Role of various mechanisms of electron loss by ions in axial channeling

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We have investigated the role of three mechanisms of electron loss by fast ions in a crystal during axial channeling, via coherent interaction (without excitation of phonons) and incoherent interactions (with excitation of phonons) with the screened nuclei of the crystal, as well as via inelastic interaction with the electrons of the crystal. The theory constructed permits prediction of the conditions under which each of these mechanisms of electron loss can turn out to be the principal mechanism. It is shown in particular how the rapid orientation dependence of the ionization probability which exists beyond the Lindhard axial-channeling angle under certain conditions and is due only to the periodic arrangement of the atomic strings, is replaced within the Lindhard angle by a weaker dependence due mainly to redistribution of channeled ions in impact parameter.

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INTRODUCTION

In passage of charged particles through a single crystal, individual collisions of particles with crystal atoms are correlated as the result of the periodic arrangement of the atoms in the lattice. This changes, under certain conditions, the probability of electron bremsstrahlung in the crystal (see for example Refs. 1–5), the probability of Coulomb excitation of levels of an ion moving along a crystal axis,[6–11] the probability of scattering of charged particles during channeling,[12,13] and finally the probability of loss of electrons by the ion (ionization) in axial channeling[14,15] and planar channeling.[16,17]

As was shown in Ref. 14, in axial channeling the action of the atoms of a crystal axis on the electron shells of an ion is equivalent in the dipole approximation to action of a flux of monochromatic photons with energy $\hbar\omega_n \approx 2\pi v n\hbar/d$, where v is the ion velocity, d is the lattice period, and $n = 1, 2, \ldots$. Therefore at sufficiently high ion velocities and not too high binding energies $|\varepsilon_N|$ of an electron in an ion with charge Z it can turn out[14,15] that the minimum energy of the equivalent photon $\hbar\omega_{\min} = \hbar\omega_1 \approx 2\pi v\hbar/d$ is significantly greater than $|\varepsilon_N|$. In accordance with the behavior of the cross section for the photoeffect, this means that coherent ionization is highly suppressed.[14,15] In regard to incoherent ionization due to deviations from strict periodicity as the result of thermal vibrations of atoms, it is suppressed in view of the smallness of these deviations. According to Ref. 15, the smallness parameter with respect to the ionization probability in an equivalent amorphous target at a given impact parameter ρ is $\varepsilon u^2|\varepsilon_z|^2/\hbar^2 v^2$, where u is the amplitude of the thermal vibrations of the crystal atoms. These conclusions are valid in some intermediate region of channeled-particle velocities in which, on the one hand, the dipole approximation[1)] is satisfied ($v > Zv_0$), and on the other hand the longitudinal momentum $q_{\parallel\text{eff}} \sim |\varepsilon_z|\hbar\omega$ transferred in the ionization process is greater than the transverse momentum $q_\perp \sim 1/\rho$ (in Ref. 15 the authors took into account only longitudinal thermal vibrations of the atoms of the crystal axis). Therefore the first purpose of the present work is to construct for the energy loss by ions in an axial channel of a crystal a theory that is valid both in the region of relatively small ion velocities and in the high-velocity region. A method of describing in a unified manner the entire range of ion velocities was developed in our previous work and has been applied to the case of planar channeling.[16] The method used here permits, in particular, going over from the axial-channeling case to a disoriented crystal and tracing how the effect predicted in Ref. 16 of a strong orientation dependence[2)] of the ionization probability in the absence of axial channeling is significantly weakened as the entry direction approaches the axial-channeling directions.

The results of the theory developed (see Secs. 2 and 3) permit detailed study of the conditions of appearance and suppression of coherent and incoherent ionization in an axial channel at high ion velocities. It has been shown that under certain conditions the ionization probability decreases by more than Z_2 times (Z_2 is the charge of the nuclei of the crystal) in comparison with the similar probability in an equivalent amorphous target.

Therefore the second purpose of the article is to take into account the contribution made to the probability of electron loss by an ion by inelastic interaction of an electron of the ion with an electron of the crystal, leading to simultaneous ionization (or excition) of a crystal atom and the fast ion. In an amorphous material this process is in order of magnitude Z_2 times less probable than ionization of only one of the interacting particles. In a crystal this process, as we have mentioned above and as will be shown in Secs 2 and 3, can be strongly suppressed as a consequence of the periodicity in location of the atoms on the axis. However, the probability of ionization as the result of inelastic electron-electron interaction with change of the electron state of the crystal cannot be suppressed as the result of the periodic arrangement of the atoms on a crystal axis, since the propagation of the electronic excitation of even the outer shells over the crystal is much slower than the ion motion. (Propagation of an excitation of inner shells is in general unlikely because of competing effects that stop this excitation, such as the Auger effect or radiation.) The role of this mechanism

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in the loss of electrons by an ion in the crystal was the subject of our attention in Ref. 17, where, among other things, we gave a qualitative estimate of the contribution of this mechanism to the ionization probability. In a previous article[16] we developed a quantitative theory for the case of planar channeling. In Sec. 3 of the present article in the framework of the general formalism (Sec. 1) we have constructed the theory of ionization in axial channeling as the result of inelastic electron interaction with excitation of both particles.

