Theory of ionization of fast atomic particles in a crystal

V. A. Bazylev and A. V. Demura
I. V. Kurchatov Institute of Atomic Energy

(Submitted 2 February 1982)
Zh. Eksp. Teor. Fiz. **83**, 668–683 (August 1982)

A theory is developed for the ionization of atomic particles channeled by the interplanar potential of a crystal. With allowance for the thermal vibrations of the nuclei, we have studied the suppression of the probability of loss of electrons by an ion in elastic interaction with the lattice atoms both in channeling and in a disoriented crystal. An anomalous dependence of the ionization probability on the angle between the ion momentum and the axes (or planes) of the crystal is predicted. It is shown that, in contrast to the ionization of fast atomic particles in an amorphous material, in a crystal this process can occur as the result of inelastic interaction with the electron subsystem of the crystal.

PACS numbers:61.80.Mk

INTRODUCTION

The establishment of the equilibrium charge of ions in a crystal in channeling differs substantially from that in an amorphous medium. This occurs for two reasons. The first is that in channeling there is a redistribution of the ion flux in impact parameter.[1] The second reason lies in the change of the very probability of loss of electrons by an ion for a given impact parameter as the result of the correlation of individual collisions of an ion with the atoms of the crystal (Refs. 2 and 3).[1)]

In an earlier article[3] Bazylev and Zhevago developed a theory of loss of electrons by an ion passing through a crystal along one of its crystallographic axes (axial channeling). In the framework of time-dependent perturbation theory in the dipole approximation, the loss probability was expressed in terms of the cross section for the photoelectric effect and the density of the flux of "photons" equivalent to a string of atoms of the crystal. The intensity and spectrum of the equivalent photons, according to Ref. 3, depend on the distance between the atoms in the string, the amplitude of their longitudinal thermal vibrations, the charge of the crystal atoms, and the ion velocity.

Questions which remain to be investigated are the loss of electrons by an ion from excited states, when the dipole approximation is violated, and also the influence of transverse thermal vibrations of the crystal atoms on the equivalent photon spectrum, which becomes important at sufficiently high ion velocities when the transfer of longitudinal momentum is small in comparison with that of the transverse momentum. In addition, no theory has been developed for the loss of electrons by ions in planar channeling. At the same time, in motion of an ion in planar channeling, important correlations exist not only between individual collisions with atoms of a single string, but also with the different strings of which the plane consists.

A final unstudied question is that of the role of other mechanisms in the loss of electrons by ions; for example, the role of inelastic interaction between the electrons of the crystal and the electrons of the ion. As we shall show below, these mechanisms can become important in the loss of electrons by an ion in a crystal.

The purpose of the present work is to construct for the loss of electrons by ions in channeling a theory that contains answers to the questions posed. A stationary formulation of the problem is used.

§ 1. INTERACTION OF A MULTIPLY CHARGED ION WITH A CRYSTAL

Let an ion with charge eZ enter a crystal at an angle θ_0 to the crystallographic planes. Let this angle θ_0 be less than or of the order of the Lindhard critical angle θ_L (see for example Ref. 6), so that the motion of the ion is controlled by the continuous potential averaged over the plane

$$U_{\text{cont}}(x)=n_s \sum_k \int d^2\boldsymbol{\rho}\, V_a([(x-kd)^2+\rho^2]^{1/2}), \tag{1.1}$$

where V_a is the potential of a crystal atom and n_s is the density of atoms in the channeling plane considered; $\boldsymbol{\rho}=\{x,y\}$ is the two-dimensional radius vector in the plane and $k=0, \pm 1, \pm 2\ldots$.

The complete Hamiltonian of the ion + crystal system has the form

$$\hat{H}=\hat{H}_i+\hat{H}_c+\hat{H}_{ic}. \tag{1.2}$$

Here $\hat{H}_i$ is the Hamiltonian of the ion entering into the crystal and consists of the Hamiltonian of the free motion of the ion as a whole and the Hamiltonian of the m bound electrons of the ion; $\hat{H}_c$ is the crystal Hamiltonian; $\hat{H}_{ic}$ is the Hamiltonian of the interaction of the ion with the crystal:

$$\hat{H}_{ic}=e^2 \sum_a \left\{ \frac{Z_1 Z_2}{|\mathbf{R}-\mathbf{R}_a|} - \sum_{s=1}^{Z_2} \frac{Z_1}{|\mathbf{R}-\mathbf{r}_a^s|} - \sum_{s=1}^{m} \frac{Z_2}{|\mathbf{r}_z^s-\mathbf{R}_a|} + \sum_{s=1}^{m} \sum_{s'=1}^{Z_2} \frac{1}{|\mathbf{r}_z^s-\mathbf{r}_a^{s'}|} \right\}. \tag{1.3}$$

In Eq. (1.3) we have used the following notation: $\mathbf{R}$, $\mathbf{r}_z^s$, $\mathbf{R}_a$, $\mathbf{r}_a^{s'}$ are the radius vectors respectively of the nucleus of the ion, the electrons of the ion, the nuclei of the crystal atoms, and the electrons of a crystal atom, eZ_2 and eZ_1 are the charges of the nuclei of the crystal and the ion, m is the number of bound electrons of the ion, and $eZ=e(Z_1-m)$ is the charge of the ion.

0038-5646/82/080371-09$04.00

Assume that conditions exist under which the charge state of the ion is sufficiently well defined:

a) The binding energy of the electrons in the ion is significantly greater than the energy of interaction of these electrons with the atoms of the nearest planes of the crystal (which is satisfied for $Z^2/n^2 \gg 1$);

b) The ion velocity v is significantly greater than the velocity v_z of the electron in those orbits of the ion for which the average distance of the electrons from the ion is greater than the minimum distance $x_{\min}$ between the ion and the channeling plane.[2] This condition is satisfied if $v \gg v_0 Z/n$, $a_0 n^2/Z \gtrsim u$, where v_0 and a_0 are the atomic units of velocity and length, n is the quantum number of a bound electron in the ion, and u is the amplitude of thermal vibrations of the atoms of the crystallographic plane.

If we are interested in the process of loss by the ion of one of its bound electrons, then under the conditions given above the Hamiltonian of interaction of the ion with the crystal (1.3) can be represented in the form

$$\hat{H}_{ic} = \hat{U}_{cont} + \hat{V}_{ec}, \tag{1.4}$$

$$\hat{V}_{ec} = e^2 \sum_a \left\{ \sum_{s'} (1/|\mathbf{r}_z^s - \mathbf{r}_a^{s'}|) - Z_2/|\mathbf{r}_z^s - \mathbf{R}_a| \right\},$$

where $\hat{U}_{\text{cont}}$ is the interaction energy of the ion as a whole with the continuous potential of the crystal planes and $\hat{V}_{ec}$ is the interaction energy of the considered electron of the ion with the nuclei and electrons of the crystal. Under the conditions of channeling and a stable charge state of the ion, the difference between the true Hamiltonian (1.3) and the approximate one given by (1.4), the physical meaning of which is that the ion as whole feels the individual impacts with the nuclei and with the ions of the crystallographic plane, leads to a redistribution of the flux of channeled ions in the energy of their transverse motion. For sufficiently small crystal thicknesses this process can be neglected, but for greater thicknesses it is easily taken into account in the final results (see below).

