}{R^2(\lambda_{3p}^2+q_0^2)^5},$$
$$\rho_{3d}=\frac{480\lambda_{3d}^8q_0^4}{R^2(\lambda_{3d}^2+q_0^2)^7}, \quad q_0=\sqrt{2}\delta\theta_0, \quad \lambda_s=(-2\delta^2\varepsilon_s)^{1/2}, \quad s=n,l. \tag{16}$$

The ground state can be described with high accuracy in the harmonic approximation[13]

$$F_0=\frac{1}{2}\beta_0^2r^2, \quad \varepsilon_0=-1+\frac{\beta_0}{\delta}, \quad \rho_0=\frac{4}{\beta\delta R^2}\exp\left\{-\frac{2\delta\theta_0^2}{\beta}\right\}. \tag{17}$$

In Fig. 2 we have shown the population of the bound states as a function of the initial angle of incidence for the case of channeling of electrons with $E=4$ MeV in the ⟨110⟩ direction of a silicon crystal. The energy-level values ε_{2p}, ε_{3p}, and ε_{3d} agree with the experimentally observed values for the chosen values of β_l and R_l. In the ground-state energy there is a small difference due to the fact that the level ε_{1s} is in the region of appreciable anharmonicity. As can be seen from Fig. 2, the formulas (16) accurately reproduce the behavior

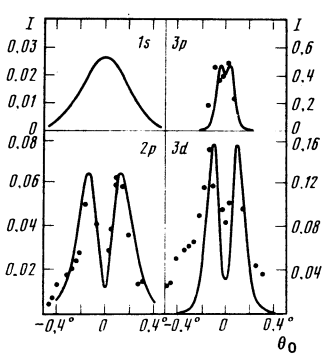

FIG. 2. Initial population of bound states as a function of the angle of incidence of an electron beam with $E=3.1$ MeV in the ⟨110⟩ direction in silicon at $T=300$ K. The constants for the curves are: $\delta=2.42$, $\beta_0=1.4$, $\beta_1=0.45$, $\beta_2=0.5$, $R_1=R_2=13$, $\varepsilon_{2p}=-0.23$, $\varepsilon_{3p}=-0.06$, $\varepsilon_{3d}=-0.08$, $\varepsilon_{1s}=-0.43$.

of the experimental curves $\rho_s(\theta_0)$, including the location of the node in the wave function Ψ_{3p} at the point $\theta_0 = (-\varepsilon_{3p})^{1/2}$. The theoretical curves shown include the angular spread in the directions of the incident beam $\Delta\theta = 0.02°$, and therefore $\rho_s \neq 0$, in spite of the fact that $\rho_s \sim \theta_0^{2l}$ at small angles of incidence and $l \neq 0$; on the other hand, the 1s state has a maximum at $\theta_0 = 0$.

3. THE DIFFUSION APPROXIMATION

Multiple scattering of channeled particles by nuclei and valence electrons leads to a gradual increase and diffusion of the transverse energy and eventually to dechanneling. If we are not interested in the relaxation of the plane wave at the surface into a superposition of bound states, i.e., in the damping of the nondiagonal elements of the density matrix, the solution of this problem in general form is given by the time evolution of the diagonal elements of the density matrix.[6,8]

In our discussion we shall neglect the energy loss, since the relative change of energy in the dechanneling length is small. In addition, we shall not take into account radiative transitions and scattering by valence electrons, since the main mechanism of dechanneling is nuclear scattering. Allowance for the latter formally reduces to transitions between bound states due to the difference of the true potential of the string of atoms displaced from their sites and the averaged continuous potential. Assuming the distribution of atomic sites of the string along the z axis to be random, the equation for the diagonal elements of the density matrix is written in the form[10]

$$\frac{\partial \rho_s}{\partial z} = \frac{(Ze^2)^2}{\hbar^2 v^2 d} \sum_{s'} (\langle |f^{s's}|^2 \rangle - \langle |f^{ss}|^2 \rangle)(\rho_{s'} - \rho_s), \quad v = pc^2/E. \tag{18}$$

