Energy loss of charged particles in crystals

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A quantum dielectric formalism is applied to analysis of the energy loss of charged particles moving in a crystal in the channeling regime and in a random direction. An analytical model of the dielectric matrix of the crystal is constructed. On the basis of this model, general formulas in the Born approximation describing the slowing down of a fast charged particle in a crystal with allowance for the nonuniformity of the electron density and the band structure of the crystal are obtained for the first time. A relation is found between the energy loss of channeled particles and the electron density in the channels of the crystal. The difference between the energy loss rates of hyperchanneled particles in axial and planar channels is rigorously demonstrated for the first time. Some features of the behavior of the energy loss of channeled particles in the low-velocity region are explained. The theory is applicable for calculation of the energy loss from low velocities (of the order of the velocity of the Fermi electrons) up to ultrarelativistic velocities of the incident particles. The theory is compared with the principal known experiments. Satisfactory agreement between theory and experiment is obtained and at the same time a number of experimental results are explained on the basis of the proposed theory.

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1. INTRODUCTION

The theory of the energy loss of charged particles in crystals has attracted considerable attention from investigators in recent years. For a number of applications, in particular for the interpretation of experiments on backscattering of protons and α particles and in studies of electron densities on the basis of the energy spectra of channeled particles, it is necessary to know the energy loss both in an unoriented crystal and in the channeling regime.

At the energies 0.5–4 MeV usually used for backscattering of protons and α particles, energy loss to valence electrons is dominant. In the channeling regime the contribution of the inner electrons, for example in silicon, begins to be felt only at energies above 3–5 MeV/amu. Therefore the subject of the present work will be mainly the calculation of the contribution of valence electrons to the slowing down of fast charged particles in crystals.

The slowing down of charged particles by a free electron gas was investigated by Lindhard and Winther.[1] The assumption of spatial uniformity of the electron gas limits the possibility of application of the results of their work only to the case of amorphous material. Kagan and Kononets[2] used the density matrix formalism to study the evolution of the energy distribution of channeled particles as they penetrate into the interior of a crystal.

The energy loss of the particles has been discussed with inclusion of the spatial inhomogeneity of the electron distribution in crystals in several articles,[3-5] but as a result of the complexity of the models and the expressions, it has been possible to make calculations only by computer and for individual energy values. A simpler method of taking into account the nonuniformity of the electron density has been suggested in Ref. 6.

Recently Golovchenko and Esbensen[7] have discussed the slowing down of fast channeled ions in terms of the first Born approximation with use of a harmonic oscillator model in calculations of the generalized oscillator strengths of atoms. This model unfortunately is limited to the case of free atoms in lattice sites and does not permit separation of the contribution of single-particle and collective excitations of electrons (such a separation is necessary in study of the multiple scattering of channeled particles), and also requires most frequently of all the introduction of an empirical value of the mean ionization potential and correction for the effect of density of the medium at relativistic velocities. Certain aspects of this theory will be discussed in Section 3.

Experimental results on the energy loss of channeled particles[8-14] exist for a wide range of energies. Construction of a theory of energy loss which is rather simple and is convenient for calculations is therefore one of the purposes of the present work. In addition, we intend to study the relation between the energy loss and the local electron density which is probed by the channeled particle. Establishment of such a relation is important in determination of the electron density in a lattice by means of the channeling method.

In the second section of the article a simple model of the band structure of a semiconductor and the sum rules for the elements of the dielectric matrix are used to obtain expressions for the diagonal and nondiagonal elements of the dielectric matrix. In the third section we derive a formula for calculation of the Fourier components of the energy loss of charged particles in an inhomogeneous electron gas. For incident-particle velocities significantly above the velocity of a Fermi electron gas we obtain a simple formula for the slowing down in a spatially inhomogeneous electron gas. In conclusion of Section 3 the formula for the energy loss is generalized to the case of relativistic particles. The relativistic formula obtained in this work takes into account the polarization of the medium, and there is no need for special introduction of a correction for the density effect.

Section 4 presents the results of calculations of the energy loss of light ions using the proposed model of the

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dielectric matrix and compares them with the results of other authors.

2. THEORY, MODEL OF THE DIELECTRIC MATRIX OF A SEMICONDUCTOR

Channeled particles probe only certain regions in a crystal, since the flow of positively charged particles is concentrated mainly near the center of the channel. In this case it is necessary to take into account the effects of the local field— the change of the microscopic electric field and of the local electron density within a unit cell. In this way we can establish a relation between the energy loss of ions in channeling and the local electron density, which is important in study of the electron density of crystals by the method of light-ion channeling.

The energy loss of a charged particle with charge Z_1 and velocity v in a nonuniform electron gas of valence electrons of a crystal with inclusion of the effects of the local field is expressed in the Born approximation by the following formula[15]:

$$S(\mathbf{r})=-\frac{dE}{dx}(\mathbf{r})=\frac{Z_1^2e^2}{\pi^2v}\int\frac{d^3\mathbf{q}}{q^2}\int d\omega\,\omega\sum_{\mathbf{G}}\mathrm{Im}\{\mathbf{K}_{\mathbf{G},0}(\mathbf{q},\omega)\}e^{i\mathbf{G}\mathbf{r}}\delta(\omega-\mathbf{q}\mathbf{v}), \tag{1}$$

where $K_{\mathbf{G},0}(\mathbf{q},\omega)$ is the inverse dielectric matrix,[16] which depends on the frequency ω and the wave vector $\mathbf{q}$; $\mathbf{G}$ is the reciprocal-lattice vector. For a solid with a periodic structure the operators K and ε are usually taken in the representation in which K and ε are matrices with columns and rows labeled by the reciprocal-lattice vectors $\mathbf{G}$ and $\mathbf{G}'$ in such a way that the relation between them is as follows:

$$\sum_{\mathbf{G}''}\varepsilon_{\mathbf{G},\mathbf{G}''}(\mathbf{q},\omega)K_{\mathbf{G}'',\mathbf{G}'}(\mathbf{q},\omega)=\delta_{\mathbf{G},\mathbf{G}'}, \tag{2}$$