Let us find the probability of loss of an electron by a channeled ion. We shall consider first the condition in which the electronic state of the crystal does not change. As the zeroth approximation to the Hamiltonian (1.2) with inclusion of (1.4) we take

$$\hat{H}_0 = \hat{H}_i + \hat{H}_c + \hat{U}_{\text{cont}}. \tag{1.5}$$

Then the wave functions of the zeroth approximation are written in the form

$$\psi_0 = \exp(i\mathbf{k}_\parallel \boldsymbol{\rho}) \varphi_{\varepsilon\perp}(x) \varphi_z(\mathbf{r}_z^s) \varphi_{cn} \varphi_{ce}, \tag{1.6}$$

where $\mathbf{p}_\parallel = \hbar \mathbf{k}_\parallel$ is the two-dimensional momentum of the ion in the channeling plane, $\varphi_{\varepsilon\perp}(x)$ is the wave function of the transverse motion of the ion and satisfies the one-dimensional Schrödinger equation with the continuous potential U_{cont}:

$$\left[-\frac{1}{2M}\frac{d^2}{dx^2} + \hat{U}_{\text{cont}}(x) \right] \varphi_{\varepsilon_\perp}(x) = \varepsilon_\perp \varphi_{\varepsilon_\perp}(x), \tag{1.7}$$

$\varphi_z(\mathbf{z}_z^s)$ is the wave function of the bound electrons of the ion, and $\varphi_{cn(e)}$ is the wave function of the nuclei (or electrons) of the crystal. The zeroth approximation energy E_0 is made up of the energy of the longitudinal motion of the ion $E_\parallel = p_\parallel^2/2M$, the energy of the transverse motion $\varepsilon_\perp$, the binding energy ε_z of the electrons in the ion, and the phonon and electron energy of the crystal $\varepsilon_c = \varepsilon_{cn} + \varepsilon_{ce}$,

$$E^0 = E_\parallel + \varepsilon_\perp + \varepsilon_z + \varepsilon_c. \tag{1.8}$$

Considering the second term of Eq. (1.4) as a perturbation leading to transition of one of the bound electrons of the ion into the continuum, we shall write the probability W of this process per unit path of the ion in the crystal in the form

$$W = \frac{2\pi}{\hbar v} \int \frac{d^2\mathbf{p}_\parallel'}{(2\pi\hbar)^2} \int \frac{d^3\mathbf{p}_e}{(2\pi\hbar)^3} \sum_{i_\perp, f_\perp, f_c} P\varepsilon_\perp^i |\langle \psi_0^f | \hat{V}_{ec} | \psi_0^i \rangle|^2 \times \delta(\Delta E_\parallel + \Delta\varepsilon_\perp + \Delta\varepsilon_z + \Delta\varepsilon_0). \tag{1.9}$$

Here $\mathbf{p}_\parallel'$ is the final momentum of the ion in the channeling plane, $(p_\parallel'^2/2M = E_\parallel')$; $\mathbf{p}_e$ is the momentum of the electron which has escaped from the ion, and $\varepsilon_z' = p_e^2/2m$; the summation over $i_\perp$, $f_\perp$, and f_c denotes summation respectively over all initial and final states of the continuous motion of the channeled ion (the sum over the bound states + the integral over the transverse momentum in the continuum) and over all final states of the nuclei of the crystal; the symbol Δ in the argument of the Dirac δ function signifies the difference in the energies in the initial and final states; $P\varepsilon_\perp^i$ is the probability of populating a state with transverse energy $\varepsilon_\perp^i$ in the channel on entry of the ion into the crystal, which according to the sudden perturbation theory has the form of an expansion of the initial plane wave in the final wave functions of the transverse motion in the planar channel of the crystal[7,8]:

$$P_{s^i_\perp} = \left| d^{-1} \int_0^d \exp(ik_\parallel \theta x) \varphi_{\varepsilon^i_\perp}(x)\, dx \right|^2. \tag{1.10}$$

We then make use of the relation

$$\langle \varphi_{ce} | \hat{V}_{ec} | \varphi_{ce} \rangle = e \int d^3\mathbf{q} S(\mathbf{q}) U_q \exp(-i\mathbf{q}\mathbf{r}_z^s), \tag{1.11}$$

where U_q is the three-dimensional Fourier component of the potential of a crystal atom and

$$S(\mathbf{q}) = \sum_a \exp(i\mathbf{q}\mathbf{R}_a)$$

is the structure factor of the crystallographic plane. We go over from the coordinate $\mathbf{r}_z^s$ of the electron executing an inelastic transition to the coordinate $\mathbf{r}_z$ reckoned from the nucleus of the ion ($\mathbf{r}_z^s = \mathbf{R} + \mathbf{r}_z$). In Eq. (1.9) we integrate over $d^2\mathbf{p}_\parallel' = M\, d\theta\, dE_\parallel'$, where θ is the angle between the initial and final momenta of the ion in the channeling plane. In the matrix element of the expression (1.9) with allowance for (1.11) we integrate over the ion coordinates $\boldsymbol{\rho}$ in the channeling plane. As a result we obtain the following expression for the probability (1.9):

$$W = \frac{8\pi^3 M}{\hbar^3 v} e^2 \int d\theta \int \frac{d^3\mathbf{p}_e}{(2\pi\hbar)^3} \times \sum_{i_\perp, f_\perp, f_e} P_{\varepsilon^i_\perp} |\langle \varphi^f_{\varepsilon_\perp} \varphi_{cn}^f | F_{\Delta \mathbf{k}_\parallel} | \varphi^i_{\varepsilon_\perp} \varphi_{cn}^i \rangle|^2, \tag{1.12}$$

$$F_{\Delta\mathbf{k}_\parallel}=\int dq_\perp S(\mathbf{q})\,U_q e^{iq_\perp x}\langle\varphi_z{}^f|e^{-i\mathbf{q}\mathbf{r}_z}|\varphi_z{}^i\rangle|_{q^2=q_\perp^2+|\Delta\mathbf{k}_\parallel|^2}, \qquad (1.13)$$

$$|\Delta\mathbf{k}_\parallel|^2=(\Delta\varepsilon_\perp+\Delta\varepsilon_z+\Delta\varepsilon_c)^2/\hbar^2v^2+k_\parallel{}^2\theta^2. \qquad (1.14)$$

In the formulation considered for this problem, the characteristic changes of the energy of the transverse motion of the ion and of the energy of the phonon state of the crystal $\Delta\varepsilon_\perp$ and $\Delta\varepsilon_c$ are significantly less than the change in the energy of an electron of the multiply charged ion $\Delta\varepsilon_z$. Therefore the momentum $|\Delta k_\parallel|$ transferred to the ion in the channeling plane according to Eq. (1.14) will not depend either on the energy of the final state of the transverse motion of the ion or on the energy of the final state of the phonon spectrum even for very small scattering angles θ of the ion in the plane. Consequently we can assume that the entire expression (1.13) for $F_{\Delta k_\parallel}$ will not depend on what state the crystal has gone over to or on how the transverse state of the channeled ion changes. As a result, in view of the completeness of the systems of functions of the crystal and the transverse states of the ion, we can use the relation

$$\sum_{f_\perp}\sum_{f_c}|\langle\varphi_{\varepsilon_\perp}^{f}\varphi_{cn}{}^f|F_{\Delta\mathbf{k}_\parallel}|\varphi_{\varepsilon_\perp}^{i}\varphi_{cn}{}^i\rangle|^2$$

$$=\langle\varphi_{\varepsilon_\perp}^{i}\varphi_{cn}{}^i||F_{\Delta\mathbf{k}_\parallel}|^2|\varphi_{\varepsilon_\perp}^{i}\varphi_{cn}{}^i\rangle. \qquad (1.15)$$

We interchange next the order of the averaging of the quantity $|F_{\Delta k_\parallel}|^2$ over the given initial state of transverse motion of the ion and of the summation over all possible such initial states with a definite probability of population $P\varepsilon_\perp^i$. After this procedure, using the fact that the quantity $|F_{\Delta k_\parallel}|^2$ is independent of the initial state of the transverse motion of the ion, it is easy to see that the expression

$$p(x)=\sum_{i_\perp}P_{\varepsilon_\perp^i}|\varphi_{\varepsilon_\perp}^{i}(x)|^2 \qquad (1.16)$$

is the average probability of distribution of the flux of ions in impact parameter in the channeling plane. As a result the expression (1.12) for the probability will take the form

$$W=\int p(x)\,w(x)\,dx, \qquad (1.17)$$

where the probability $w(x)$ of loss of an electron by the ion at a given distance x of the ion from the channeling plane[3] is determined by the formula

$$w(x)=\frac{8\pi^3Me^2}{\hbar^3v}\int d\theta\int\frac{d^3\mathbf{p}_e}{(2\pi\hbar)^3}\langle|F_{\Delta\mathbf{k}_\parallel}|^2\rangle_{\delta\mathbf{R}_a}. \qquad (1.18)$$