§1. LOSS OF ELECTRONS BY AN ION IN ELASTIC INTERACTION WITH CRYSTAL ATOMS

Considering the interaction V_{ea} of an electron of a channeled ion with a crystal atom as a perturbation, following Ref. 16, we shall write the probability of loss of an electron by a multiply charged ion per unit path of the ion in the crystal in the form

$$W=\frac{2\pi}{\hbar}\int\frac{dp_{\parallel}'}{(2\pi\hbar)}\int\frac{d^3p_e}{(2\pi\hbar)^3}\sum_{i_\perp,f_\perp,f_c}P_{\varepsilon_\perp^i}|\langle\Psi_0{}^f|V_{ea}|\Psi_0{}^i\rangle|^2 \times\delta(\Delta E_{\parallel}+\Delta\varepsilon_\perp+\Delta\varepsilon_z+\Delta\varepsilon_c). \quad (1)$$

Here $\mathbf{p}_{\parallel}'$ is the final one-dimensional momentum of the ion in the axial channel of the crystal, $\mathbf{p}_e$ is the momentum of the electron which has left the ion, and the summation is carried out over all initial states $i_\perp$ and final states $f_\perp$ of the transverse motion of the channeled ion and over all final states of the phonon subsystem of the crystal f_c; the symbol Δ in the argument of the Dirac δ function represents the difference in energies in the initial and final states of the system; the total energy of the system is made up of the energy of longitudinal motion of the ion $E_{\parallel}$ $E_{\parallel}=p_{\parallel}^2/2M$, the energy of transverse motion $\varepsilon_\perp$, the binding energy of the electron in the ion ε_z, and the phonon energy of the crystal ε_c; the zero-approximation wave function ψ is the product of the wave function of the free longitudinal motion of the ion $\exp(ip_\perp z\hbar^{-1})(v)^{-1/2}$, the wave function of the transverse motion $\varphi_{\varepsilon\perp}(\boldsymbol{\rho})$, which satisfies the one-dimensional Schrödinger equation of an iron with transverse energy $\varepsilon_\perp$ in the continuous potential of the crystal axis $U_{\text{cont}}(\boldsymbol{\rho})$, the wave function of the electron in the ion $\varphi_z(r_2)$, and the wave function of the nuclei of crystal φ_c. Then

$$P_{\varepsilon_\perp^i}=\left|d^{-2}\int\exp(i\mathbf{p}_\perp\boldsymbol{\rho})\varphi_{\varepsilon_\perp^i}(\boldsymbol{\rho})\,d^2\rho\right|^2$$

is the probability of population of a state with transverse energy $\varepsilon_\perp^i$ in a channel on entry of the ion into the crystal at an angle θ to axes the distance between which is d.[18,19]

Using the formula

$$V_{ea}=\langle\varphi_{ce}|V_{ec}|\varphi_{ce}\rangle=e\int d^3\mathbf{q}S(\mathbf{q})U_q\exp\{-i\mathbf{q}(\mathbf{R}+\mathbf{r}_z)\},$$

where V_{ec} is the interaction energy of the separated electron of the ion with the nuclei and electrons of the crystals and φ_{ce} is the wave function of the electrons of the crystal, $\mathbf{R}$ is the position vector of the nucleus of the ion,

$$U_q=\frac{1}{(2\pi)^3}\int d^3\mathbf{r}\,e^{i\mathbf{qr}}V_a(r)$$

$V_a(r)$ is the potential of a crystal atom, and

$$S(\mathbf{q})=\sum_a e^{i\mathbf{qR}_a}$$

is the structure factor of the crystal (R_a is the position vector of the atoms of the lattice), after integrating in the matrix element V_{ea} over the longitudinal coordinate z and then over $dp_{\parallel}'$, one can obtain

$$W=\frac{4\pi^2e^2}{(\hbar v)^2}\int\frac{d^3\mathbf{p}_e}{(2\pi\hbar)^3}\sum_{i_\perp,f_\perp,f_c}P_{\varepsilon_\perp^i}|\langle\varphi_c{}^f\varphi_{\varepsilon_\perp}^f|F_{q_\parallel}|\varphi_c{}^i\varphi_{\varepsilon_\perp}^i\rangle|^2,$$

$$F_{q_\parallel}=\int d^2\mathbf{q}_\perp S(\mathbf{q})U_q\exp(i\mathbf{q}_\perp\boldsymbol{\rho})\langle\varphi_z{}^f|\exp(-i\mathbf{qr}_z)|\varphi_z{}^i\rangle|_{q^2=q_\perp^2+q_\parallel^2}$$

$$q_\parallel{}^2=(\Delta\varepsilon_z+\Delta\varepsilon_c+\Delta\varepsilon_\perp)^2/(\hbar v)^2. \quad (1')$$

Since at high multiplicities of the ion charge Z the momentum transferred in an inelastic transition will not depend on the energy of the transverse motion of the ion or the energy of the crystal electrons in the final state, it is possible to sum expression (1') over $f_\perp$ and f_c, using the completeness of the systems of functions $\varphi_{\varepsilon\perp}(\boldsymbol{\rho})$ and φ_c. After summation over f_c one obtains the average over the initial state of the nuclei, which actually means averaging over the thermal vibrations of the nuclei.[4] In addition, after summation over $f_\perp$ it is easy to sum over $i_\perp$, using the fact that

$$\sum_i P_{\varepsilon_\perp^i}|\varphi_{\varepsilon_\perp^i}(\boldsymbol{\rho})|^2=p(\boldsymbol{\rho})$$

represents the probability of the distribution of the channeled ions with respect to the impact parameter and the crystal axes. As the result, after averaging over the thermal vibrations of the nuclei, following the procedure of Ref. 16, we obtain