where $\varepsilon_{\mathbf{G},\mathbf{G}'}$ is the dielectric response matrix introduced by Adler and Wiser.[17] The component $\varepsilon_{0,0}(\mathbf{q},\omega)$ of the dielectric matrix corresponds to the ordinary dielectric function $\varepsilon(\mathbf{q},\omega)$. The components of the inverse dielectric matrix entering into the stopping formula, in the case of weak binding when the nondiagonal elements of the matrix $\varepsilon_{\mathbf{G},\mathbf{G}'}$ are significantly smaller than unity, are easily expressed in terms of the elements of the matrix $\varepsilon_{\mathbf{G},\mathbf{G}'}$:

$$K_{\mathbf{G},0}=\delta_{\mathbf{G},0}\frac{1}{\varepsilon_{0,0}}-(1-\delta_{\mathbf{G},0})\frac{\varepsilon_{0,\mathbf{G}}}{\varepsilon_{0,0}}, \tag{3}$$

$$\varepsilon_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega)=\delta_{\mathbf{G},\mathbf{G}'}-\frac{4\pi e^2}{\Omega|\mathbf{q}+\mathbf{G}||\mathbf{q}+\mathbf{G}'|}\times\sum_{\mathbf{k},l,l'}\frac{f_0[E_{l'}(\mathbf{k}+\mathbf{q})]-f_0[E_l(\mathbf{k})]}{E_{l'}(\mathbf{k}+\mathbf{q})-E_l(\mathbf{k})-\hbar\omega+i\hbar\alpha}\times\langle\mathbf{k}+\mathbf{q},l'|e^{i(\mathbf{q}+\mathbf{G})\mathbf{r}}|\mathbf{k},l\rangle\langle\mathbf{k},l|e^{-i(\mathbf{q}+\mathbf{G}')\mathbf{r}}|\mathbf{k}+\mathbf{q},l'\rangle, \tag{4}$$

where $|\mathbf{k},l\rangle$ and $E_l(\mathbf{k})$ are the eigenstates and eigenvalues of the unperturbed Hamiltonian of the crystal, f_0 is the Fermi-Dirac distribution function, Ω is the crystal volume considered, and α is a small positive quantity.

The first term in the expression (3) is the inverse dielectric function of a uniform electron gas, and the second term is nonzero for $\mathbf{G}\neq 0$ and expresses in this way the effects of nonuniformity of the local field in the crystal lattice.

The elements of the dielectric response matrix $\varepsilon_{\mathbf{G},\mathbf{G}'}$ are complex numbers and can be written in the form

$$\varepsilon_{\mathbf{G},\mathbf{G}'}=\varepsilon_{\mathbf{G},\mathbf{G}',1}+i\varepsilon_{\mathbf{G},\mathbf{G}',2}. \tag{5}$$

Since in what follows we shall use only $K_{\mathbf{G},0}$ and $\varepsilon_{0,\mathbf{G},1}$, $\varepsilon_{0,\mathbf{G},2}$, we shall omit the index 0.

The imaginary part of the inverse dielectric function is

$$\mathrm{Im}\,K_{\mathbf{G}}=\frac{-\varepsilon_2}{\varepsilon_1^2+\varepsilon_2^2}\left\{\delta_{\mathbf{G},0}+(1-\delta_{\mathbf{G},0})\left(\frac{\varepsilon_1}{\varepsilon_2}\varepsilon_{\mathbf{G},2}-\varepsilon_{\mathbf{G},1}\right)\right\}. \tag{6}$$

To calculate the energy loss it is necessary to know the dielectric function $\varepsilon_{\mathbf{G}}(\mathbf{q},\omega)$ over a wide range of variation of $\mathbf{q}$ and ω and also for several vectors $\mathbf{G}$, and therefore the numerical integration over the wave vector $\mathbf{k}$ becomes laborious and it is necessary to resort to simplified models of the band structure of the crystal. In this work we shall propose a model for the crystal band structure which is most appropriate for semiconductor and metallic crystals. The energy bands are assumed to be identical for all valence electrons; the multiplicity of degeneracy is equal to the number of valence electrons per atom in the crystal. The conduction band is separated from the valence band by some average energy gap E_g which does not depend on the direction of the wave vector $\mathbf{k}$. The dispersion of an electron in the bands is assumed to obey the following law[18]:

$$\begin{aligned}E_l(\mathbf{k})&=\hbar^2k^2/2m \quad \text{for } k<k_F,\\ E_l(\mathbf{k})&=\hbar^2k^2/2m+E_g \quad \text{for } k>k_F,\end{aligned} \tag{7}$$

where k_F is the Fermi wave vector. Equation (7) differs from the result for a free electron gas by inclusion of the energy gap in the semiconductor band structure. The behavior of $E_1(\mathbf{k})$ as $k\to k_F$ is not taken into account, since inclusion of it affects the final result only to a small extent, as a result of the fact that the energy loss is determined by the set of excitations over the entire spectrum of frequencies and wavelengths.

With the aid of the semiconductor model described we shall find the real part $\varepsilon(\mathbf{q},\omega)$ and the imaginary part $\varepsilon_2(\mathbf{q},\omega)$ of the dielectric function for the case $\mathbf{G}=0$. As for a free electron gas,[1] the sum in Eq. (4) can be replaced by integration over a sphere of radius k_F; we must take into account, however, that the matrix element now may differ from unity. On the assumption that the structure of the dielectric function is determined mainly by the density of electron states in the energy interval considered and not by the dependence of the matrix element $\langle\mathbf{k}+\mathbf{q},l'|e^{i\mathbf{q}\mathbf{r}}|\mathbf{k},l\rangle$ on the variation of the wave vector $\mathbf{k}$ within the sphere of integration, we take the square of the matrix element outside the integral sign. Analytical integration leads to the following result for the imaginary part of the dielectric function:

$$\varepsilon_2=-\frac{3}{2}\pi\frac{w_p^2}{z^3}M^2(z)(w-w_g), \tag{8a}$$

if $w_g<w<z(1-z)+w_g$;

$$\varepsilon_2=-\frac{3'}{8}\pi\frac{w_p^2}{z^3}M^2(z)\left\{1-\frac{1}{z^2}(z^2-w+w_g)^2\right\}, \tag{8b}$$

if $z(z-1)+w_g<w<z(z+1)+w_g$ and $w>w_g$;

$$\varepsilon_2=0, \tag{8c}$$

if $w\leq w_g$ or $w\leq z(z-1)+w_g$, or $w\geq z(z+1)+w_g$.