Averaging over the initial state of the nuclei of the crystal actually amounts to averaging over the displacements of the nuclei from their equilibrium positions as a consequence of thermal vibrations (Ref. 4).[4)] Assuming that the longitudinal and transverse thermal vibrations are independent, calculations too cumbersome to present here can yield, as was done in Ref. 10,

$$\langle|F_{\Delta\mathbf{k}_\parallel}|^2\rangle_{\delta\mathbf{R}_a}=n_s\sum_k\{\langle|D_k|^2\rangle_{x_a}-|\langle D_k\rangle_{x_a}|^2$$

$$\times\exp[-\Delta k_\parallel{}^2u^2]\}$$

$$+\frac{(2\pi)^2}{\Delta}n_s\exp[-\Delta k_\parallel{}^2u^2]$$

$$\times\left|\left\langle\sum_k D_k\right\rangle_{x_a}\right|^2\sum_g\delta(\Delta\mathbf{k}_\parallel-\mathbf{g}), \qquad (1.19)$$

where the angle brackets with the subscript x_a denote averaging over the Gaussian distribution

$$\langle D\rangle_{x_a}=(2\pi u^2)^{-1/2}\int_{-\infty}^{+\infty}dx_aD\exp(-x_a{}^2/2u^2),$$

and the function D_k is equal to

$$D_k=\int dq_\perp U_q\exp\left[iq_\perp\left(x-\left(k-\frac{1}{2}\right)d-x_a\right)\right](e^{i\mathbf{q}\mathbf{r}_z})_{if}. \qquad (1.20)$$

In Eqs. (1.19) and (1.20) we have used the following notation: n_s is the density of atoms in the plane, **g** are the various vectors of the reciprocal lattice in the crystallographic plane, and Δ is the area of the unit cell, which is equal to the product of the two translation vectors. In accordance with the result (1.19) the probability $w(x)$ can be represented in the form of the sum of two terms (see also Ref. 3):

$$w(x)=w_{coh}(x)+w_{inc}(x). \qquad (1.21)$$

Here $w_{\rm coh}(x)$ is the coherent part of the probability of electron loss by the ion in the crystal, and is associated with the periodic arrangement of the atoms in the crystal plane [$w_{\rm coh}(x)$ arises on substitution of the second term in Eq. (1.19) into expression (1.18) and subsequent integration over the angle θ of scattering of the ion in the channeling plane and over the energy of the electron lost by the ion]:

$$w_{coh}(x)=\frac{(2m)^{3/2}2\pi^2n_se^2}{\hbar^4\Delta v}\sum_g\int d\Omega_e\left|\left\langle\sum_k D_k\right\rangle_{x_a}\right|^2$$

$$\times e^{-g^2u^2}\lambda_{gk}\eta(\lambda_{gk}), \qquad (1.22)$$

$d\Omega_e$ is the interval of solid angle in the direction of emission of the electron from the ion, $|g_k|$ is the projection of the momentum vector of the reciprocal lattice onto the initial direction of the momentum of the ion, $|\varepsilon_z^i|$ is the binding energy of the electron in the ion, the quantity $\left|\left\langle\sum_k D_k\right\rangle x_a\right|^2$ in Eq. (1.20) is taken at the value $|q_\parallel|=|\mathbf{g}|=|\Delta\,\mathbf{k}_\parallel|$ and at a wave function of the final state φ_z^f corresponding to an energy ε_z^f of the electron far from the ion; $\varepsilon_z^f=\lambda_{gk}^2=|g_k|\hbar v-|\varepsilon_z^i|$; the summation over k signifies a sum over the coordinates of the two nearest planes, which form the planar channel, if the ion is moving between the two planes; if the ion crosses all the planes, the summation is carried out over all $k=0$, ±1, and ±2; in the sum over all possible reciprocal-lattice vectors **g** it is sufficient here and below to retain the single minimal vector $\mathbf{g}_{\min}$, for which one has the inequality $|g_k^{\min}|\hbar v\geqslant|\varepsilon_z^i|$; $\eta(y)$ is the unit function of Heaviside:

$$w_{inc}(x)=\frac{Mn_s e^2}{\hbar^6 v}\int d\theta \int d^3\mathbf{p}_e$$

$$\times\sum_{k}\{\langle|D_k|^2\rangle_{x_a}-|\langle D_k\rangle_{x_a}|^2\exp[-\Delta k_{\parallel}{}^2u^2]\} \quad (1.23)$$

is the incoherent part of the probability of electron loss by the ion and is associated with the thermal vibrations of the crystal atoms; the quantity D_k is taken at a value $q_{\parallel}$ equal to

$$q_{\parallel}=|\Delta\mathbf{k}_{\parallel}|=[(\Delta\varepsilon_z/\hbar v)^2+k_{\parallel}{}^2\theta^2]^{1/2}. \quad (1.24)$$

§ 2. COHERENT IONIZATION OF AN ATOMIC PARTICLE IN A PLANAR CHANNEL OF A CRYSTAL

a) Let us discuss in more detail the general expression for the probability of coherent ionization (1.22) of an ion in planar channeling. We shall investigate first the case of loss of an electron by an ion from an unexcited state, when the following inequality is satisfied ($\langle r_z\rangle \approx n^2a_0/Z$):

$$g\langle r_z\rangle\ll 1, \quad \langle r_z\rangle/|x\pm d/2|\ll 1.$$

Then, expanding the function $\exp(i\mathbf{q}\cdot\mathbf{r}_z)$ in Eq. (1.20), substituting the first nonvanishing term into Eq. (1.22), and integrating over the angles of emission of the electron, we obtain

$$w_{coh}(x)=\hbar v\frac{8\pi^3 n_s c}{\Delta\hbar^2 v^2}\sum_{\mathbf{g}}\frac{\sigma_{\mathrm{p}}(\omega_{\mathbf{g}})}{\omega_{\mathbf{g}}}\Big|\sum_{k}T_g{}^k(x)\Big|^2 e^{-g^2u^2}, \quad (2.1)$$

$$T_g{}^k=\int dq_{\perp}U_q(g^2+q_{\perp}{}^2)^{1/2}\exp[-q_{\perp}{}^2u^2/2-iq_{\perp}(x-(k-{}^1/_2)d)|. \quad (2.2)$$

As can be seen from Eq. (2.2), in the dipole approximation (2.1) the coherent probability of loss of an electron by an ion is expressed in terms of the cross section $\sigma_{\mathrm{p}}(\omega_g)$ for the photoelectric effect in the electron shells of the ion. Here the role of the photon frequency is played by the quantity $\omega_g = |g_k|v$, and the role of the photon flux density $j_{\omega_g}(x)$ at a given distance x of the ion from the plane is played by the quantity

$$j_{\omega_g}(x)=\frac{8\pi^3 n_s c}{\hbar\Delta\omega_{\mathbf{g}}}\exp[-g^2_{min}u^2]\Big|\sum_{k=0,1}T^k_{g_{min}}(x)\Big|^2, \quad (2.3)$$

where $g_{\min}$ is the minimum length of the reciprocal lattice vector whose projection on the initial direction of the ion momentum in the plane satisfies the inequality $g_{\min}\geqslant|\varepsilon_z^i|/\hbar v$. Here Eq. (2.1) can be represented in the form (see also Ref. 2)

$$w_{coh}(x)=\sum_{\mathbf{g}}\sigma_{\mathrm{p}}(\omega_{\mathbf{g}})j_{\omega_{\mathbf{g}}}(x)/v. \quad (2.4)$$

The quantity T_g^k depends on the amplitude u of the transverse thermal vibrations of the atoms in the crystal plane and can be represented in a rather simple form in a number of limiting cases. For example, if the inequality ($\varkappa^{-1}$ is the screening radius of the crystal atom)

$$g_{min}>[(x\pm d/2)/u^2, \varkappa], \quad g_{min}u>1, \quad |x\pm d/2|<u \quad (2.5)$$

is satisfied [which is practically always the case for not too high ion velocities v and a sufficiently large binding energy of the electron in the ion $\varepsilon_z^i(g_{\min}\geqslant|\varepsilon_z^i|/\hbar w)$], the expression for T_g^k takes the form

$$T_g{}^k=\frac{\sqrt{2\pi}}{u}gU_g\exp\Big[-\frac{(x-(k-{}^1/_2)d)^2}{2u^2}\Big]. \quad (2.6)$$

We note here that the inequalities (2.5) are compatible with (2.1) only for high values of the ion charge multiplicity Z.