$$W=\int d^2\rho p(\boldsymbol{\rho})w(\boldsymbol{\rho}),$$

$$w(\boldsymbol{\rho})=\frac{4\pi^2e^2}{(\hbar v)^2}\int\frac{d^3\mathbf{p}_e}{(2\pi\hbar)^3}\langle|F_{q_\parallel}|^2\rangle_{\delta\mathbf{R}_a}|_{q_\parallel^2=(\Delta\varepsilon_z/\hbar v)^2},$$

$$\langle|F_{q_\parallel}|^2\rangle_{\delta\mathbf{R}_a}=n_l\left[\sum_i\{\langle|D_q{}^i|^2\rangle_{\delta\rho_a}-\exp(-q_\parallel{}^2u^2)|\langle D_q{}^i\rangle_{\delta\rho_a}|^2\}+\frac{2\pi}{\Delta}\exp(-q_\parallel{}^2u^2)\left|\left\langle\sum_i D_q{}^i\right\rangle_{\delta\rho_a}\right|^2\sum_{\mathbf{g}}\delta(\mathbf{q}_\parallel-\mathbf{g})\right],$$

$$D_q{}^i=\int d^2\mathbf{q}_\perp U_q\exp[i\mathbf{q}_\perp(\boldsymbol{\rho}-\boldsymbol{\rho}_i-\boldsymbol{\rho}_a)] \times(\exp[-i\mathbf{qr}_z])_{fi}|_{q^2=(\Delta\varepsilon_z/\hbar v)^2+q_\perp^2}. \quad (2)$$

Here the angle brackets with the subscripts $\delta\mathbf{R}_a$, $\delta\rho_a$ denote respectively averaging over themal vibrations of the crystal atoms along the longitudinal and transverse coordinates and only along the transverse coordinate; Δ is the "volume" of the one-dimensional unit cell of the crystal, n_1 is the density of atoms in the crystal string, $\mathbf{g}$ is the one-dimensional reciprocal-lattice vector, $\boldsymbol{\rho}_i$ is the radius vector of the location of the i-th string of the crystal, and $w(\boldsymbol{\rho})$ is the sum of the

coherent probability $w_{coh}(\rho)$ $w_{inc}(\rho)$ of ionization of the channeled atomic particle:

$$w(\rho)=w_{coh}(\rho)+w_{inc}(\rho). \tag{3}$$

The coherent part of the ionization probability which is due to phononless scattering by the vibrating atoms of a string, is written in the form

$$w_{coh}(\rho)=\frac{2^{1/2}m^{3/2}n_1e^2}{dv\hbar^4}\sum_g\int d\Omega_e\left|\left\langle\sum_i D_q^{(i)}(\rho)\right\rangle_{\delta\rho_a}\right|^2_{q_\parallel=g}\times e^{-g^2u^2}(g\hbar v-|\varepsilon_z|)^{1/2}\eta(g\hbar v-|\varepsilon_z|). \tag{4}$$

Here $g=2\pi n/d$ $(n=1, 2,...)$, m is the electron mass, $d\Omega_e$ is the solid angle defined by the direction of $\mathbf{p}_e$, in the sum over i we need consider only the closest strings forming the axial channel, and in the sum over g we need consider only the minimum g which satisfies the condition $g\geqslant|\varepsilon_z|/\hbar v$; $\eta(x)$ is the Heaviside unit function, and the wave functions φ_z^i and φ_z^f in the matrix element $(e^{iqr_z})_{if}$ describe respectively the initial state of the electron in the ion with energy ε_z and the final state of the electron of the ion with a definite energy $\varepsilon_z^f=g\hbar v-|\varepsilon_z|$ in the continuum.

The incoherent part of the probability due to production (and annihilation) of phonons we shall write in the form

$$w_{inc}(\rho)=\frac{n_te^2}{2\pi v^2\hbar^5}\int d^3\mathbf{p}_e\sum_i\{\langle|D_q^{(i)}|^2\rangle_{\delta\rho_a}-e^{-q_\parallel^2u^2}|\langle D_q^{(i)}\rangle_{\delta\rho_a}|^2\}|_{q_\parallel=|\Delta\varepsilon_z|/\hbar v}. \tag{5}$$

We note in conclusion of this section that in obtaining Eq. (5) we summed over the final states of the phonon subsystem of the crystal and therefore the phonon variables enter into the result (5) only in the form of an average over the thermal vibrations of the atoms.

§2. LOSS OF ELECTRONS BY AN ION AS THE RESULT OF PHONONLESS SCATTERING

If $g\langle r_z\rangle\ll1$, where $\langle r_z\rangle$ is the mean radius of the electron orbit in the ion, the coherent part of the probability can be represented in the dipole approximation in the form

$$w_{coh}(\rho)=\frac{2\pi n_tc}{d\hbar v}\sum_g\frac{\sigma_p(\omega_g)}{\omega_g}\left|\left\langle\sum_i T_g^{(i)}\right\rangle_{\delta\rho_a}\right|^2e^{-g^2u^2}, \tag{6}$$

$$T_g^{(i)}=\int d^2\mathbf{q}_\perp U_q q\exp[i\mathbf{q}_\perp(\rho-\rho_i-\rho_a)]|_{q=(g^2+q_\perp^2)^{1/2}}, \tag{7}$$

where $\delta_p(\omega)$ is the cross section of photoionization of the ion.