We have introduced the reduced quantities $w=\hbar\omega/4E_F$

and $z=q/2k_F$, where E_F is the Fermi energy, w_g and w_p are the energy gap and the energy corresponding to the plasma frequency of the electron gas in reduced units, and $M^2(z)$ is the square of the matrix element of interband transitions, averaged over the region of integration.

To find the value of the matrix elements $M^2(z)$ we use the well known sum rule for the imaginary part of the dielectric function[19]:

$$\int_0^\infty \varepsilon_2(\mathbf{q},\omega)\,\omega\,d\omega=-{}^1/_2\pi\omega_p^2, \tag{9}$$

where ω_p is the plasma frequency determined from the relation $\omega_p^2=4\pi e^2n/m$ and n is the electron density; e and m are respectively the charge and mass of the electron. Substituting the expression for the imaginary part of the dielectric function into Eq. (9), we obtain the square of the matrix element as a function of the reduced wave vector z:

$$M^2(z)=z\Big/\left[z+\frac{1}{2}(3-z^2)w_g\right], \quad z<1,$$
$$M^2(z)=z^2/(z^2+w_g), \quad z\geqslant 1. \tag{10}$$

The cited expressions for the mean square of the matrix element together with Eq. (8) accurately satisfy the rule (9) for all values of z. For $w_g=0$, i.e., in the absence of a gap in the valence-electron energy spectrum, the matrix element becomes equal to unity, and the expression for $\varepsilon_2(z,w)$ goes over to the formula for the imaginary part of the dielectric function of a free electron gas obtained by Lindhard.[1]

The real part of the dielectric function we shall obtain by a Kramers-Kronig transformation[19]:

$$\varepsilon_1(q,\omega)=1+\frac{2}{\pi}\int_0^\infty \varepsilon_2(q,\omega')\frac{\omega'\,d\omega'}{\omega^2-\omega'^2}. \tag{11}$$

From Eq. (10) it follows that

$$\varepsilon_1(z,w)=1-\frac{3}{8}\frac{w_p^2M^2(z)}{z^3}[4f_1(z,w)+f_2(z,w)], \tag{12}$$

where

$$\left.\begin{aligned} f_1&=\theta(1-z)\left\{w_g\ln\frac{w^2-w_s^2}{w^2-w_g^2}\right.\\ &\left.+w\ln\left[\left|\frac{w+w_s}{w-w_s}\right|\left|\frac{w-w_g}{w+w_g}\right|\right]-2z(1-z)\right\},\\ f_2&=\left[\left(z+\frac{w_g}{z}\right)^2-1\right]\ln\frac{w^2-w_m^2}{w^2-w_s^2}+\frac{1}{z^2}\left[w_m^2-w_s^2+w^2\ln\frac{w^2-w_m^2}{w^2-w_s^2}\right]\\ &+2\left(1+\frac{w_g}{z^2}\right)\left\{w\ln\left[\left|\frac{w+w_m}{w-w_m}\right|\left|\frac{w-w_s}{w+w_s}\right|\right]-2(w_m-w_s)\right\}. \end{aligned}\right\} \tag{13}$$

The designations are the same as in Eq. (8); $w_m=z(z+1)+w_g$; $w_s=z(1-z)+w_g$ for $z<1$, and for $z\geqslant 1$ we have $w_s=z(z-1)+w_g$;

$$\theta(x)=0 \text{ for } x<0, \quad \theta(x)=1 \text{ for } x>0.$$

For $z\geqslant 1$ the dielectric function is determined only by the function $f_2(z,w)$; the function $f_1(z,w)=0$ for $z\geqslant 1$. For $w_g=0$ we obtain the dielectric function of a free electron gas:

$$\varepsilon_1(z,w)=1+\frac{3}{8}\frac{w_p^2}{z^3}\left\{4z+\left[1-\left(z-\frac{w}{z}\right)^2\right]\right.$$
$$\left.\times\ln\left|\frac{w-z(z+1)}{w-z(z-1)}\right|+\left[1-\left(z+\frac{w}{z}\right)^2\right]\ln\left|\frac{w+z(z+1)}{w+z(z-1)}\right|\right\}.$$

The nondiagonal elements of the dielectric matrix $\varepsilon_{G,1}$ and $\varepsilon_{G,2}$ are found by using the sum rule for them given by Johnson.[20] As in the case of ε_1 and ε_2 we shall assume that the product of the matrix elements can be averaged over the region of integration and taken outside the integral sign in carrying out the summation in Eq. (4):

$$\{\langle \mathbf{k}+\mathbf{q},l'|e^{i\mathbf{q}r}|\mathbf{k},l\rangle\langle\mathbf{k},l|e^{-i(\mathbf{q}+\mathbf{G})r}|\mathbf{k}+\mathbf{q},l'\rangle\}_{\mathbf{k}}=M_1M_2(\mathbf{q},\mathbf{G}). \tag{14}$$

The curly brackets with the subscript k indicate averaging over k within the region of integration over k. For centrally symmetric crystals (and semiconductors with a lattice of the diamond type belong to this class) $M_1M_2(\mathbf{q},\mathbf{G})$ is a real number, and therefore with allowance for Eq. (14) we can write the following simple relations between ε_1, ε_2 and $\varepsilon_{G,1}$, $\varepsilon_{G,2}$:

$$\varepsilon_{G,1}=\frac{q}{|\mathbf{q}+\mathbf{G}|}\frac{M_1M_2(\mathbf{q},\mathbf{G})}{M^2(q)}[\varepsilon_1(q,\omega)-1], \tag{15a}$$

$$\varepsilon_{G,2}=\frac{q}{|\mathbf{q}+\mathbf{G}|}\frac{M_1M_2(\mathbf{q},\mathbf{G})}{M^2(q)}\varepsilon_2(q,\omega). \tag{15b}$$

The sum rule in Ref. 20 for the imaginary part of the nondiagonal element of the dielectric matrix appears as follows:

$$\int_0^\infty \varepsilon_{G,2}(\mathbf{q},\omega)\,\omega d\omega=-{}^1/_2\pi\omega_p^2f(\mathbf{G})e(\mathbf{q})\hat{e}(\mathbf{q}+\mathbf{G}), \tag{16}$$

where $f(\mathbf{G})$ is the Fourier component of the valence-electron density in the crystal, normalized so that $f(0)=1$; $\hat{e}(\ldots)$ designates a unit vector in the direction of the argument.