For the greater part of the channeled ions, not all distances of the ion to the plane are achieved: ($|x\pm d/2|_{\min}\gg u$). However, the momentum transferred to the ion in the ionization process is large ($gu>1$) for not too high ion velocities; if the probability is not to be small, small impact distances of the ion to the plane are required. Therefore for well channeled, not too fast ions the probability of loss of an electron by the ion is smaller than for quasichanneled superbarrier ions, which all cross the crystallographic planes. The weight of the superbarrier states is high if the entry angle is comparable with the Lindhard angle (or if the crystal thickness is sufficiently great so that ions from sub-barrier states go over to superbarrier states as the result of diffusion in their transverse energy).

As follows from Eqs. (2.2), (2.3), and (2.6), the coherent part of the probability of electron loss by an ion disappears if the longitudinal thermal vibrations u or the transverse vibrations increase (or the momentum $q_{\parallel}=g_{\min}$ transferred to the ion increases). If the momentum transfer $g_{\min}$ is not too great:

$$g_{min}\ll|x\pm d/2|/u^2, \quad g_{min}\ll\varkappa, \quad (2.7)$$

which is the case for high ion velocities and sufficiently low binding energies of the electron in the ion, the transverse thermal vibrations $u_{\perp}$ and the longitudinal ones $u_{\parallel}$ can be neglected. In this case T_g^k can be written in the following form:

$$T_g{}^k(x)=\frac{d}{dx}V_g\Big[x-\Big(k-\frac{1}{2}\Big)d\Big], \quad (2.8)$$

where

$$V_g(x)=(2\pi)^{-2}\int V_a([\rho^2+x^2]^{1/2})\exp(ig\rho)d^2\rho$$

is the two-dimensional Fourier component of the potential of the atom. Further, if the inequalities

$$g_{min}\ll|x\pm d/2|/u^2 \text{ and } g_{min}>\varkappa, \quad (2.9)$$

are satisfied, then

$$T_g{}^k=gV_g[x-(k-{}^1/_2)d]. \quad (2.10)$$

Various models of the lattice atom potential can be used for specific calculations. In particular, a sufficiently accurate potential is that of Molière,

$$V_a(r)=\frac{eZ_2}{r}\sum_{i}\alpha_i\exp(-\varkappa_i r),$$

where $\varkappa_i=\beta_i/a$, $a=0.885Z_2^{-1/2}$, a_0 is the Thomas-Fermi radius of the atom, $a_0=\hbar^2/me^2$, and $\alpha_i=\{0.1, 0.55, 0.35\}$ and $\beta_i=\{6.0, 1.2, 0.3\}$ are the Molière constants. In this case the quantities U_g and V_g in Eqs. (2.6), (2.8), and (2.10) are determined by the formulas [see the definition (1.11)]

$$U_g=\frac{1}{2\pi^2}eZ_2\sum_{i=1,2,3}\alpha_i/(g^2+\varkappa_i^2),$$
$$V_g=\frac{1}{2\pi}eZ_2\sum_i\alpha_i\exp(-[g^2+\varkappa_i^2]^{1/2}|x|)/(g^2+\varkappa_i^2)^{1/2}. \tag{2.11}$$

One can also use a model similar to that of Barrett,[11] in which $\alpha_i=\{0.4, 0.6\}$ and $\beta_i=\{2.984, 0.474\}$, or to that of Firsov,[12] which is valid in particular even for very light crystals.

Let us now investigate the dependence of the coherent part of the probability of electron loss by an ion (2.2) on the direction of the ion momentum in the channeling plane with respect to the principal crystallographic axes of which the plane consists. For definiteness let the nuclei in the channeling plane be at the sites of a plane rectangular lattice with period d. Further, let the ion momentum vector in the plane make not too large an angle χ with the vectors which connect the neighboring nuclei of the crystallographic plane, and let the ion velocity v be such that the minimum energy of the equivalent photon $\hbar\omega_g^{\min}=2\pi\hbar v\sin\chi/d$ significantly exceeds the electron binding energy in the ion $|\varepsilon_z^i|$. If, at a constant angle of entry of the ion with respect to the channeling plane, the angle χ between the direction of the momentum and the vector connecting the neighboring nuclei of one of the principal crystallographic axes of the lattice decreases ($\chi\ll 1$), the probability of electron loss by the ion begins to rise rapidly. For example, for a hydrogenlike ion the rate of rise is proportional to $\chi^{-9/2}$. However, at some critical value $\chi_{\rm cr}$ of the angle,

$$\chi_{\rm cr}^{(1)}=|\varepsilon_z^i|d/2\pi\hbar v \tag{2.12}$$

the ionization probability undergoes a downward jump and then again begins to rise to a value $\chi_{\rm cr}^{(2)}=\chi_{\rm cr}^{(1)}/2$, and so forth. The absolute value of the probability in the next nth maximum is either almost the same as or smaller than in the preceding maximum, in accordance with Eq. (2.2).

We shall consider next the case of loss of an electron by an ion from an excited state for relatively low ion velocities when the inequalities

$$\langle r_z\rangle/|x\pm d/2|\gtrsim 1,\qquad g_{\min}\langle r_z\rangle\gg 1, \tag{2.13}$$

are satisfied. Then the dipole approximation is inapplicable, and the ionization probability is no longer expressed in terms of the cross section for the photoelectric effect. In this case, since the effective values of $q_\perp$ in Eq. (1.20) are small in comparison with g for well channeled particles, the matrix element in Eq. (1.20) can be taken outside the integral sign at the point $\mathbf{q}=\mathbf{g}$. As a result the probability of electron loss by the ion can be expressed in terms of the cross section for ionization of an ion with unit charge moving with velocity v in the Born approximation $\sigma^e(\mathbf{q}, \vec{\varkappa}_e)$,5) expressed in the variables of the momentum transfer $\mathbf{q}$ and the momentum of the electron emitted from the ion $\vec{\varkappa}_e$ at definite values of these parameters ($\mathbf{q}=\mathbf{g}$, $\vec{\varkappa}_g=\vec{\varkappa}_e$, $\vec{\varkappa}_g=(2m)^{1/2}(|g_k|\hbar v-|\varepsilon_z|)^{1/2}\hbar$)

$$w_{\rm coh}(x)=\frac{8\pi^5 n_s\hbar}{\Delta v m e^2}\sum_{\mathbf{g}}\frac{\sigma^e(\mathbf{g},\varkappa_{\mathbf{g}})}{\varkappa}g^4\Big|\sum_k P_g^k\Big|^2, \tag{2.14}$$

$$P_g^k=\int dq_\perp U_q\exp[-q_\perp^2u^2/2 - iq_\perp(x-(k-{}^1/_2)d)]_{q=(g^2+q_\perp^2)^{1/2}}. \tag{2.15}$$

The formulas (2.2) and (2.14), as must be the case, come together in the region $gr_z\sim 1$. Here if $\varkappa_g\langle r_z\rangle\gg 1$, which is the case for ion velocities $v\gg v_z Z/ga_0n^3$ and corresponds in order of magnitude to the condition that the equivalent photon energy exceed substantially the electron binding energy in the ion, we have for the cross section $\sigma^e(gr\sim 1, \varkappa_g)\sim\varkappa_g^{-8}$. Therefore qualitatively all results of this section relating to the anomalous behavior of the probability as a function of the entry angle of the ion with respect to the principal crystallographic axes remain valid, since $\varkappa_g\sim\chi^{1/2}$. We note that this effect can be observed also under conditions of strong nondipole nature ($g\langle r_z\rangle\gg 1$), provided that $\varkappa_g\gg g$, which is the case for still greater ion velocities $v\gg v_z g a_0 n/Z\chi$. However, for low ion velocities, $v\ll v_z\, g a_0 n/Z\chi$, we have for the cross section $\sigma^e(\mathbf{g},\vec{\varkappa})\sim\varkappa_g$, and consequently according to Eq. (2.14) the probability of electron loss by the ion will not depend on $\varkappa_g$ and therefore also not on the angle χ.