For the fraction of well-channeled ions the distances $|\rho-\rho_i|_{\text{eff}}$ to the strings which form the axial channel in the crystal are greater than the amplitude u of the transverse vibrations of the atoms. Then we can use the expression

$$|\langle T_g^i\rangle_{\delta\rho_a}|^2=g^2|V_g(|\rho-\rho_i|)|^2+\left|\frac{d}{d\rho}V_g(|\rho-\rho_i|)\right|^2, \tag{8}$$

which together with Eq. (6) leads to the result obtained in Ref. 15 by the method of time-dependent perturbation theory. Here

$$V_g=(2\pi)^{-1}\int dze^{igz}V_a(r)$$

is the one-dimensional Fourier component of the potential of a crystal atom.

For higher charge states of the channeled ion Z and unexcited states of the electron in this ion $n=1$, and also for relatively low velocities of the ion in the crystal, it may turn out to be necessary to transfer a rather large momentum g in the longitudinal direction. If in this case we have the inequality

$$gu\gg\max[1, |\rho-\rho_i|_{\text{eff}}u^{-1}],$$

then the following expression is valid:

$$\langle T_g^i(|\rho-\rho_i-\rho_a|)\rangle_{\delta\rho_a}=\frac{2\pi gU_g}{u^2}\exp\left\{-\frac{|\rho-\rho_i|^2}{2u^2}\right\}. \tag{9}$$

If we consider the case of loss of an electron by an ion from an excited state, in which

$$\langle r_z\rangle\varkappa\gtrsim1, \qquad g_{min}\langle r_z\rangle\gg1, \tag{10}$$

$(a_{TF}=\simeq)\varkappa^{-1}$ is the Thomas-Fermi radius of the crystal atom), then the probability of loss of the electron by the ion can be expressed in terms of the ionization cross section in the Born approximation $\sigma(q, \varkappa_q)$ by an atomic particle of unit charge moving with velocity v, written in the variables of the momentum transfer q and the momentum $\varkappa_q$ of the electron emitted from the ion with the following values of these parameters: $q=g$, $\varkappa_q=\varkappa_g=(2m(g\hbar v-|\varepsilon_z|))^{1/2}/\hbar$, i.e.,

$$w_{coh}(\rho)=\frac{2\pi^3n_t\hbar}{dvme^2}\sum_g\frac{\sigma(g,\varkappa_g)}{\varkappa_g}e^{-g^2u^2}g^4\left|\left\langle\sum_i P_g^i\right\rangle_{\delta\rho_a}\right|^2, \tag{11}$$

$$P_g^i=\int d^2\mathbf{q}_\perp U_q\exp[i\mathbf{q}_\perp(\rho-\rho_i-\rho_a)]|_{q=(q_\perp^2+g^2)^{1/2}}. \tag{12}$$

In the sums it is usually sufficient to take one term with the minimum reciprocal-lattice vector satisfying the condition $g_{min}\hbar v\geqslant|\varepsilon_z|$ and the strings closest to the ion (or one string).

For the condition

$$gu\gg\max[1, |\rho-\rho_i|_{\text{eff}}u^{-1}|$$

we have

$$\langle P_g^i\rangle_{\delta\rho_a}=\frac{2\pi U_g}{u^2}\exp\left\{-\frac{|\rho-\rho_i|^2}{2u^2}\right\}. \tag{13}$$

If the inverse inequality is satisfied, then

$$\langle P_g^i\rangle_{\delta\rho_a}=V_g(|\rho-\rho_i|). \tag{14}$$

For specific calculations it is possible to use the Moliere potential:

$$V_a=eZ_2\sum_{i=1}^3\alpha_ie^{-\varkappa_ir}r^{-1},$$

where

$$\varkappa_i=\beta_i a_{TF}^{-1}, \quad a_{TF}=0.885Z_2^{-1/3}\,a_0;$$
$$\alpha_i=\{0.1;\ 0.55;\ 0.35\}; \quad \beta_i=\{6.0;\ 1.2;\ 0.3\}.$$

In this case U_g and V_g which enter into Eqs. (8), (9), (13), and (14) are given by the formulas

$$U_g=(2\pi^2)^{-1}eZ_2\sum_{i=1}^{3}\alpha_i(g^2+\varkappa_i^2)^{-1},$$
$$V_g=\pi^{-1}eZ_2\sum_{i=1}^{3}\alpha_i K_0(\rho(\varkappa_i^2+g^2)^{1/2}). \tag{15}$$

It is also possible to use the Barrett model,[20] which $\alpha_i=\{0.4;\ 0.6\}$, $\beta_i=\{2.984;\ 0.474\}$, or the Firsov model,[21] which is valid, in particular, even for very light crystals.

As follows from Eqs. (4), (6), and (11), in the dipole approximation the coherent ionization can be suppressed if the energy of the equivalent photon is significantly greater than the binding energy of the electron in the ion (in accordance with the behavior of the cross section for the photoeffect), and in the nondipole region it can be suppressed as a result of the smallness of the cross section for ionization of the ion by a charge for a high energy of the electron emitted from the ion.

Let us analyze now the dependence of the ionization probability on the entry angle θ of the particle into the crystal with respect to the lattices axes. If the entry angle is less than or of the order of the critical angle for axial channeling, this dependence is due only to the dependence $p(\boldsymbol{\rho})$ of the probability of distribution of the ions in the impact parameters relative to the crystal axes. This occurs because the trajectory of a channeled ion is strongly curved in the field of the continuous potential of the crystal axis. The spectrum of the perturbation due to collision of an ion with atoms of different strings in the same direction (or merely with different strings) is not represented here by a definite frequency which is sufficient for ionization and which furthermore must depend on the entry angle.