Substituting the expression (15b) into Eq. (16), we obtain

$$M_1M_2(\mathbf{q},\mathbf{G})=\frac{|\mathbf{q}+\mathbf{G}|}{q}M^2(q)f(\mathbf{G})\hat{e}(\mathbf{q})\hat{e}(\mathbf{q}+\mathbf{G}). \tag{17}$$

It should be noted that the relation (17) does not depend on the model used for the dielectric function but is valid both for weakly bound and strongly bound electrons.

3. STOPPING FORMULAS IN AN INHOMOGENEOUS ELECTRON GAS

The formula for the energy loss of a charged particle in a crystal is conveniently written in the form of a Fourier series in the reciprocal-lattice vectors:

$$S(\mathbf{r})=\sum_{\mathbf{G}}S(\mathbf{G})e^{i\mathbf{G}r}. \tag{18}$$

Taking into account Eqs. (6), (15), and (17) and introducing a spherical coordinate system in wave-vector space in such a way that the azimuthal angle φ is measured from the direction of the vector G and the polar angle from the direction of motion of the particle, we obtain

$$S(\mathbf{G})=\frac{Z_1^2e^2}{\pi^2v^2}\int_0^\infty\frac{dq}{q}\int_0^{qv}d\omega\omega\frac{-\varepsilon_2}{\varepsilon_1^2+\varepsilon_2^2}f(\mathbf{G})\int_0^{2\pi}d\varphi\hat{e}(\mathbf{q})\hat{e}(\mathbf{q}+\mathbf{G}). \tag{19}$$

Since analytical expressions (8) and (12) exist for the dielectric function ε_1 and ε_2, the energy loss can be obtained from Eq. (19) in terms of the dielectric approach for an arbitrary velocity of the incident particle. For velocities significantly greater than the Fermi velocity, we can obtain from Eq. (19) analytic expressions for the

Fourier components of the energy loss. In a homogeneous electron gas[1] for high velocities the energy loss is

$$S(\mathbf{G}=0)=-\left(\frac{dE}{dx}\right)_{\text{hom}}=\frac{Z_1^2e^2\omega_p^2}{v^2}\ln\frac{2mv^2}{\hbar\omega_p}, \tag{20}$$

where m is the electron mass.

In contrast to the case $\mathbf{G}=0$, for nonzero Fourier components of the energy loss the integral over φ in Eq. (19) will depend on the magnitude of the momentum transfer $\hbar q$. For large momentum transfers $q \gg G$ the unit vector $\hat{e}(\mathbf{q}+\mathbf{G}) \approx \hat{e}(\mathbf{q})$ and the integral over the angle φ in Eq. (19) is equal to 2π, as for a homogeneous electron gas. In regions of low momentum transfer, where $q \ll G$, the unit vector $\hat{e}(\mathbf{q}+\mathbf{G}) \approx \hat{e}(\mathbf{G})$ and the unit integral over the angle φ is close to zero. We can assume approximately that collisions with a momentum transfer less than $\hbar G$, where $\mathbf{G}$ is the reciprocal-lattice vector considered, do not contribute to the $\mathbf{G}$-th Fourier component of the energy loss.

Utilizing the sum rule for the imaginary part of the inverse dielectric function, it is easy to obtain from Eq. (19)

$$S(\mathbf{G})=\frac{Z_1^2e^2\omega_p^2}{v^2}f(\mathbf{G})\ln\frac{2mv}{\hbar G}. \tag{21}$$

Equation (18) for high velocities of the incident particle $v \gg v_F$ with allowance for Eqs. (20) and (21) can be written in the form

$$S(\mathbf{r})=\frac{Z_1^2e^2\omega_p^2}{v^2}\left\{\left[\frac{1}{2}+\frac{1}{2}\rho(\mathbf{r})\right]\ln\frac{2mv^2}{\hbar\omega_p}+\frac{1}{2}\sum_{\mathbf{G}\neq 0}f(\mathbf{G})e^{i\mathbf{G}\mathbf{r}}\ln\frac{2m\omega_p}{\hbar G^2}\right\}, \tag{22}$$

where

$$\rho(\mathbf{r})=1+\sum_{\mathbf{G}\neq 0}e^{i\mathbf{G}\mathbf{r}}f(\mathbf{G})$$

is the relative density of valence electrons at the point $\mathbf{r}$.

The equations (21) and (22), in contrast to the corresponding formulas of Ref. 7, were obtained without the additional assumption that the generalized harmonic oscillator strengths of the atomic electrons are analogous to the generalized harmonic oscillator strengths. They differ also in that in them the principal parameter characterizing the energy loss is ω_p, and not the mean ionization potential.

Equation (22) is convenient for analysis of the energy loss of light channeled ions; it permits direct calculations of the energy loss in any of the axial or planar channels of the crystal if the electron density distribution in the crystal is known. If the velocity of the channeled ion is so high that the inner electrons begin to be excited, then it is necessary to take into account their contribution also.[21] The energy of a proton corresponding to the Fermi velocity of the valence electrons of silicon is 23 keV, and therefore for protons with an energy of several hundred keV the condition of applicability of Eqs. (20)–(22), $v \gg v_F$, is completely satisfied.