In the quasiclassical approach it is possible to use the diffusion approximation, choosing as independent variables the quantities ε_s and $M = \hbar l$. For this purpose we shall expand the right-hand side of Eq. (18) in series in powers of $\varepsilon_{s'} - \varepsilon_s$ and $M' - M$. As a result we obtain

$$\frac{\partial \rho_s}{\partial z} = -\frac{\partial A_{10}\rho_s}{\partial \varepsilon} + \frac{1}{2}\frac{\partial^2 A_{20}\rho_s}{\partial \varepsilon^2} + \frac{1}{2}\frac{\partial^2 A_{02}\rho_s}{\partial M^2} + \frac{\partial^2 A_{11}\rho_s}{\partial \varepsilon \partial M}. \tag{19}$$

This equation was obtained in Ref. 15 on the basis of a classical discussion. The kinetic coefficients in Eq. (19) are

$$A_{ik} = \frac{Ze^2}{\hbar v^2 d} \sum_{s'} (\langle |f^{s's}|^2 \rangle - \langle |f^{ss}|^2 \rangle)(\varepsilon_{s'} - \varepsilon_s)^i (M' - M)^k. \tag{20}$$

In view of the axial symmetry of the problem the average moment A_{01} is zero.

Summation over the states in Eq. (20) in the averages over energy A_{10} and A_{20}, which have the significance of the average increase and diffusion of the transverse energy, reduces to the convolution of the product of the operators, including the functional derivative with respect to time[8]:

$$A_{10} = A_0(\langle f_r'^2 \rangle - \langle f \rangle_r'^2)_{av}, \quad A_0 = \frac{1}{2}\left(\frac{Ze^2}{a}\right)^2 \frac{1}{EU_0 d},$$
$$A_{20} = 4A_0(\langle f_r'^2 \rangle - \langle f \rangle_r'^2)(\varepsilon - \Phi))_{av}. \tag{21}$$

The use of parentheses with the subscript $(\ldots)_{av}$ signifies an average over the period of radial oscillations of a particle, which is the form taken by the diagonal matrix element in the quasiclassical approximation.

The coefficients of the diffusion in angular momentum are expressed in terms of the angular momentum operator $l = -i\partial/\partial\varphi$, where φ is the angle between the vectors $\mathbf{r}$ and $\mathbf{u}$. We finally obtain

$$A_{02} = A_0(\langle f_\varphi'^2 \rangle)_{av}, \quad A_{11} = 2A_0(\langle f_r' f_\varphi' \rangle(\varepsilon - \Phi)^{1/2})_{av}. \tag{22}$$

We note that the coefficients (21) coincide with their classical analogs. For example, the average increase of the transverse energy is expressed in terms of the mean square angular spread,

$$A_{10} = \left(\frac{\delta \varepsilon}{\delta z}\right)_{av} = \frac{E}{2d}(\langle \theta^2 \rangle - \langle \theta \rangle^2)_{av}, \quad \theta = -\frac{Ze^2}{Ea}\frac{\partial f}{\partial \mathbf{r}}, \tag{23}$$

where θ is the scattering angle in a binary collision.

The kinetic coefficients A_{ik} diverge logarithmically at the lower limit of the integration over the impact parameter. This divergence, which is usual for the diffusion approximation, is removed by limiting the region of integration over r' in Eqs. (21) and (22) on the low end to some small value r_{min} which actually separates the regions where the multiple collisions are few or numerous. The removal of the singularity can in principle be carried out by two means, which differ in the order of integration in Eq. (21): in calculation of the averages over the trajectories, and in averaging over the thermal displacements. The second method is more convenient for calculation, although it does not permit one to go over in the final results to the limit $\bar{u}^2 \to 0$, since the region of its applicability is limited by the condition $\bar{u}^2 \gg r_{min}^2$ which, incidentally, is always satisfied.