The situation changes, however, for ion entry angles into the crystal significantly greater than the axial-channeling critical angle θ_L. In this case the motion of the ion is on the whole close to rectilinear. Therefore the spectrum of the perturbation contains in addition to the frequency $\omega=2\Pi v/d$ other definite frequencies equal to the reciprocal of the time of flight between neighboring axes (or planes) of the crystal ($\omega=\mathbf{gv}$, where $\mathbf{g}$ is the three-dimensional reciprocal-lattice vector). These frequencies, and consequently also the ionization probability, already depend substantially on the angle θ with respect to the axes (or planes) of the crystal.[16] We shall obtain this result from Eqs. (2) and (4). Actually, for $\theta\gg\theta_L$ the probability of the distribution in impact parameter no longer depends on $\boldsymbol{\rho}$, namely: $p(\boldsymbol{\rho})=d^{-2}$. (For simplicity and convenience we have taken a cubic crystal.) Then we represent the square of the modulus, which enters into Eq. (4), in the form of a quadruple integral over $d^2\mathbf{q}_\perp$ and $d^2\mathbf{q}_\perp'^{\diamond\diamond}$ (see Eq. (2)). We then integrate over $d^2\boldsymbol{\rho}$, using the well known representation of the two-dimensional Dirac delta function. Then, after use of the formula

$$\Big|\sum_n \exp(i\mathbf{q}_\perp\boldsymbol{\rho}_n)\Big|^2=\sum_{\mathbf{g}_\perp}\frac{(2\pi)^2}{d^2}\delta(\mathbf{q}_\perp-\mathbf{g}_\perp),$$

where $\boldsymbol{\rho}_n$ is the two-dimensional vector of the location of the crystal strings in the plane perpendicular to this string and $\mathbf{g}_\perp$ is the two-dimensional reciprocal-lattice vector of this plane, we obtain for the ionization probability W in the two limiting cases the expressions obtained in Ref. 16 by another method:

$$W=\frac{(2\pi)^5 n_V}{d^3 v}\sum_{\mathbf{g}} g^2|U_g|^2 e^{-g^2u^2}\begin{cases} c\sigma_p(\mathbf{gv})/\hbar\mathbf{gv}, & g\langle r_z\rangle\ll 1;\\ \dfrac{\pi^2\hbar}{me^2}\dfrac{\sigma_e(\mathbf{g},\varkappa_g)}{\varkappa_g}g^2, & g\langle r_z\rangle\gg 1.\end{cases}$$

Here $n_V=n_1/d^2$ is the density of atoms of the crystal, $\mathbf{g}$ is the three-dimensional reciprocal-lattice vector, and U_g is the three-dimensional Fourier component of the potential of the crystal atom. These formulas show a rapid dependence, which appears in view of the dependence of σ_p on $\mathbf{g}\cdot\mathbf{v}$ and of σ_e on $\varkappa_g$, of the ionization probability (and in particular its anomalous behavior if the ion has more than one electron in its orbit) on the entry angle of the particle into the crystal with respect to its axes; we mentioned this dependence and its behavior above. Thus, the relatively weak orientation dependence of the probability of electron loss by an ion within the Lindhard critical angle in axial channeling, which is due mainly to the effect of redistribution of the flux of ions in impact parameter, is replaced beyond the Lindhard angle by a stronger dependence due only to the periodicity of the principal axes of the crystal.

For observation of these effects it is necessary that the disturbance spectrum that is equivalent to the lattice be discrete, i.e., that the crystal be ideal. Thermal vibrations lead to an incoherent perturbation which can be equal in strength to the action of the coherent perturbation. It is *a priori* clear what conditions are necessary for the smallness of the incoherent perturbation which is due to deviations from periodicity. First it is necessary that the change in the potential of an atom at distances of the order of the thermal-vibration amplitudes u be significantly less than the value of the potential itself. Since the effective range of the potential is $\varkappa^{-1}$, this requirement is satisfied for $\varkappa u\ll 1$, i.e., for sufficiently light crystals. Second, it is necessary that the mean radius of the electron orbit in the ion $\langle r_z\rangle$, be greater than u. Otherwise the main contribution to the ionization probability will be from the region of small distances from the ion to the nuclei of the crystal $r\lesssim u$, for which the condition of periodicity of the potential and consequently of discreteness of the perturbation spectrum is not satisfied.

As an illustration of the theory developed above, we can mention, for example, the relative magnitudes and locations of the orientation peaks due to coherent ionization of the ion O^{+5} in a disoriented target, i.e., in the absence of channeling, under conditions in which the dipole approximation $\mu\gg Zv_e$ is applicable (see the figure).

In the diamond crystal chosen as a target, the necessary conditions given above for appearance of orientation effects are satisfied.

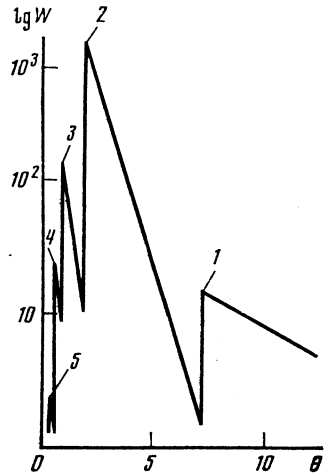

FIG. 1. Illustration of relative magnitudes and locations of orientation peaks associated with coherent ionization of an O^{+5} ion in traversal of a diamond crystal at a small angle θ to the (111) plane. The abscissa shows the angle θ in degrees between the direction of the velocity and the (111) plane, and the ordinate gives the logarithm of the number of ionization events per unit path for one particle in relative units. The numbers identifying the peaks have the following meanings: 1 and 2 are ionization from K and L shells, respectively, by the first harmonic; 3, 4 and 5 are ionization from the L shell by the second, third, and fourth harmonics, respectively.