Very fast relativistic particles whose velocities are close to the velocity of light interact with matter as with an electron plasma. The energy loss of such particles is not determined by the structure of the target atoms, but depends on the electron density of the material. In order that Eq. (22) be applicable for particles with velocities close to the velocity of light, we shall include in it a change to take into account relativity. Gould[22] has shown that in the slowing down of relativistic particles in a homogeneous electron plasma the maximum momentum transfer is increased by a factor $\gamma=(1-\beta^2)^{-1/2}$ in comparison with the nonrelativistic case, while the minimum momentum remains the same as in the nonrelativistic case— equal to $\hbar\omega_p/v$. In addition, for close collisions it is necessary to take into account the effect of electron spin, which leads to an additional term in the stopping formula equal to $-\beta^2/2$, where $\beta=v/c$ and c is the velocity of light in vacuum. Thus, the energy loss of a very fast relativistic particle with charge Z_1 in an inhomogeneous electron gas is

$$S(\mathbf{r})=\frac{Z_1^2e^2\omega_p^2}{v^2}\left[\ln\frac{2m\gamma a^2}{\hbar\omega_p}-\frac{\beta^2}{2}+\sum_{\mathbf{G}\neq 0}e^{i\mathbf{G}\mathbf{r}}f(\mathbf{G})\ln\frac{2m\gamma v}{\hbar G}\right]. \tag{23}$$

The plasma frequency and the Fourier components of the electron density for relativistic particles must be taken with inclusion of all electrons, and not only valence electrons, since in slowing down of very fast relativistic particles all electrons are drawn into the interaction, regardless of their binding with the nuclei of the atoms. The stopping formula of this work differs from those of Ref. 7 in that in Eqs. (20)–(23) we have the plasma frequency of the electron gas, and not the mean ionization potential of the atoms. The use of Eq. (23) does not require the additional introduction of a correction for the density effect, since in the dielectric approach the influence of screening is taken into account from the very beginning.

In spite of the fact that very fast relativistic charged particles interact with the electrons of matter at distances greater than the average interatomic distance in the crystal, the dependence of the energy loss on the location of the trajectory in the crystal is preserved, and consequently the loss experienced by channeled particles should differ from the energy loss of particles moving in an unoriented crystal.

For $\gamma \lesssim 10$ it is necessary to take into account the binding of the inner electrons with the nucleus, particularly in calculations of the contribution of distant collisions.

4. RESULTS OF NUMERICAL CALCULATIONS. COMPARISON OF THEORY WITH EXPERIMENT

In the preceding section for velocities $v \gg v_F$ we obtained simple analytical formulas for the slowing down of a charged particle in an inhomogeneous gas of valence electrons. At lower incident-particle velocities the integration in Eq. (19) must be carried out numerically with inclusion of Eqs. (8), (12), and (15) for the elements of the dielectric matrix.

In Fig. 1 we have shown the results of a numerical calculation of the energy loss of a proton with energy up to 250 keV in a homogeneous electron gas with an energy gap characteristic of the valence electrons of silicon. The value of the energy gap was chosen as 4.8 eV,[23] and in this case the results of the calculation for $\varepsilon_1(q, 0)$

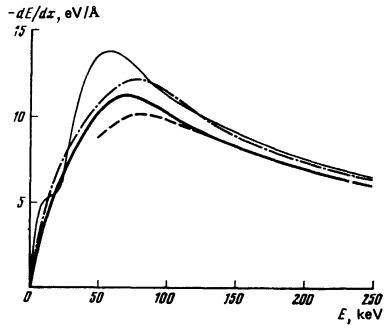

FIG. 1. Energy loss of protons in a homogeneous electron gas with parameters corresponding to a gas of silicon valence electrons: dot-dash—from the data of Ref. 23, thin solid line—Ref. 5, heavy line—results of the present work, dashed curve—experimental energy loss of protons in the ⟨111⟩ axial channel of silicon.[10]

agree with the results of Penn[24] for $q \gtrsim 0.2$. Our data in this energy interval lie somewhat below those obtained by Brandt and Reinheimer[23] and Desalvo and Rosa.[5] The discrepancy is due to the different choice of the matrix element of interband transitions $M^2(q)$. In the present work the matrix element exactly satisfies the sum rule for the imaginary part of the dielectric function for all q, whereas in Refs. 23 and 5 for $q \lesssim 2k$ the sum rule (9) is satisfied only approximately.

The energy loss values calculated by us are in good agreement with the experimental energy loss in the ⟨111⟩ axial channel of silicon.[10] The distribution of valence electrons in this channel is close to uniform, since the Fourier component of the valence electron density $f(220)$ which determines the inhomogeneity of the electrons in the ⟨111⟩ channel is close to zero.[25,26] The contribution to the total energy loss due to excitation of inner electrons is negligible at the energies considered, and therefore the energy loss calculated for valence electrons is in good agreement with the experimental energy loss of ions channeled in the ⟨111⟩ axial channel of silicon.

In most experimental studies of channeling, the average energy loss of a particle which has passed through a thin oriented single crystal is measured. Usually one takes as the average energy loss the energy loss of a channeled particle measured on the basis of the peak of the energy spectrum of particles at the exit from the crystal.[8-11] Only a few studies have used small-angle detectors after the passage through the crystal to separate the fraction of the best-channeled particles.[12]

The energy loss values measured in the peak and at the edge of the spectrum may differ substantially. This is particularly true of the energy loss in the most open channels of silicon, ⟨110⟩. As a result of the rapid variation of the electron density over the cross section of the channel, the energy loss depends strongly on the trajectory of the ion in the channel. The spread in the energies of particles which have passed through a crystal oriented in the ⟨110⟩ direction is several times greater than the spread of the spectrum of unchanneled particles. As a result the energy loss values determined at the edge and at the peak of the spectrum differ significantly.

In Fig. 2 we have given a comparison of the theoretical and experimental energy loss values for light ions in the silicon ⟨110⟩ channel. We have given the universal stopping function[11] $B(E)/AZ_{eff}^2$(MeV^2/cm), where

$$B(E) = -\frac{dE}{dx}E,$$

as a function of the energy per amu (A is the mass and Z_{eff} is the effective charge of the incident particle). The effective charge of ^{4}He$^+$ ions, which is determined by the capture and loss rates of the moving particle, was taken from Ref. 27. In the figure we have shown data of experiments on proton stopping by Appleton *et al.*[8] and Della Mea *et al.*[11] and also the energy loss of ^{4}He$^+$ measured by Eisen *et al.*[12] at the peak and at the edge of the energy spectrum.