The expression (2.15) for p_g^k, which essentially determines the flux density of unit-charges (which transfer to the ion a momentum $\mathbf{g}$ and to the emitted electron a momentum $\varkappa_g$), a density equivalent to the crystal lattice in the plane, can be simplified in a number of limiting cases of small or large transverse vibrations of the crystal atoms and momentum transfers, as has been done above [see Eqs. (2.6)–(2.11)]. This expression can also be obtained analytically for a number of specific models of the atom potential [see Eq. (2.11)].

Under the condition (2.5) we have

$$P_g^k(x)=\frac{\sqrt{2\pi}}{u}U_g\exp\Big[-\frac{(x-(k-{}^1/_2)d)^2}{2u^2}\Big]. \tag{2.16}$$

If the inequalities (2.7) and (2.9) are satisfied, then

$$P_g^k(x)=V_g[x-(k-{}^1/_2)d]. \tag{2.17}$$

b) We shall obtain next the expression for the probability of coherent ionization if the particle entry angle into the crystal significantly exceeds the critical angle of planar channeling. In this case the eigenfunctions of the transverse motion are essentially plane waves and according to Eqs. (1.10) and (1.16) $p(x)$ is equal to $1/d$. To obtain a general expression for the probability we shall represent $\Big|\Big\langle\sum_k D_k(x)\Big\rangle\Big|^2$ [see Eq. (1.20)] in the form of a double integral over $dq_\perp$ and $dq_\perp'$; we shall then integrate over dx, using the equality

$$\int\exp[i(q_\perp-q_\perp')x]dx=2\pi\delta(q_\perp-q_\perp'),$$

and then the formula

$$\Big|\sum_k\exp(ikq_\perp d)\Big|^2=\frac{2\pi}{d}\sum_{g_\perp}\delta(q_\perp-g_\perp).$$

As a result we obtain from Eqs. (1.17)–(1.20)

$$W=\frac{2^{9/2}\pi^4 m^{1/2}n_V e^2}{d\Delta\hbar^4 v}\sum_{\mathbf{g}}\int d\Omega_e|(e^{i\mathbf{g}\mathbf{r}_z})_{if}|^2|U_g|^2\lambda_{\mathbf{g}}e^{-g^2u^2}\eta(\lambda_{\mathbf{g}}), \tag{2.18}$$

where $n_V = n_s/d$ is the density of crystal atoms and **g** is the vector of the three-dimensional reciprocal lattice. In the dipole approximation $(g\langle r_z\rangle \ll 1)$ the probability takes the form

$$W=\sum_{\mathbf{g}} \sigma_{\mathrm{p}}(\omega_g) j_g/v, \qquad j_g=32\pi^5 \frac{|U_g|^2 g^2 c n_V}{\hbar d^3 \omega_{\mathbf{g}}} e^{-g^2u^2}. \tag{2.19}$$

The result given by Eqs. (2.18) and (2.19) shows that the role of the equivalent photon frequency is played by the quantity $\omega_{\mathbf{g}} = |g_k|v = 2\pi v d^{-1} n \sin\theta$, where θ is the angle at which the ion crosses the crystallographic planes. Therefore there is an anomalous behavior of the probability (2.19) as a function of this angle θ.

In the case $g\langle z_r\rangle \gg 1$, as was done in obtaining Eq. (2.15), from Eq. (2.18), we have

$$W=\frac{32\pi^7\hbar n_V}{d\Delta v m e^2}\sum_{\mathbf{g}} \frac{\sigma(\mathbf{g}, \varkappa_{\mathbf{g}})}{\varkappa_{\mathbf{g}}} g^4 |U_g|^2 e^{-g^2u^2}. \tag{2.20}$$

§ 3. INCOHERENT IONIZATION OF AN ATOMIC PARTICLE IN PLANAR CHANNELING

a) In the preceding section we found in particular that, for sufficiently high ion velocities in the crystal and at directions of the ion momentum in the channeling plane far from the directions of the principal axes of the crystallographic planes, the coherent probability of electron loss by the ion can be highly suppressed. This occurs as a result of the fact that too large an energy is transferred to the electron, and there are no smaller energies in the spectrum of the coherent perturbation by the crystal. As a result the role of incoherent ionization becomes dominant. Let us investigate in more detail the general expression (1.23) for high ion velocities:

$$v>Zv_0. \tag{3.1}$$

Under the condition (3.1) we can assume that the effective longitudinally transferred momentum $\mathbf{q}_\parallel$ will not depend on the electron energy $(q_\parallel = k\theta)$, and in addition we can utilize a series expansion of $\exp(i\mathbf{q}\cdot\mathbf{r})$. Further, if the effective distances of the ion to the plane are greater than the amplitude of the thermal vibrations of the atoms $(|x \pm d/2| \gg u)$, and $\theta_{\mathrm{eff}} \ll (ku)^{-1}$, we can expand the probability of electron loss by the ion in powers of u, using the equality

$$\langle|D_k|^2\rangle-|\langle D_k\rangle|^2\exp(-q_\parallel^2u^2)=u^2\left\{q_\parallel^2|D_k|^2+\left|\frac{\partial D_k}{\partial x}\right|^2\right\}_{x_a=0}. \tag{3.2}$$

As a result, after some transformations, we can obtain from Eq. (1.23)

$$w_{inc}(x)=\frac{j(x)}{v}\int_{\omega_{\mathrm{thr}}}^{\infty}\frac{\sigma_{\mathrm{p}}(\omega)\,d\omega}{\omega}. \tag{3.3}$$

Here the density of the equivalent photon flux is

$$j(x)=\frac{2\pi u^2 n_s c}{\hbar v}\sum_{k=0,1}\int d\mathbf{q}_\parallel\left\{\mathbf{q}_\parallel^2|T^k_{\mathbf{q}_\parallel}(x)|^2+\left|\frac{d}{dx}T^k_{\mathbf{q}_\parallel}(x)\right|^2\right\}_{u=0}, \tag{3.4}$$

where for $T^k_{\mathbf{q}_\parallel}(x)$ the formulas (2.8), (2.10), and (2.11) which determine $T^k_{\mathbf{q}_\parallel}(x)$ in terms of the atom potential for the conditions (2.7) and (2.9) are valid; $\hbar\omega_{\mathrm{thr}}$ is the threshold ionization energy.

The order of magnitude of the incoherent probability of electron loss by the ion (3.3) can be estimated from the formula

$$w_{inc}\sim\sigma_{\mathrm{p}}(\omega_{\mathrm{thr}})(Z_2^2e^2/\hbar v)(c/v)(u^2n_s/b^3), \tag{3.5}$$

where $b = \min[|x \pm d/2|, \varkappa^{-1}]$ and $\varkappa$ is the screening parameter of the crystal atom. From the estimate (3.5) it follows that the probability (3.4) is suppressed relative to the coherent probability at the maximum $w^{\max}_{\mathrm{coh}}(x)$, which is realized when the equivalent photon energy $h\omega_g$ is close to the threshold ionization energy $|\varepsilon^i_z|$ [see Eq. (2.2)]. In the case $v > Zv_0$, as a rule, we have $\hbar\omega_g \gg |\varepsilon^i_z|$. Therefore the coherent probability (2.2) in this case is decreased by a factor $(h\omega_g/|\varepsilon^i_z|)^{9/2}$ in comparison with this value at the maximium. As a result under the conditions

$$(\hbar\omega_g/|\varepsilon_z^i|)^{7/2}\gg(u/b)^{-2}, \quad v\gg Zv_0, \tag{3.6}$$

the probability of electron loss by an ion is determined by the incoherent part (3.4).