The region of impact parameters $r' < a$ is characterized by a Coulomb behavior of the interaction potential of an electron with an atom, for which $f'^2 = 4/r^2$. Therefore the result of averaging the angular spread over the thermal displacements can be represented

$$\langle f_r'^2 \rangle - \langle f \rangle_r'^2 = 8\alpha \ln \xi e^{-\alpha r^2} + R_{res}, \quad \xi = 2r_{min}\alpha^{1/2}e^{1/4}, \tag{24}$$

where the residual term R_{res} is already independent of r_{min}. At small impact parameters of the electron with the string, the main contribution to Eq. (24) is from the first term, and for large r it is from the second term; here in the limit $\alpha r^2 \gg 1$ Eq. (24) goes over to the well known form[9]

$$R_{res} = \frac{1}{2\alpha}\left(f''^2 + \frac{f'^2}{r^2}\right). \tag{25}$$

A straightforward calculation of the residual term for the Lindhard potential gives for $\alpha C^2 \gtrsim 1$

$$R_{res} = 4\alpha e^{-\alpha r^2}\left[\mathrm{Ei}(\alpha r^2) - \ln(\alpha r^2) + \gamma - \frac{2}{\alpha(r^2+C^2)}\right] - \frac{1}{r^2}(1 - e^{-\alpha r^2})^2 - \frac{1}{\alpha}\frac{r^4 + C^4}{(r^2+C^2)^2}. \tag{26}$$

The value of r_{min} represents the value of impact parameter at which the scattering angle becomes of the order $\hbar/pd_{min}$,[16] where d_{min} is the radius of the nucleus. Hence it follows that $r_{min} \approx Z^{5/3}/137^2$.

If we limit the integration over r' in Eq. (24) at the upper end to some value r_{max} corresponding to a minimum momentum transfer $p_\perp \sim \hbar/a$,[16] we arrive at the well known result of the theory of Kitagawa and Ohtsuki.[17] In fact, from the condition of cutoff of the scattering cross section at angles less than θ_{min},

$$\theta_{min}=2Ze^2/Er_{max}\sim\hbar/pa, \tag{27}$$

it follows that $r_{max}=2Z/137$, and for small Z this value can be much less than the amplitude of the thermal vibrations. With this condition the angular spread (24) does not depend on the density gradient of the atoms of the string in the transverse plane and is determined by its local value at the point r. In other words, in a target with small Z, particles located a distance r from the axis of the string are scattered exactly in the same way as in an amorphous medium with an atomic density $P=\pi^{-1}\alpha e^{-\alpha r^2}$:

$$\frac{\delta\varepsilon}{\delta z}=A_0 P f_{at}'^2,$$
$$f_{at}'^2=\frac{8\pi Ze^2}{E}\ln\xi_{at}, \tag{28}$$
$$\xi_{at}=r_{max}/r_{min}=(181/Z^{1/3})^2.$$

This approximation, which was first developed in Ref. 17, was used for calculation of the planar dechanneling of relativistic positrons.[18] It should be emphasized that the method indicated for choice of the integration limits is crude, even within logarithmic accuracy, from the point of view of an exact solution of the initial integral equation (18). It would be more acceptable to use a self-consistent procedure for calculation of r_{min} as a function of the thickness of the crystal, but as the result of the complexity of such a problem it would be possible to solve it only in the case of an amorphous medium.[7]

In Fig. 3 we have shown the results of calculation of $\delta\varepsilon/\delta z$ for a tungsten single crystal at $T=300$ K in various approximations. The difference of the exact result according to Eqs. (24) and (26) (curve 1) from the approximate result (28) is most significant in the region $r^2>1/\alpha$, where it is determined by the residual term R_{res} (curve 3) and reaches many orders of magnitude. For $r<1/\alpha$ this difference depends on the quantities ξ and ξ_{at} in the argument of the logarithm in (24) and (28).