The experiment of Eisen *et al.*[12] was carried out with a small-angle detector, and therefore the energy loss measured at the edge of the spectrum can be interpreted as the energy loss of a well channeled particle moving along the channel axis. The energy loss of well channeled ions was calculated with allowance for the nonuniformity of the distribution of the local electron density in the ⟨110⟩ channel of silicon. The Fourier components of the electron density were taken from Ref. 25 and the (111) Fourier component from Ref. 26, where the accuracy of the measurement is appreciably better. The energy loss to valence electrons with allowance for the nonuniformity of electron density is approximately 40% lower than the energy loss in a homogeneous gas of valence electrons. The energy loss measured at the peak of the energy spectrum of particles channeled in the silicon ⟨110⟩ axial channel agrees quite well with the energy loss in a homogeneous gas with the parameters corresponding to silicon valence electrons.

In Fig. 3 we have given the stopping function for particles moving in the silicon ⟨111⟩ axial channel. The experiments of Refs. 8, 10, and 11 were carried out with

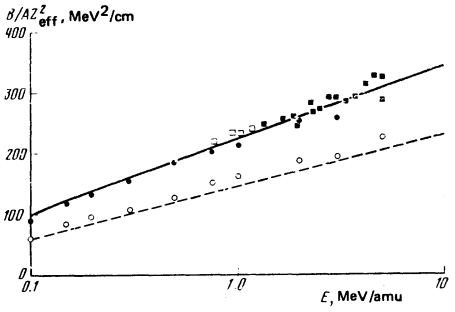

FIG. 2. Universal stopping function for protons and ions channeled in the ⟨110⟩ axial channel of silicon: •—energy loss measured at the peak,[12] ○—energy loss measured at the edge of the spectrum,[22] ■ and □—results of Ref. 11 on channeling of protons and deuterons, respectively. The solid line is the energy loss in a homogeneous gas of valence electrons; the dashed line takes into account the inhomogeneity of the electron density distribution in the channel. The deviation of Z_{eff} from 2 for helium ions, calculated with the formula from Ref. 27, increases with decrease of the ion energy; for $E = 500$ keV $Z_{eff} = 1.87$, while for $E = 100$ keV $Z_{eff} = 1.48$.

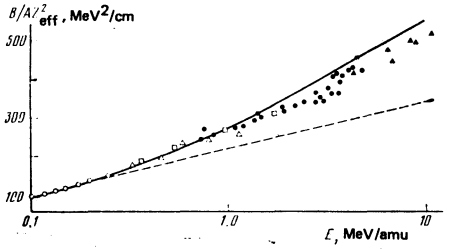

FIG. 3. Universal stopping function for protons, deuterons, and He ions channeled in the ⟨111⟩ axial channel of Si. The points are from the following experiments: ▲—data of Ref. 10, ●—Ref. 8, ○, □, and △—data of Ref. 11 respectively for protons, deuterons, and helium ions; the dashed curve is the contribution of valence electrons.

wide-angle detectors: the energy loss was measured at the peak of the spectrum. The ⟨111⟩ axial channel of silicon is narrower than the ⟨110⟩ channel and therefore at incident-particle energies of several MeV per amu it is necessary to take into account the contribution of inner electrons. The loss to inner electrons was calculated in the dipole approximation[28] for particles moving along the channel axis. The calculated stopping function satisfactorily describes experiment.

The model of energy-loss calculation developed in Section 2 for light ions permits discussion of the relation between the energy loss of channeled particles and the local electron density. The energy loss of a particle, like the electron density in a crystal, is expressed by a Fourier series in the reciprocal-lattice vectors. In Fig. 4 we have shown the electron density and the energy loss of 100-keV protons in the ⟨110⟩ axial channel of silicon, calculated numerically in accordance with Eqs. (18) and (19). The energy loss distribution for the most part follows the shape of the electron density distribution, but the energy loss is not sensitive to small details of the valence-electron density distribution. Since the density of valence electrons varies smoothly in space, the Fourier components of the electron density $f(G)$ fall off rapidly with increase of the length of the reciprocal-lattice vector. As can be seen from Eq. (21), $S(G)$ falls off with increase of G still more rapidly, and therefore the function $S(\rho)$ is determined mainly just by the Fourier components of the vector G_{min} of smallest

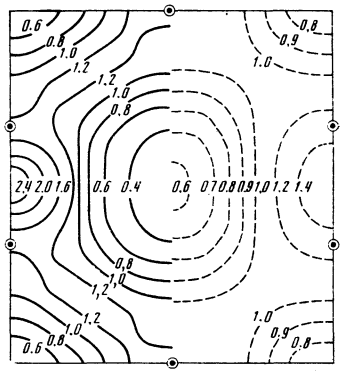

FIG. 4. Distribution of density of valence electrons (solid line) and of energy loss (dashed line) of 100-keV protons in the ⟨110⟩ axial channel of silicon. The values have been normalized so that when averaged over the crystal they are equal to unity.

absolute value. If we neglect corrections originating from vectors $G > G_{min}$, the energy loss depends linearly on the electron density ρ:

$$S_{rel}=S(\mathbf{r})/S_{hom}\approx\beta\rho_{rel}+(1-\beta), \tag{24}$$

where

$$\beta=S(G_{min})/S(0)f(G_{min}), \quad \rho_{rel}=\rho(\mathbf{r})/\rho_{av}.$$

In Fig. 5 we have shown the relative energy loss in the silicon ⟨110⟩ channel as a function of the relative density of valence electrons. The smooth line is given by Eq. (24) and the circles show the relation between S and ρ at various points over the channel cross section. It is evident from the figure that although not all points lie on the straight line, nevertheless on the average the dependence of S on ρ is satisfactorily described by the straight line (24).

At very high velocities where $v \gg \hbar G/2m$ and $v^2 \gg \hbar\omega_p/2m$, as can be seen from Eqs. (22) and (24), the coefficient $\beta \to 1/2$, which is an expression of the rule of equipartition of energy loss in close and distant collisions. For particle velocities of the order of several times the velocity v_F or lower, depending on the band structure of the material, deviations from the equipartition rule can be observed both in the separation of the energy loss into plasma and single-particle components[4] and in the distribution into local and nonlocal energy losses.