For the part of the beam of ions scattered at a small angle $(\theta\approx 0)$ in the channeling plane, the longitudinally transferred momentum will no longer depend on the equivalent photon energy. Therefore the probability of electron loss by an ion can be written in the form

$$\left.\frac{dw_{inc}(x)}{d\theta}\right|_{\theta=0}=2\pi\frac{u^2n_sck_\parallel}{\hbar v^2}\int_{\omega_{\mathrm{thr}}}\frac{d\omega}{\omega}\sigma_{\mathrm{p}}(\omega)L(x,\omega),$$

$$L(x,\omega)=\sum_{k=0,1}\left\{\frac{\omega^2}{v^2}|T^k_{\omega/v}(x)|^2+\left|\frac{d}{dx}T^k_{\omega/v}(x)\right|^2\right\}_{u=0}. \tag{3.7}$$

It follows from this that the ionization probability is also suppressed [the estimate (3.5) is valid, but $b = \min\{v/\omega, \varkappa^{-1}\}$]. For the part of the ion beam whose distances to the channeling plane are less than or of the order of the amplitude of the thermal vibrations $|x \pm d/2| \lesssim u$ or for ions scattered at a large angle θ, the expansion (3.2) is inapplicable; however, for the condition (3.1) one can as before use the expansion of $\exp(i\mathbf{q}\cdot\mathbf{r}_z)$ in series and express $w_{\mathrm{inc}}(x)$ in terms of the cross section for the photoelectric effect [see Eq. (3.3)]. The role of the equivalent-photon flux density here is played by the quantity

$$j(x)=2\pi\frac{Mn_sc}{\hbar^2}\sum_k\int d\theta\{\langle|T^k_{q_\parallel}(x)|^2\rangle_{\delta x_a} -|\langle T^k_{q_\parallel}(x)\rangle_{\delta x_a}|^2\exp(-q_\parallel^2u^2)\},$$

$$q_\parallel^2=|\varepsilon_z^i|^2/\hbar^2v^2+k_\parallel^2\theta^2. \tag{3.8}$$

If the size of the electron orbit in the ion is greater than the amplitude of the thermal vibrations, the probability (3.3) with $j(x)$ from (3.8) is less than the coherent probability of electron loss by the ion at the maximum $w^{\max}_{\mathrm{coh}}(x)$ for ions scattered at a very small angle in the channeling plane $(\theta \lesssim |\varepsilon^i_z|/\hbar k_\parallel v)$, and of the order of $w^{\max}_{\mathrm{coh}}(x)$ fore the part of the beam scattered at a relatively large angle $[\theta \sim (ku)^{-1}]$.

For relatively small ion velocities $v < Zv_0$ the coherent ionization (2.2) can be small already for another reason. Indeed, when the condition $\hbar\omega_g \gtrsim |\varepsilon_z^i|$ is satisfied for small velocities the transfer of a rather large reciprocal-lattice vector g can become necessary. Here according to (2.2) the probability is small ($\sim\exp(-g^2u^2)$) as the result of the influence of the thermal vibrations of the atoms. Therefore the role of incoherent ionization increases and can become dominant. We shall consider the coherent part of the probability (3.4) for small ion velocities in the crystal. First let

$$v_z \ll v \ll Zv_0, \tag{3.9}$$

which can occur for excited states of a multiply charged ion. The right-hand side of the inequality (3.9) determines the strong non-dipole nature of the process [$gr_z \gg 1$ in Eq. (1.20)]. The matrix element $\langle\varphi_z^f|\exp(i\mathbf{g}\cdot\mathbf{r})|\varphi_z^i\rangle$ is appreciably different from zero (as the result of rapid oscillations of the integrand) only for the condition $\varphi_z^f \sim e^{ipr_z/\hbar}$, where $\mathbf{p} = \hbar\mathbf{q}(\mathbf{p})$. These equalities can occur if the energy of the electron which has left the ion is significantly greater than its binding energy in the initial state, which is assured by the left part of the inequality (3.9). In addition, for the part of the beam scattered at a small angle ($\theta < |\varepsilon_z^i|/\hbar v k_\parallel$) in the channeling plane we can assume $q(p) \approx q_\parallel(p) = \Delta\varepsilon_z/\hbar v$, and take the matrix element in Eq. (1.20) outside the integral over $dq_\perp$; then, using the resonance matrix element for $\hbar\mathbf{q}(\mathbf{p}) = \mathbf{p}$, it is possible to integrate in (1.23) over the electron momentum in the final state $d^3\mathbf{p}_e'$. If here one has the inequality

$$umv/\hbar \ll 1, \tag{3.10}$$

then, expanding the probability in a series in this parameter, it is possible to obtain the following expression for the incoherent probability of electron loss by an ion in the crystal:

$$w_{inc}(x) = \frac{2^5\pi^3 n_s k_\parallel u^2 m^2 e^2}{\hbar^4} \sum_{k=\pm1} \left\{ \left| V_{2mv/\hbar}\left(x - \frac{kd}{2}\right)\right|^2 + \frac{\hbar^2}{4m^2v^2}\left|\frac{d}{dx} V_{2mv/\hbar}\left(x - \frac{kd}{2}\right)\right|^2 \right\} \Delta\theta_{\text{eff}}, \tag{3.11}$$

where $V_g(x)$ is the two-dimensional Fourier component of the atom potential, for which the equations (2.11) are valid, and $\hbar q = 2mv$ is the solution of the equation $\hbar\mathbf{q}(\mathbf{p}) = \mathbf{p}$; $\Delta\theta_{\text{eff}}$ is the interval of effective angles of detection of the scattered ions in the plane, which satisfies the condition

$$\Delta\theta_{\text{eff}} \leqslant |\varepsilon_z^i|/\hbar v k_\parallel.$$

As follows from Eq. (3.11), the ionization probability is small, in this case not only as the result of smallness of the Fourier component of the potential $V_q(x)$ at large distances x from the plane, but also as the result of the influence of the periodic arrangement of the atoms in the channeling plane (see above, and also Ref. 10). The inequalities (3.9) and (3.10) can be satisfied simultaneously for sufficiently highly excited states and high charge multiplicity of the ion. For the condition

$$umv/\hbar \gg 1, \tag{3.12}$$

the influence of the periodic arrangement of the atoms in the plane can be neglected. As a result the second term in (1.23) does not have to be taken into account and instead of Eq. (3.11) for the ionization probability one can obtain the expression

$$w_{inc}(x) = \frac{(2\pi)^3 n_s k_\parallel e^2}{\hbar^2 v^2} \sum_k \left\langle \left| V_{2mv/\hbar}\left(x - \frac{kd}{2}\right)\right|^2 \right\rangle_{\delta x_a} \Delta\theta_{\text{eff}}. \tag{3.13}$$

Equations (3.11) and (3.13) can be used to explain the results of experiments if the ion beam has a very low divergence and the angular resolution of the apparatus is sufficiently high.