An orientation-peak structure similar to that shown in the figure in the ionization probability per unit length arises also in the case of planar channeling. However, it should be noted that in planar channeling the structure of the orientation peaks will be much more distinct than in the case of a disoriented target, since the incoherent background due to production (or annihilation) of phonons is highly suppressed in channeling (see Ref. 16 and Sec. 3 below).

§3. LOSS OF AN ELECTRON BY AN ION AS THE RESULT OF INCOHERENT INTERACTION WITH VIBRATING ATOMS OF A CRYSTAL

The formula for the incoherent part of the probability (5) is also simplified in a number of limiting cases. Let $v \gg Zv_0$; then for well-channeled ions ($|\rho - \rho_i|_{\text{eff}} \gg u$), upon fulfillment of the inequality

$$\varkappa \langle r_z \rangle \ll 1, \tag{16}$$

which is satisfied for unexcited states of a multiply charged ion ($n \ll Z^{1/2}$), we obtain from (5), after carrying out the necessary expansions and integration,

$$w_{inc}(\rho) = \frac{n_l u^2 c}{v^2 \hbar} \int_{\omega_{\text{thr}}}^{\infty} \frac{d\omega}{\omega} \sigma_p(\omega) \left\{ \left(\frac{\omega}{v}\right)^2 \left[\left(\frac{\omega}{v}\right)^2 \left| V_{\omega/v}(|\rho-\rho_i|) \right|^2 + \left| \frac{d}{d\rho} V_{\omega/v}(|\rho-\rho_i|) \right|^2 \right] + \left(\frac{\omega}{v}\right)^2 \left| \frac{d}{d\rho} V_{\omega/v}(|\rho-\rho_i|) \right|^2 + |\Delta V_{\omega/v}(|\rho-\rho_i|)|^2 \right\}. \tag{17}$$

This result coincides with Eq. (17) of Ref. 15 if in Eq. (17) above we neglect the last two terms in the curly brackets, which stem from allowance for the transverse thermal vibrations (in Eqs. (17) and (18) Δ is the two-dimensional Laplacian).

When the condition

$$v \gg Z^2 v_0 a_{\text{TF}} (n^2 a_0)^{-1}$$

is satisfied, however, the incoherent part of the probability is determined by the transverse (and not longitudinal) thermal vibrations. Therefore for well channeled particles ($|\rho - \mathbf{r}_i|_{\text{eff}} \gg u$) we obtain from Eq. (5)

$$w_{inc}(\rho) = \frac{n_l u^2 c d^2}{\hbar v^2} \sum_i \left| \Delta U_{cont}(|\rho-\rho_i|) \right|^2 \int_{\omega_{\text{thr}}}^{\infty} \sigma_p(\omega) \frac{d\omega}{\omega}. \tag{18}$$

Then let $v_z \ll v \ll Zv_0$, which is satisfied for excited states of a multiply charged ion. In this case the exponential $\exp(i\mathbf{q}\cdot\mathbf{r}_z)$ oscillates strongly and the main contribution to the integral over $d^3\mathbf{p}_e$ is from $\mathbf{p}_e$ values in the vicinity of the solution of the equation $\mathbf{p}_e^0 = \mathbf{q}(\mathbf{p}_e^0)\hbar$. Replacing $\varphi_z^f(r_z)$ by $\exp(i\mathbf{p}\mathbf{r}_z\hbar^{-1})$ in (2) and expanding $\mathbf{q}(\mathbf{p})$ near p_e^0, we can then integrate over $d^3\mathbf{p}_e$ in (5).

If here the inequality $umv\hbar^{-1} \ll 1$ is valid, then we can obtain from (5) for the probability of loss of an electron by an ion the following result:

$$w_{inc}(\rho) = 16\pi^2 \frac{u^2 m^2 e^2}{\hbar^4} n_l \sum_i \left[|V_{2mv/\hbar}(|\rho-\rho_i|)|^2 + \frac{\hbar^2}{4m^2v^2} \times \left| \frac{d}{d\rho} V_{2mv/\hbar}(|\rho-\rho_i|) \right|^2 \right]. \tag{19}$$

However, if the inequality $umv\hbar^{-1} \gg 1$, is satisfied, the influence of the periodic location of the atoms on the crystal axis can be neglected. According to Eq. (5), in which it is necessary to take into account only the first term in the curly brackets, this leads to the formula

$$w_{inc}(\rho) = \frac{(2\pi)^2 n_l e^2}{(\hbar v)^2} \sum_i \langle |V_{2mv/\hbar}(|\rho-\rho_i-\rho_a|)|^2 \rangle_{\delta\rho_a}. \tag{20}$$

As follows from Eqs.(17), (18), and (19), the probability of incoherent ionization is suppressed by the periodicity of the atoms in strings in comparison with the probability of ionization in an amorphous target[3] (for a given impact parameter), and also in comparison with the probability of coherent ionization at the maximum. This is a consequence of the smallness of the deviations of the crystal lattice from ideal. Therefore an ion moving far from a string and with sufficiently high velocity, when the transverse and longitudinal momentum transfers are relatively small, will feel these deviations only slightly. The suppression parameter is the ratio

$$u^2/\max\left[(\rho-\rho_i)^2, (\hbar v)^2 |\varepsilon_z|^{-2}, \varkappa^{-2}\right].$$

In addition, the probability is small in comparison with the probability in an amorphous target, as a result of the redistribution of the flux of channeled ions over impact parameter[22] (the Fourier component of the atom potential $V_q(\rho)$ is small if $\rho_{\text{eff}} \gg \varkappa^{-1}$, as is the case for channeling).