We note that the coefficient β, which is equal to the fraction of the energy loss proportional to the local electron density, at finite velocities is always less than the fraction of the energy loss due to single-particle excitations. Thus, for protons with energy $E=100$–500 keV moving in the ⟨110⟩ and ⟨111⟩ axial channels of silicon, numerical calculation with Eq. (19) gives respectively $\beta=0.50$ and $\beta=0.24$, while the fraction of the energy loss to single-particle excitations α differs appreciably from β. At $E=150$ keV, for example, $\alpha=0.70$. At lower energies β increases, as a result of the fact that at such velocities plasma oscillations are not excited, but only single-particle oscillations. Here the localization of these excitations is strengthened, since at low energies only excitations with a wave vector close to $2k_F$ contribute to the stopping, while excitations with $k < 2k_F$ turn out to be suppressed. This explains the decrease of the ratio of the energy loss of channeled ions to the energy loss in an unoriented target at low energies in the experiment of Eisen *et al.*[12]

The difference between the coefficients α and β is due

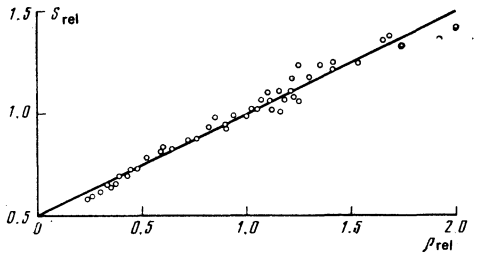

FIG. 5. Relative energy loss in the silicon ⟨110⟩ channel as a function of the relative density of valence electrons.

to the nonlocality of single-particle excitations at low and intermediate velocities. This difference is greater, the greater is the ratio $G_{min}/2k_F$, which is equal to the ratio of the characteristic dimension of the excitations at low velocities to the channel dimension. For example, for the most open channels of aluminum $G_{min}/2k_F$ is 16% greater than in the case of semiconductors with a lattice of the diamond type. This leads to the result that the dependence of the energy loss on the local electron density in an aluminum crystal is weaker: $\beta = 0.4$ at $E = 100$ keV/amu. The value of the energy gap affects β to a smaller extent. Thus, for diamond at $E = 100$ keV/amu β is only 5% higher than for silicon.

Since the electron density in the {111} planar channel is determined mainly by the same Fourier component $f(111)$ as in the ⟨110⟩ axial channel, the ratio between S and ρ in the {111} planar channel is the same as that in the ⟨110⟩ axial channel, which is given by Eq. (24). The electron densities near the axis in the axial and planar channels are different, amounting to $\rho_{rel} = 0.25$ in the ⟨110⟩ axial channel and $\rho_{rel} = 0.68$ in the {111} planar channel. Therefore the energy loss of well channeled charged particles with energy 100 keV/amu amounts to $S_{rel} = 0.63$ for an axial channel and $S_{rel} = 0.84$ for a planar channel; thus, a 25% decrease of the energy loss occurs in the transition from planar to axial channeling. In the experiment of Eisen *et al.*[12] a 20% decrease of the energy loss of hyperchanneled helium ions with energy 100 keV/amu was observed in ⟨110⟩ axial channels in comparison with the case of {111} planar channels of silicon.

At the present time it has been shown experimentally[13,29] and theoretically (see for example Ref. 30) that channeling is preserved even at relativistic energies of the incident particle. Esbensen *et al.*[29] have measured the energy loss of π mesons, K mesons, and protons with energies 2–15 GeV both in unoriented crystals and in the channeling regime. The energy loss of relativistic particles was measured on the basis of the pulse-height spectra obtained from crystals which simultaneously served as a detector. Since the electrons knocked out of the crystal by the incident particle do not contribute to the measured energy loss spectrum, it is necessary to calculate the energy loss limited in energy transfer. The maximum energy transfer T_0 depends on the size of the crystal and for the crystals studied by Esbensen *et al.*,[29] according to the calculations of the authors, amounts to 500 keV. The maximum momentum transfer then is $(2mT_0)^{1/2}$ instead of $2m\gamma v$ and the expression under the logarithm in Eq. (23) acquires the form $(2mT_0)^{1/2}v/\hbar\omega_p$.

In Fig. 6 the energy loss calculated with Eq. (23) for well channeled positively charged particles in silicon planar channels is compared with values obtained experimentally. The local relative density in the channels was calculated from the experimental data of Refs. 25 and 26. Correction was also made for the width of the energy-loss spectrum, with inclusion of the Landau distribution.[31] The theory correctly predicts a decrease of the energy loss in the case of channeling for very fast relativistic particles with momentum $p/Mc \gtrsim 10$ in the region where the stopping is determined not by the structure of the atoms but by the total electron density.

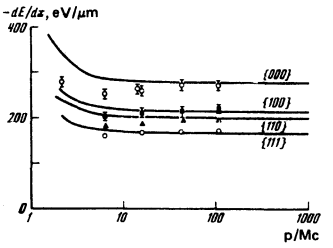

FIG. 6. Energy loss of positively charged particles ($M > m$) in the silicon planar channels {111}, {110}, and {100} and in an unoriented crystal {000}; the experimental points are from Ref. 29.

At lower incident-particle energies the energy loss calculated with Eq. (23) is higher than the experimental value, since the effects of binding of the target electrons with the nuclei of the atoms begin to be felt.

5. CONCLUSION

In this work we have proposed a simple analytical model for the dielectric function $\varepsilon(\mathbf{q}, \omega)$. Using the sum rule for the nondiagonal elements of the dielectric matrix, we have obtained a relation between the nondiagonal elements of the dielectric matrix $\varepsilon_{\mathbf{G},0}(\mathbf{q}, \omega)$ and the dielectric function. As a result of the analytical model developed for the dielectric matrix, the theory of the slowing down of channeled light ions using a quantum dielectric formalism takes a simple form.

In the region of not very high energies, channeled light ions are slowed down only by the valence electrons of the atoms of a crystal, and therefore the proposed theory completely describes the energy loss of such particles. Equation (22) expresses the relation between the local electron density and the energy loss. The energy loss is approximately proportional to the local density of valence electrons. The proportionality coefficient connecting the relative energy loss and the electron density is less than the ratio of the energy loss due to single-particle excitations to the total energy loss. In narrow channels the fraction of the energy loss which is proportional to the local density is small, and the energy loss depends to a greater degree on the average electron density.