The probability of electron loss by an ion, integrated over all ion scattering angles in the channeling plane, can be obtained also by using the resonance matrix element $(e^{i\mathbf{q}\mathbf{r}_z})_{if}$ for $\hbar\mathbf{q} = \mathbf{p}$. Here it is only necessary to assume that the longitudinally, transferred momentum is determined by elastic deflection of the ion in the plane ($q_\parallel = k\theta$). Then the energy of the electron emitted from the ion is determined by the ion scattering angle in the plane (to each scattering angle θ there corresponds an electron energy in the continuum $p_\parallel^2\theta^2/2m$). If the distances from the ion to the crystal plane are significantly greater than the amplitude of the thermal vibrations of the atoms of the plane $|x \pm d/2| \gg u$, will take the form

$$w_{inc}(x) = \frac{(2\pi)^3 n_s e^2}{\hbar^2 v^2} \sum_{k=\pm1} \int dq\,(1 - e^{-q^2u^2}) \left| V_q\left(x - \frac{kd}{2}\right)\right|^2. \tag{3.14}$$

For a number of models of the atom potential the integral over the scattering angles in the plane dq can be performed analytically [see Eq. (2.11)]; however, regardless of the dependence on a specific model of the atom potential it is evident that for a sufficiently light crystal ($\varkappa u \ll 1$) there also exists an effect of suppression of the probability of electron loss by the ion as a consequence of the periodic arrangement of the atoms in the crystal plane.

However, if $(1 - e^{-q^2u^2}) \sim 1$, the effect of the periodic arrangement of the atoms in the plane can be neglected, i.e., it is not necessary to take into account the second term in Eq. (1.23), and for the probability of electron loss by the ion we obtain

$$w_{inc}(x) = \frac{(2\pi)^3 n_s e^2}{\hbar^2 v^2} \sum_{k=\pm1} \int dq \left\langle \left| V_q\left(x - \frac{kd}{2}\right)\right|^2 \right\rangle_{x_a}. \tag{3.15}$$

b) Above we have obtained and studied expressions for the probabilities $w(x)$ of coherent and incoherent ionization of atomic particles in a crystal in planar channeling, as a function of the distance x of the ion to the crystallographic planes. The physical meaning of the quantity $w(x)p(x)$ is that it describes the loss of electrons by that part of the total ion beam whose average density (averaged over the thickness T and consequently dependent on T) at a distance from the center of the channel is $p(x)$. Recognizing that there is a correspondence of the average of the quantity $p(x)$ over the thickness with the angle of emission of the ions from the crystal,[6] the differential probability $w(x)p(x)$ can be verified experimentally. The quantity $p(x)$ depends on the divergence of the ion beam, the entry angle of the ions into the crystal with respect to the plane, and the depth of penetration of the ions into the crystal. For entry angles greater than the Lindhard angle θ_L, at very small depths and, on the other hand, at very large depths we have $p(x) = 1/d$; for a well channeled beam of particles with an entry angle $\theta \ll \theta_L$ this quantity is greater at the center of the channel and less near the planes. If we analyze the charge state not of the entire ion beam but only of a part of it, for example, with a small angle of emission from the crystal with respect to the plane, we can study also the dependence of the density of channeled ions near the center of the channel on the crystal thickness T.

If the entry angle of the ion into the crystal with respect to the plane is significantly greater than the Lindhard angle, it is possible to obtain from Eq. (1.23) a simpler expression for the probability. For this purpose, as in the derivation of Eq. (2.18), we represent $|D_k|^2$ in the form of a double integral over $dq_\perp dq'_\perp$ and integrate over dx. The dependence of the resulting integrand on $q_\perp$ and θ will be a dependence on the combination $q'^2 = q_\perp^2 + k_\parallel^2 \theta^2$. Therefore one integration can be carried out by using the transformation $k_\parallel \int dq_\perp d\theta = 2\pi \int q'\, dq'$. As a result we obtain from Eq. (1.23) $(n_V = n_s/d)$

$$W = \frac{4\pi^2 M n_V e^2}{k_\parallel v \hbar^6} \int d^3\mathbf{p}_e \int_0^\infty q' |U_q|^2 |(e^{i\mathbf{q}\mathbf{r}_z})_{if}|^2 (1 - e^{-q^2u^2})\, dq',$$

$$q^2 = q'^2 + (\Delta\varepsilon_z/\hbar v)^2. \tag{3.16}$$

Assume that the condition (3.1) is satisfied and let $\langle r_z \rangle \ll u$; in this case we obtain from (3.16) a result which differs from the corresponding expression for an amorphous target only in the argument of the logarithm:

$$W = \frac{2}{\pi} Z_2^2 \frac{e^2}{\hbar v} n_V \frac{c}{v} \ln\left(\frac{u}{\langle r_z \rangle}\right) \int_{\omega_{\text{thr}}}^\infty \sigma_p(\omega) \frac{d\omega}{\omega}. \tag{3.17}$$

However, if $\varkappa^{-1} > \langle r_z \rangle \gg u$, the ionization probability turns out to be suppressed in comparison with (3.17) by the parameter $u^2/\langle r_z \rangle^2$:

$$W = 8\pi Z_2^2 \frac{e^4 n_V u^2}{(v\hbar)^2} \ln\left(\frac{\langle r_z \rangle}{u}\right). \tag{3.18}$$

A similar result is obtained for $\langle r_z \rangle \gg \varkappa^{-1} \gg u$:

$$W = 8\pi Z_2^2 \frac{e^4 n_V u^2}{(v\hbar)^2} \ln((\varkappa u)^{-1}). \tag{3.19}$$

§ 4. ROLE OF OTHER MECHANISMS IN THE LOSS OF AN ELECTRON BY A CHANNELED ION

In the process of establishment of the equilibrium charge of atomic particles (ions) in amorphous solids, the probability of ionization is detrmined by interactions, with the nuclei and electrons of the material, in which the electronic state of the solid is not changed. The simultaneous electronic excitation of the ions and the atoms of the material is significantly less probable than the electronic excitation of only the ion passing through the material.

A different situation exists in passage of atomic particles through crystals in the channeling regime. As was shown above, under certain conditions the probability of electron loss by an ion, as the result of an interaction of the ion with the crystal in which the electronic state of the crystal does not change, turns out to be rather strongly suppressed. The suppression effect is particularly important at high ion velocities when the coherent process of stripping of the ion is small as the result of the fact that the minimal energy of the photon which is equivalent to the crystal lattice is significantly greater than the binding energy of the electron in the ion, and the incoherent process is small as a result of the fact that the deviations from periodicity are small and for not too large momentum transfers the ion losing the electron does not feel these deviations. As the result the loss of electrons by an ion in channeling has important contributions from other mechanisms of electron loss by ions.

Electron loss by ions as the result of inelastic interaction with the electron subsystem of the crystal

The formalism developed in §1 permits one actually to follow by simple manipulations the derivation of the general expression for the probability.

Since the electronic excitation of a crystal atom is propagated over the crystal significantly more slowly than the ion is moving, the process of electron loss by the ion is incoherent over the periodic distribution of the electron density in the crystal. As a result one can obtain the following expression for the probability of electron loss by an ion per unit pathlength in the crystal in planar channeling as a result of inelastic interaction of the electron of the ion with the electrons of the crystal:

$$w(x) = \frac{M n_s}{v \hbar^6} \sum_k \int \left\langle \{|R^2|_{aa} - |R_{aa}|^2\} \right\rangle \delta x_a d^3\mathbf{p}_e d\theta, \tag{4.1}$$

$$R = \frac{e^2}{2\pi^2} \sum_s \int dq_\perp q^{-2} \exp\left\{-iq_\perp \left(x - \frac{kd}{2}\right) + i\mathbf{q}\mathbf{r}_a^s\right\} (e^{-i\mathbf{q}\mathbf{r}_z})_{if},$$

$$q^2 = q_\perp^2 + (\Delta\varepsilon_z/\hbar v)^2 + k_\parallel^2 \theta^2, \tag{4.2}$$

where $\Delta\varepsilon_z$ is the change in energy of the electron of the ion; R_{aa} is the diagonal matrix element between the initial wave functions of the electrons of the crystal atom; the sum over s stands for the sum over the electrons of the crystal atom.