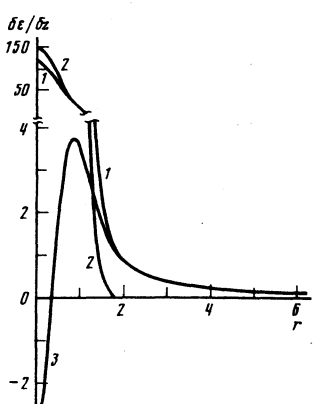

FIG. 3. Rate of increase of electron transverse energy as a function of the distance to the string (in units of A_0).

In the limit $r_{max}^2\ll 1$ it is easy to obtain analytic expressions for the averages over the thermal vibrations in the remaining kinetic coefficients A_{02} and A_{20} with accuracy to terms of order r_{max}. Thus,

$$\langle f_\varphi'^2\rangle=\frac{r^2}{2}P(r)f_{at}'^2,$$
$$\langle f_r'^2\rangle-\langle f\rangle_r'^2=\frac{3}{8}P(r)f_{at}'^2,\quad \langle f_r'f_\varphi'\rangle=0. \tag{29}$$

Returning to the question of choice of r_{max}, we note that a similar situation exists in scattering of relativistic particles by valence electrons. The region of impact parameters in collision of an electron with an atom which gives the main contribution to the angular spread is bounded above by the value $r_{max}=2a_0/137$ (Ref. 19) (a_0 is the radius of the orbit of the valence electron). Similarly for conduction electrons, in which the angular spread is determined by single-particle excitations (close collisions), $r_{max}=8Zv_F/\omega_p$, where v_F is the velocity of the electron at the Fermi surface and ω_p is the plasmon frequency.

The diffusion approximation is justified if the dechanneling length z_s, due to a single collision accompanied by change of the direction of motion of the particle by an angle of the order of the critical angle, is much greater than the diffusion dechanneling length $z_d\sim z_s/\ln\xi$. The Coulomb logarithm is $\ln\xi\sim 5-8$, and therefore diffusion over the transverse states is the main mechanism of dechanneling (cf. Ref. 19).

Let us turn now to calculation of the average over the period of radial motion, which is

$$L=\frac{1}{\psi_{cr}}\int_{r_1}^{r_2}\frac{dr}{(\varepsilon-\Phi)^{1/2}}. \tag{30}$$

Here r_1 and r_2 are the classical limits of the particle motion. To facilitate determination of the average over the trajectories it is necessary to take into account two different modes of motion of the particle. If the angular spread changes insignificantly within a period, for example, near the bottom of the effective potential Φ_M when $r_1\approx r_2$, the average over the period is approximately equal to the value of the function at the point of the minimum of the potential r_m. Another, opposite situation is realized when the particle motion occurs under conditions of a rapid dependence of the angular spread on the distance to the string. In this case the main contribution to the spread is from the region of values of r close to the distance r_1—the closest approach to the string, where $\delta\varepsilon/\delta z$ is maximal. Taking into account that the trajectory near r_1 is parabolic, so that

$$r(z)=r_1+\frac{\psi_{cr}^2}{4}|\Phi_{r_1}'|z^2, \tag{31}$$

we obtain

$$e^{-\alpha r^2}=\frac{2}{L}\int_0^\infty dz e^{-\alpha r^2(z)}=\frac{1}{\psi_{cr}L}\left(\frac{2r_1}{|\Phi_{r_1}'|}\right)^{1/2}\exp\left(-\frac{\alpha r_1^2}{2}\right)K_{1/4}\left(\frac{\alpha r_1^2}{2}\right). \tag{32}$$

For the Lindhard potential the distance r_1 is found from the expression

$$r_1^2=\frac{-t+(t^2+2\varepsilon Mb)^{1/2}}{2\varepsilon b}\approx\frac{M^2}{2t},\quad t=1+\varepsilon-\frac{bM^2}{2}. \tag{33}$$

Using the asymptote of the Macdonald function K_α for $\alpha r^2 \gg 1$, we can obtain the average increase of the energy in the most interesting case of long-lived states:

$$A_{10}=\frac{4A_0\ln\xi}{\psi_{cr}L}\left(\frac{2\pi\alpha}{r_1|\Phi_{r_1}'|}\right)^{1/2}e^{-\alpha r_1^2}. \tag{34}$$

From this expression it follows that with increase of the angular momentum and of the absolute value of the transverse energy, the electron-dechanneling length increases exponentially.