Therefore for very fast ions in an axial channel of a crystal it is possible to have a different principal mechanism of electron loss as a consequence of the simultaneous inelastic interaction of an electron of an ion with the electrons of the crystal. For this one must have the following conditions satisfied:

$$\frac{\sigma_p(|\varepsilon_z|/\hbar v)}{\sigma_p(2\pi v/d)}, \quad \frac{\min\{\varkappa^{-2}, \rho_{\text{eff}}^2, (\hbar v/|\varepsilon_z|)^2\}}{u^2} > Z_2;$$

here the probability of ionization of an ion in a crystal by elastic interactions turns out to be suppressed in comparison with the similar probability in an amorphous target by more than Z_2 times. These conditions are realized, for example, in a diamond crystal for an O^{+5} ion with $v \gtrsim 2 \cdot 10^9$ cm/sec.

In the case of a disoriented crystal ($\theta \gg \theta_L$) the flux of ions is uniformly distributed over the impact parameter ρ. It is then possible to integrate Eq. (5) over $d^2\rho$ and then over $d^2\mathbf{q}_\perp$. As a result of Eqs. (5) and (2) we obtain the formula derived and studied in Ref. 16 as the limiting transition from planar channeling ($k_\parallel = Mv/\hbar$):

$$W = \frac{4\pi^2 M n_e e^2}{k_\parallel v \hbar^6} \times \int d^2\mathbf{p}_e \int dq' q' |U_q|^2 |(e^{i\mathbf{q}\mathbf{r}_z})_{if}|^2 (1-e^{-q^2u^2}) |_{q^2=q'^2+(\Delta\varepsilon_z/\hbar v)^2}. \tag{21}$$

§4. IONIZATION OF ATOMIC PARTICLES AS THE RESULT OF INELASTIC INTERACTION WITH THE ELECTRON SUBSYSTEM OF A CRYSTAL

Let us investigate the process of ionization as the result of simultaneous inelastic transitions in the electron shells of the channeled ion and the atoms of the crystal.

Using the formalism developed in Sec. 1 and replacing the variables characterizing the phonon state of the crystal by variables which characterize the electronic state, it is easy to obtain the following formula for the desired probability instead of the similar expression (5) for the incoherent probability (the coherent part of the probability is equal to zero because, as was stated above, the electronic excitation is not capable of following the ion):

$$w(\rho) = \frac{n_i e^4}{2\pi v^2 \hbar^3} \sum_i \int d^2\mathbf{p}_e \langle |M^{(i)}|_{aa}^2 - |M_{aa}^{(i)}|^2 \rangle_{\delta\rho_a}, \tag{22}$$

where M^i_{aa} is the diagonal matrix element between the initial wave functions of the electrons of a crystal atom;

$$M^{(i)} = \frac{1}{2\pi^2} \sum_s \int d^2\mathbf{q}_\perp q^{-2} \times \exp[iq_\perp(\rho - \rho_i - \rho_a) - i\mathbf{q}\mathbf{r}_a^s] (e^{i\mathbf{q}\mathbf{r}_z})_{i,f} |_{q^2=q_\perp^2+(\Delta\varepsilon_z/\hbar v)^2},$$

$r_a^{(s)}$ are the coordinates of the electrons of the crystal atom, and the summation over s signifies a sum over the electrons in the crystal atom ($s = 1, 2, \ldots, Z_2$).

Let $v \gg Zv_0$. Then also we have $|\rho - \rho_i| \gg a_{\text{TF}} \gg \langle r_z \rangle$. Then in Eqs. (22) and (23) we can make the following substitutions:

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

$$|M|_{aa}^2 - |M_{aa}|^2 \to Z_2 \left| \int d^2\mathbf{q}_\perp q^{-1} \exp[i\mathbf{q}_\perp(\rho - \rho_i)] \right|^2. \tag{23}$$

As a result we obtain for the probability of loss of an electron by an ion per unit path in the crystal the expression

$$w(\rho) = \frac{n_i Z_2 e^2 c}{\pi^2 \hbar v^2} \int_{\omega_{\text{thr}}}^{\infty} \frac{d\omega}{\omega} \sum_i \frac{\sigma_p(\omega)}{|\rho - \rho_i|^2} \exp\left[-\frac{2\omega}{v}|\rho - \rho_i|\right]. \tag{24}$$

This result shows that the spectrum of photons that are equivalent to the field of the electrons of the crystal depends substantially on the distance to the strings where the maximum electron density occurs, and the intensity of the photon flux is proportional to the number of electrons of the crystal atom Z_2. This is natural, since the electrons of the crystal atom are bound considerably more weakly than an electron of the ion, and in the process of the simultaneous inelastic transition the former can be considered as free.

If $|\rho - \rho_i| \gg \langle r_z \rangle a_{\text{TF}}$, which can be the case for sufficiently heavy crystals and excited states of a multiply charged ion, and the ion velocity is given by $Zv_0 \gg v \gg v_z$, we can assume in Eq. (23) that $\exp(-i\mathbf{q}\mathbf{r}_a^s) \approx 1 - i\mathbf{q}\mathbf{r}_a^s$, take the matrix element $(\exp(i\mathbf{q}\mathbf{r}_z))_{if}$ outside the integral over $d\mathbf{q}_\perp$, integrate in Eq. (23) over $d^3\mathbf{p}_e$ using the resonance of this matrix element near $\mathbf{p}_e^0 = \mathbf{q}_\parallel(\mathbf{p}_e^0)\hbar$, and after several manipulations obtain

$$w(\rho) = \frac{4n_i e^2 \langle d^2 \rangle}{(\hbar v)^2} \sum_i \frac{\exp\left[-\frac{4mv}{\hbar}|\rho - \rho_i|\right]}{|\rho - \rho_i|^2}. \tag{25}$$

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

As follows from Eqs. (24) and (25) and from their comparison with Eqs. (17), (19), and (20), in light crystals for well channeled, sufficiently fast ions the probability of electron loss by the ions can exceed the similar probability for an elastic interaction.