Assume that condition (3.1) is satisfied. Also let the average radius of the electron orbit in the ion $\langle r_z \rangle$ be significantly less than the Thomas-Fermi radius of the crystal atom a_{TF}, where most of the electrons are concentrated. This condition is satisfied for ions with sufficiently high charge multiplicity Z (and for ground states) and for relatively light crystals $Z_2 < 30$. We shall also assume that the distance of the ions to the plane averaged over the thickness $(x \pm d/2)$ of the crystal is greater than a_{TF}. Then in Eqs. (4.1) and (4.2) we can make the following substitutions:

$$\exp(i\mathbf{q}\mathbf{r}_z) \to \mathbf{q}\mathbf{r}_z,$$

$$\langle |R^2|_{aa} - |R_{aa}|^2 \rangle \delta x_a \to Z_2 \left| \int dq_\perp \frac{\exp[iq_\perp(x - kd/2)]}{[q_\perp^2 + (\Delta\varepsilon_z/\hbar v)^2 + k_\parallel^2 \theta^2]^{1/2}} \right|^2. \tag{4.3}$$

We shall calculate the integral over $dq_\perp$ in (4.3) by means of a contour C which encloses the branch point in the upper half-plane[7]:

$$q_\perp^0 = i[k_\parallel^2 \theta^2 + (\Delta\varepsilon_z/\hbar v)^2]^{1/2}.$$

The result can already by integrated over the scattering angle of the ion in the channeling plane and for the probability of electron loss by the ion we obtain

$$w(x)=\frac{1}{\pi^2}n_s Z_2\frac{e^2}{\hbar v}\frac{c}{v}\int_{\omega_{\rm thr}}\frac{d\omega}{\omega}\sigma_{\rm P}(\omega)\frac{K_0[2|x-d/2|\omega/v]}{|x-d/2|}. \qquad (4.4)$$

Here $K_0(z)$ is the Macdonald function.

This result shows, on the one hand, that all electrons of the crystal atom can be considered as free, since in the process of inelastic interaction a sufficiently large momentum is transferred to them, and on the other hand, that their action on the electron of the ion is equivalent to a flux of photons whose spectrum and intensity depend on the distance of the ion to the maximum of the electron density of the crystal.

However, if the radius of the electron orbit in the ion is significantly greater than the Thomas-Fermi radius of the crystal atom, which is the case for heavy crystals and for excited states of a multiply charged ion, one can make the substitution $\exp(i\mathbf{q}\mathbf{r}_a^s)\to 1+i\mathbf{q}\mathbf{r}_a^s$, and take the matrix element $(e^{i\mathbf{q}\mathbf{r}_z})_{if}$ outside the integral over $dq_\perp$. Then it is possible to integrate the square of this matrix element over $d^3\mathbf{p}_e$, using the fact that it is nonzero only for the condition $\mathbf{p}=\hbar\mathbf{q}$, and then integrate over $dq_\perp$ and $d\theta$ as was done in derivation of Eq. (4.4). As a result we obtain for the desired probability $w(x)$ the expression

$$w(x)=4\frac{n_e e^2\langle d_x^2\rangle}{\hbar^2 v^2}\frac{K_0[4|x-d/2|mv/\hbar]}{|x-d/2|}. \qquad (4.5)$$

Here $\langle d_x^2\rangle$ is the mean square of the dipole moment of the crystal atom.

If the angle θ of entry of the ion into the crystal with respect to the plane is significantly greater than the Lindhard angle $\theta_{\rm L}$, then from Eqs. (4.1), (4.2), proceeding as in the derivation of Eqs. (3.16)–(3.18), for the case $\langle r_z\rangle \ll a_{\rm TF}$ we will have for the probability

$$W=\frac{2e^2}{\pi\hbar}\frac{n_V c}{v^2}\int_{\omega_{\rm thr}}\frac{d\omega}{\omega}\sigma_{\rm P}(\omega)\ln\left(\frac{v}{\langle r_z\rangle\omega}\right). \qquad (4.6)$$

However, if $\langle r_z\rangle \gg a_{\rm TF}$, then

$$W=8\pi n_V\langle d_x^2\rangle\frac{e^2}{(\hbar v)^2}\ln\left(\frac{v\hbar\varkappa}{|\varepsilon_z^i|}\right). \qquad (4.7)$$

This result coincides with the result for the total probability of inealstic excitation of the target atoms by an electron in the Born approximation. See for example Ref. 13, formula (148.26) [formula (145.26) in the 1963 Russian edition, and formula (120.22) in the 1959 edition of the Sykes-Bell translation]. Indeed, if $\langle r_z\rangle \gg a_{\rm TF}$, the electron of the ion can be considered free in an inelastic interaction with a crystal atom, and for the condition $\theta\gg\theta_L$ the distribution in impact parameters can be considered uniform, from which Eq. (4.7) immediately follows.

[1)] These correlations affect not only the ionization of the passing particles, but also other inelastic processes occurring with these particles such as bremsstrahlung.[4,5]

[2)] For deeper orbits, i.e., for strongly bound states of the multiply charged ion, the condition $v>v_z$ may turn out to be unnecessary, since charge exchange is suppressed as a result of the impossibility of intersection of the orbits of electrons with nearby binding energies, and ionization is suppressed for the reasons discussed below.

[3)] In planar channeling of positively charged ions the coordinate x is conveniently measured from the center of the interplanar distance.

[4)] In the case in which the combined potential of the nuclei of the lattice acts as a perturbation, averaging over the thermal vibrations was carried out also ion Refs. 3 and 9.

[5)] For a hydrogenlike ion $\sigma^e(\mathbf{q},\varkappa)$ can be expressed in terms of elementary functions (see for example Ref. 13).

[6)] Ions channeled near the center of the channel are emitted from the crystal directly along the direction of a beam entering the crystal parallel to the planes; the further from the center of the distance between planes, the greater is the emission angle with respect to the plane.

[7)] For $x\pm d/2<0$ the contour C is closed into the lower half-plane.

[1] M. A. Kumakhov, Usp. Fiz. Nauk **115**, 427 (1975) [Sov. Phys. Uspekhi **18**, 203 (1975)].

[2] V. A. Bazylev and N. K. Zhevago, Phys. Lett. **74A**, 443 (1979).

[3] V. A. Bazylev and N. K. Zhevago, Zh. Eksp. Teor. Fiz. **77**, 312 (1979) [Sov. Phys. JETP **50**, 161 (1979)].

[4] M. L. Ter-Mikaélyan, Vliyanie sredy na élektromagnitnye protsessy pri vysokikh énergiyakh (Influence of the Medium on Electromagnetic Processes at High Energies), Erevan, Academy of Sciences of the Armenian SSR, 1969.

[5] A. I. Akhiezer, V. F. Boldyshev, and N. F. Shul'ga, Fiz. Elem. Chastits At. Yadra **10**, 51 (1979) [Sov. J. Part. Nucl. **10**, 19 (1979)].

[6] D. S. Gemmel, Rev. Mod. Phys. **46**, 129 (1974).

[7] Yu. Kagan and Yu. V. Kononets, Zh. Eksp. Teor. Fiz. **58**, 226 (1970) [Sov. Phys. JETP **31**, 124 (1970)].

[8] V. A. Ryabov, Zh. Eksp. Teor. Fiz. **67**, 150 (1974) [Sov. Phys. JETP **40**, 77 (1975)].

[9] V. I. Truten', S. P. Fomin, and N. F. Shul'ga, Preprint 80–32, Khar'kov Physico-technical Institute, Khar'kov, 1980, pp. 1–40.

[10] V. A. Bazylev and V. V. Goloviznin, Rad. Eff. **60**, 101 (1982).

[11] J. H.B arrett, Phys. Rev. B **20**, 3535 (1979).

[12] O. B. Firsov, Rad. Eff. **61**, 73 (1982).

[13] L. D. Landau and E. M. Lifshitz, Kvantovaya mekhanika, Moscow, Nauka, 1974. English transl., earlier edition, Quantum Mechanics, Pergamon Press, 1959.

Translated by Clark S. Robinson