In open channels such as the ⟨110⟩ axial channel and the {111} planar channel of silicon, the contribution of the energy loss proportional to the local density is greater, so that neglecting the inhomogeneity of the electron density in these channels leads to an error up to 40% for the energy loss of ions. For the first time it has been rigorously demonstrated that the energy loss of well channeled charged particles in axial channels is less than in the planar channels which intersect this axis. At low and intermediate velocities the ratio $S(\rho)$ depends on the electronic structure of the material.

Allowance for the inhomogeneity of the valence electrons is important not only at velocities at which the stopping of channeled ions is accomplished only by valence electrons, but also at higher velocities, since the

contribution of valence electrons to the stopping is always significant.

The theory presented in this work for stopping in an inhomogeneous electron gas can be applied also to the calculation of the total energy loss of channeled relativistic particles, where the stopping is determined by the effect of the density of the medium.

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[1]J. Lindhard and A. Winther, Mat.-Fys. Medd. Dan. Vid. Selsk. **34**, No. 4 (1964).
[2]Yu. Kagan and Yu. V. Kononets, Zh. Eksp. Teor. Fiz. **66**, 1693 (1974) [Sov. Phys. JETP **39**, 832 (1974)].
[3]F. Bonsignori and A. Desalvo, J. Phys. Chem. Solids **31**, 2191 (1970).
[4]F. F. Komarov and M. A. Kumakhov, Radiat. Eff. **22**, 1 (1974).
[5]A. Desalvo and R. Rosa, J. Phys. **C10**, 1595 (1977).
[6]V. V. Beloshitsky and M. A. Kumakhov, Radiat. Eff. **35**, 209 (1978).
[7]H. H. Esbensen and J. A. Golovchenko, Nucl. Phys. **A298**, 382 (1978).
[8]B. R. Appleton, C. Erginsoy, and W. M. Gibson, Phys. Rev. **161**, 330 (1967).
[9]A. R. Sattler and G. Dearnaley, Phys. Rev. **161**, 244 (1967).
[10]G. Della Mea, A. V. Drigo, S. Lo Russo, P. Massoldi, and G. G. Bentini, Atomic Collisions in Solids, **1**, ed. by S. Datz, B. R. Appleton, and C. D. Moak, Plenum Publishing Corp., p. 75, 1975.
[11]G. Della Mea, A. V. Drigo, S. Lo Russo, P. Massoldi, and G. G. Bentini, Radiat. Eff. **13**, 115 (1972).
[12]F. H. Eisen, G. J. Clark, J. Bottiger, and J. M. Poate, Radiat. Eff. **13**, 93 (1972).
[13]O. Fich, J. A. Golvchenko, K. O. Nielsen, E. Uggerhøj, G. Charpak, and F. Sauli, Phys. Lett. **57B**, 90 (1975).
[14]H. Esbensen, O. Fich, J. A. Golovchenko, K. O. Nielsen, E. Uggerhøj, C. Vraast-Thomsen, G. Charpak, S. Majewski, F. Sauli, and J. Ponpon, Nucl. Phys. **B127**, 281 (1977).
[15]F. Bonsignori and A. Desalvo, Nuovo Cimento Lett. **1**, 589 (1969).
[16]D. Falk, Phys. Rev. **118**, 105 (1960).
[17]S. L. Adler, Phys. Rev. **126**, 413 (1962); N. Wiser, Phys. Rev. **129**, 62 (1963).
[18]J. Callaway, Phys. Rev. **116**, 1368 (1959).
[19]D. Pines, Elementary Excitations in Solids, W. A. Benjamin, Inc., New York, 1963. Russ. transl., Mir, 1965, p. 369.
[20]D. L. Johnson, Phys. Rev. B **9**, 4475 (1974).
[21]K. Dettmann, Z. Phys. **A272**, 227 (1975).
[22]R. J. Gould, Physica **58**, 379 (1972).
[23]W. Brandt and J. Reinheimer, Phys. Rev. B **2**, 3104 (1970).
[24]D. R. Penn, Phys. Rev. **128**, 2093 (1962).
[25]P. M. Raccah, R. N. Euwema, D. J. Stukel, and T. C. Collins, Phys. Rev. B **1**, 756 (1970).
[26]S. Tenemura and N. Kato, Acta Cryst. **A28**, 69 (1972).
[27]W. Booth and J. S. Grant, Nucl. Phys. **63**, 481 (1965).
[28]J. P. Jackson, Classical Electrodynamics, J. Wiley, Inc., New York–London, 1962, p. 434. Russ. transl., Mir, 1965, p. 475.
[29]H. Esbensen, O. Fich, J. A. Golovchenko, S. Madsen, H. Nielsen, H. E. Schiott, E. Uggerhøj, C. Vraast-Thomsen, G. Charpak, S. Majewski, G. Odyniec, G. Petersen, F. Sauli, J. P. Ponpon, and P. Siffert, Phys. Rev. B **18**, 1039 (1978).
[30]M. A. Kumakhov, R. Wedell, and F. F. Komarov, Phys. Lett. **51A**, 151 (1975).
[31]L. D. Landau, J. Phys. USSR **8**, 201 (1944).

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Features of the suppression effect under conditions of hyperfine quadrupole splitting

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We report the first experimental investigations of the effect of suppression of a nuclear reaction under conditions of hyperfine quadrupole splitting. The investigations were performed on a perfect iron borate crystal enriched with the resonant isotope Fe^{57}. A strong effect of the interference of different nuclear transitions on the form of the Mössbauer spectrum of the gamma-quantum Laue diffraction is observed.

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In our preceding articles[1] we reported investigations of the suppression effect (SE) of a nuclear reaction in an $Fe^{57}BO_3$ crystal for pure nuclear magnetic diffraction of the Mössbauer rays. Besides the advantages of iron borate for the study of the SE described in Ref. 1, there are also other advantages that make it possible to expand the research on the effect, particularly to include the case of quadrupole splitting of the nuclear energy levels.

As was previously observed,[2] the iron borate crystal has a large number of reflections in which complete or almost complete extinction of electron diffraction is obtained as a result of mutual cancellation of waves scattered by atoms of different species, iron on the one hand, and boron and oxygen on the other. For example, complete compensation is reached in the previously investigated[2] (222) reflection, where pure nuclear diffraction was observed for the first time ever in scattering of quanta on nuclear transmitions with $\Delta m = 0$.

Another advantage of the considered crystals is the

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