In the case when there is no channeling ($\theta \gg \theta_L$) it is possible to derive from Eqs. (22) and (23), in the same way as in derivation of Eq. (21), the following formula for the probability

$$W = 8\pi n_v \left(\frac{e^2}{\hbar v}\right)^2 \int \frac{d^3\mathbf{p}_e}{(2\pi\hbar)^3} \int \frac{dq' q'}{q^4} \left| (e^{i\mathbf{q}\mathbf{r}_z})_{if} \right|^2 \times \left[\left| \sum_{s=1}^{Z_2} e^{i\mathbf{q}\mathbf{r}_a^s} \right|_{aa}^2 - F^2(q) \right] \Big|_{q^2=q'^2+(\Delta\varepsilon_z/\hbar v)^2}, \tag{26}$$

where $F(q)$ is the form factor of the crystal atom. Equation (26) was obtained in Ref. 16 by another method and was investigated in various limiting cases.

§5. APPLICABILITY OF THE THEORY, AND THE EQUILIBRIUM CHARGE OF IONS IN A CRYSTAL

The formulas obtained in the present work for the probability of electron loss by an ion in a crystal cover practically the entire region of ion velocity in which it makes any sense at all to look for this probability, i.e., the region $v \gg v_z$ where the ionization probability is greater than the probability of capture of an electron by the ion. In this region, perturbation theory in the interaction of the electron with the atoms of the material can be applied satisfactorily even in an amorphous solid (see for example Ref. 23). In a crystal, as was shown above, the probability of electron loss by an ion under certain conditions may turn out to be suppressed as a consequence of the periodic location of atoms in a string and also as a consequence of the smallness of the field at sufficiently large distances of the main part of the channeled ions from the string. (For the main part of the channeled ions small impact distances of the ions to the strings are not reached.) We recognize also that the transition of electrons from crystal atoms to rather deep orbits ($Z \gg 5$) of a multiply charged ion (charge exchange) at velocities $v \lesssim v_z$ also is suppressed as the result of the impossibility of intersection of deep orbits with nearly equal electron binding energy at large distances from the channeled ion to the atoms of the string. Therefore a stable charge state of the channeled ion can be preserved up to velocities $v \sim v_z$, so that it is possible to use perturbation theory. In particular, this is a distinction of the condition of applicability of perturbation theory for calculation of ionization probability in a crystal in channeling from the condition of applicability of perturbation theory in an amorphous solid.

The results of the theory developed in this work show that the process of establishing the equilibrium charge for ions in axial channeling differs substantially from the same process for ions in an amorphous material. In view of the rather strong suppression of the incoherent probability of electron loss and the smallness of charge exchange, we should expect a significant increase in the time of establishment of the equilibrium charge of multiply charged ions in an axial channel of a crystal at high ion velocities, when $2\pi\hbar v|d \gg |\varepsilon_z|$. However, if $2\pi\hbar v/d \sim \varepsilon_z|$, the ionization is no longer small, owing to the increased contribution of coherent ionization. Here effective charge exchange, which is sensitive mainly to the impact parameter, remains suppressed. This leads to a decrease of the time for establishment of the equilibrium charge in a crystal and to an increase of the equilibrium charge, which is especially important under conditions of only a small increase (relative to an amorphous target) of the phase space of the ion beam after traversal of the thickness of the crystal. These tendencies exist also under conditions of planar channeling,[16] and differ only in the magnitude of the effect.

A different situation will exist in the case of passage of ions through a disoriented crystal. When the following conditions are satisfied (see Sec. 2 and also Ref. 16):

$$v \gg v_z, \quad \hbar g_{min} v \gg |\varepsilon_z|, \quad \langle r_z \rangle \gg \varkappa^{-1} \gg u, \tag{27}$$

the probability of electron loss by an ion turns out to be suppressed in comparison with the similar probability in an amorphous material. However, the probability of capture of an electron by an ion for $v > v_z$ is the same as in an amorphous solid, as a consequence of the uniform distribution of ions over impact parameter, and also as a consequence of the insensitivity of charge exchange to the periodicity of the atoms in the crystal. It is then clear that the time of establishment of the equilibrium charge can only increase, while the equilibrium charge can only decrease in comparison with the similar values in an amorphous material.

However, if the inequality (27) is not satisfied, which usually occurs in heavy crystals at relatively low ion velocities and sufficiently deep electron orbits in the ion, the process of ionization and charge exchange, and consequently also the process of establishment of the equilibrium charge, are not distinguished from the similar processes in an amorphous material.

[1)] In what follows, v_0 and a_0 are the atomic units of velocity and length.
[2)] That is, of the dependence on the small ($\theta \gg 1$) (but nevertheless significantly greater than the Lindhard critical channeling angle) angle of entry of the ion with respect to the principal axes of the crystal.
[3)] By way of illustration we point out that the results for an amorphous target are obtained from the general formulas (4) and (5) in the limit $u \to \infty$.

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