Calculation of the coefficients of the diffusion in transverse energy and angular momentum with includeion of Eq. (29) gives

$$\begin{aligned}A_{02}&=-\frac{1}{2}\frac{\partial}{\partial\alpha}\frac{A_{10}}{\alpha},\\ A_{20}&=-2(|\Phi_{r_1}'|)^{1/2}e^{-\alpha r_1^2}\frac{\partial}{\partial r_1}(|\Phi_{r_1}'|)^{1/2}A_{10}e^{\alpha r_1^2}.\end{aligned} \tag{35}$$

The boundary conditions for Eq. (19) are determined from the requirement of reflection of particles at the point $r=\Phi(r_m)$. Channeled particles, on reaching the point $\varepsilon=0$, leave the channel and then take part mainly in collisions with conduction electrons. The intensity of the latter is Z^2d^2/Z_vu^2 times longer than the maximum of the intensity of the nuclear mechanism (Z_v is the number of valence electrons).

As can be seen from Eqs. (33) and (34), the longest-lived states are unfilled states near the bottom of the potential well and also states which have a large orbital angular momentum. However, the filled states with the greatest angular momenta are near $\varepsilon=0$ and therefore rapidly leave the channel. In addition, the analysis of the initial population which was carried out in Sec. 2 showed that the greatest total population I_c is achieved for very small angles of incidence (in comparison with the critical angle). Here most of the particles have orbital angular momentum close to zero. For such particles the length for rearrangement of the distribution function ρ can be evaluated from Eq. (23) as

$$z_{d\,min}^{-1}=\frac{\delta\varepsilon}{\delta z}(r=0)=8\alpha A_0\ln\xi. \tag{36}$$

For example, for electrons with $E=1$ GeV in silicon (the ⟨110⟩ direction) it amounts to $z_d=5500$ Å, and in tungsten (⟨111⟩) $z_d=540$ Å.

4. DECHANNELING OF LOW-ENERGY ELECTRONS

When the number of levels of the bound motion is small, the diffusion approximation is inapplicable and it is necessary to return to Eq. (18). This equation takes on the simplest form if the feeding of the bound state by the superbarrier states is not taken into account, especially since the probability of transitions of this type is smaller by a factor $\sim 1/R_m^2$ than the probability of transitions between bound states $w_{ss'}$. Equation (15) is then written in the form

$$\frac{\partial\rho_s}{\partial z}=\sum_{s'}w_{ss'}\rho_{s'}-\frac{\rho_s}{z_{ds}}. \tag{37}$$

The solution of this equation is expressed in terms of a linear combination of exponentials

$$\rho_s=t_{ss'}\exp(\lambda_{s'}z)\,t_{s's''}^{-1}\rho_{s''}(0) \tag{38}$$

with arguments which are eigenvalues of the matrix of transition probabilities:

$$\lambda_s\delta_{ss'}=t_{ss''}^{-1}\left(w_{s''s'''}-\frac{\delta_{s's'''}}{z_{ds''}}\right)t_{s'''s'}. \tag{39}$$

Numerical evaluation of the matrix elements for the experimental situations presented in Sec. 2 shows that with satisfactory accuracy the characteristic length of damping of the diagonal elements of the density matrix coincides with z_{ds}, which corresponds to taking into account only the "escape" from the s state in Eq. (37). Convolution of the sum of the escape probabilities gives

$$\left(\frac{z_{ds}}{d}\right)^{-1}=\left(\frac{Ze^2}{\hbar v}\right)^2(\langle f^{ss}\rangle-\langle f^{ss'}\rangle-\langle f\rangle^{ss}+\langle f\rangle^{ss'}). \tag{40}$$

For large values of angular momentum when the region of localization of a particle is removed from the string by a distance greater than the amplitude of thermal vibrations, the expression in the parentheses can be expanded in series in $\overline{u^2}$:

$$\varkappa_s=\frac{1}{2\alpha}(f'^{ss}-f'^{ss'}). \tag{41}$$

In the general case analysis of the expression (40) can be simplified by going over to a Fourier transformation of the screening function in the coordinate. Eventually we obtain

$$\begin{aligned}\varkappa_s=&\int d\mathbf{k}_1\int d\mathbf{k}_2 f_{k_1}f_{k_2}\exp\left(-\frac{k_1^2+k_2^2}{4\alpha}\right)\\ &\times\left[\exp\left(-\frac{\mathbf{k}_1\mathbf{k}_2}{2\alpha}\right)-1\right]\{[e^{i(\mathbf{k}_1-\mathbf{k}_2)\mathbf{r}}]^{ss}-[e^{i\mathbf{k}_1\mathbf{r}}]^{ss}[e^{-i\mathbf{k}_2\mathbf{r}}]^{ss}\}.\end{aligned} \tag{42}$$

We shall now calculate this quantity for the $1s$ and $2p$ states from the data of Sec. 2, using the well known Fourier transform of the function f_L:

$$f_k=\frac{1}{2\pi}\int_0^\infty drrJ_0(kr)f_L(r)=\frac{1}{\pi k}\left(\frac{1}{k}-CK_1(Ck)\right). \tag{43}$$

The diagonal matrix elements of the exponential in Eq. (42) are

$$\begin{aligned}(e^{i\mathbf{kr}})^{2p}&=-\frac{\lambda_{2p}^4}{3}\frac{d^3}{d\lambda_{2p}^3}\frac{1}{(4\lambda_{2p}^2+k^2)^{1/2}},\\ (e^{i\mathbf{kr}})^{1s}&=e^{-k^2/20\beta_0}.\end{aligned} \tag{44}$$

Numerical calculation of z_d according to Eqs. (42)–(44) in silicon gives for $E=4$ MeV and the ⟨111⟩ direction $z_d=450$ Å and for $E=3.81$ MeV and the ⟨110⟩ direction $z_d=3200$ Å, which is in agreement with the experimental values of these quantities determined from the known transition widths: $z_{d(1s)}^{exp}=270$ Å (Ref. 13) and $z_{d(2p)}^{exp}=3200$ Å.[14]

CONCLUSION

1. Analysis of the initial population showed that, to achieve the greatest fraction of channeled electrons, angles of incidence much less than the critical channeling angle are necessary. This conclusion is qualitatively different from the case of scattering of positive par-

ticles, for which angles of incidence of the order of the critical angle are sufficient. Under these conditions the longest-lived states are populated with transverse angular momentum close to zero.

2. For any angles of incidence only a fraction of the possible bound states are filled. Diffusion to unfilled states significantly increases the dechanneling length.

3. Good agreement of the theoretical and experimental values for scattering of low-energy channeled electrons can be achieved without taking into account the band structure of the spectrum of states of the transverse motion, with a potential of a simple type which permits a complete analytic calculation of the populations.

4. The kinetics of the behavior of channeled electrons in a crystal differs qualitatively from the kinetics of positrons, since the main mechanism of inelastic scattering of channeled electrons is nuclear. Correspondingly the intensity of the scattering of channeled electrons is approximately Z^2d^2/Z_0u^2 times larger than for positrons. This circumstance is important in the radiation problem, where from crystals with large Z one expects a harder spectrum and a higher intensity of γ rays at the maximum of the spectral density. Therefore a quantitative analysis of the kinetic equation is necessary for choice of the optimal conditions for radiation.

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[1)]We note in this connection that the rectangular shape of the Kronig-Penney potential permits formation of bound states for any values of angular momentum in the classical limit, which, as follows from the estimates given above, does not correspond to reality. Together with the estimate discussed above of the height of the centrifugal barrier, this makes unlikely the possibility of population of resonance levels discussed in Ref. 12.

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