Plasmon-diffraction resonance during motion of a fast charged particle in a single crystal

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A theory is developed for the emission of bulk plasmons by a charged particle as it undergoes diffraction in a crystal. The angle-integrated cross section for inelastic scattering due to emission of a bulk plasmon by the diffracted particle is subject to a pronounced orientational effect such that for appropriate directions of motion of the fast particle conditions arise that are favorable for the emission of plasmons that have very small wave vectors and that could not be emitted as a result of the usual "Čerenkov" generation of plasmons. This kind of phenomenon can be called bremsstrahlung of bulk plasmons induced by the diffraction of fast charged particles. The theoretically predicted resonances in the orientation dependence of the inelastic cross section for fast particles being diffracted in a single crystal may be the basis of a method for the direct experimental observation of bremsstrahlung of longitudinal electromagnetic waves.

§1. INTRODUCTION

For many years after the work of Bethe,[1] in which the basis of the quantum mechanical theory of diffraction of light charged particles in a crystal was worked out, the main attention in the physics of diffraction has been focused on developing and refining the concepts concerning the formation of the wave field of the charged particles in crystals, finding those specific mechanisms for the interaction of the fast particles with crystals which determine the damping of this field, studying diffraction in non-ideal crystals, and developing special theoretical formulations and approximation methods suitable for carrying out computer calculations.[2–11]

There exists also a wide literature on the diffraction of slow particles at single crystal surfaces and diffraction phenomena at high electron and positron energies such that it becomes more appropriate to use specific methods of describing the interaction of electrons and holes with matter, even to the point of using classical mechanics.[14–17] In this investigation we take diffraction to mean the interaction of fast charged particles (henceforth for brevity we shall call them electrons) with single crystals, where an adequate description of the physical processes in the bulk of the material can be obtained in the few-wave approximation. Interest in this topic has not abated even now.[18–21]

Diffraction, however, is interesting not only in its own right, but also in that it can serve as a rather fine tool for the study of those physical processes that can exist also without diffraction, but in which diffraction of electrons helps to reveal new aspects and to obtain information that is hard to obtain by other means. In recent years it has been established that by using electron diffraction it is possible, for example, to study incoherent electron-atom scattering of electron beams in which there are electrons with preferred impact parameters.[22] In the usual experiments on electron-atom scattering, an electron plane wave is incident on the atom, and the incident electron can, with equal probability, be in any angular momentum state. Crystals, however, allow the formation of wave packets which select out certain values of the orbital quantum number and thus make it possible to carry out a phase shift analysis of the electron-atom scattering. By using diffraction one can reveal spatial regions in the crystal where secondary electrons are produced most intensely.[23]

Finally, electron diffraction causes a fine structure to appear in, apparently, all of the forms of electron emission from the crystal taking place under the influence of fast electrons penetrating the crystal. The first experimental observation of this sort was made in Ref. 24. The role of diffraction in these effects was established in Ref. 25, as well as in subsequent papers.[26–28] It is now known that the diffraction of intermediate-energy electrons has an effect even on the emission of Auger electrons, which are emitted from almost the very surface of the crystal.[29–31]

In this investigation we show that diffraction of electrons makes it possible to reveal new aspects of the interaction of fast electrons with plasmons. Generally speaking, the interaction of diffracted electrons with bulk plasmons has been investigated previously,[5,11] in the first place to determine the relative contribution of this process (in comparison to the contributions of phonons and one-electron excitations) to the imaginary part of the crystal lattice potential that determines the damping of the coherent field. Here it was taken as obvious that, because the wavelength of a bulk plasmon is ordinarily much greater than the crystal lattice constant, for the interaction of an electron with a plasmon it is not very important exactly in what state the fast electron is, whether it is in a diffraction state or whether it can be described by an ordinary plane wave. This means that in, e.g., two-wave diffraction, the contributions of plasmons to the damping of type I waves and type II waves are practically the same.

The generation of plasmons is actually not very sensitive to the state of the diffracting electron if the process of generation is considered to be a Čerenkov process. But besides the Čerenkov mechanism for the generation of bulk plasmons, they can be emitted as bremsstrahlung, and the corresponding density effect can take place.[32] We shall show that the two last effects are very sensitive to the character of

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the diffraction. The specific details of the diffraction, as it turns out, allow us, in the description of the emission of plasmons during diffraction, to separate directly the elementary processes, the bremsstrahlung of bulk plasmons and the density effect. These two processes also take place, of course, in an isotropic medium. In Ref. 32 it was shown that they can have a marked effect on the halfwidth of the peak of the probability of plasma excitation by a fast electron in an isotropic medium. However, under these conditions the line shape of the plasmon peak is also determined by other factors, such as the decay of a plasmon with the excitation of interband transitions or its decay that results when the electrons that participate in the plasma oscillations collide with impurities or crystal-lattice imperfections. All of these mechanisms that enter into the expression for the halfwidth of the plasmon peak are additive, so that under experimental conditions it is not possible to separate their relative contributions. The diffraction of electrons in single crystals changes this situation.

The possibility of direct observation of bremsstrahlung of bulk plasmons and of the density effect is also of general-physics interest. Whereas these two processes in the emission of transverse electromagnetic waves can be considered quite well studied, in the emission of plasmons—longitudinal electromagnetic waves—they have never even been directly detected in spite of the important (and, according to relatively recent estimates,[33] decisive) role of plasmons in the transformation of the energy of a fast particle into energy of excitation of the medium.

In this study we shall show that the bremsstrahlung of plasmons and the density effect under conditions of diffraction of fast electrons have a quite unusual character and lead to a characteristic orientational dependence of the cross section for the excitation of a bulk plasmon. In particular, we predict the existence of a new resonance in the angle-integrated inelastic scattering cross section for a fast electron, where, for certain directions of motion of the fast electron relative to the crystallographic planes, the total cross section for the emission of a bulk plasmon shows a resonance-like increase (in thin crystals or in thick crystals where plasmons make the decisive contribution to the average coherence length).

§2. CROSS SECTION FOR PLASMON EMISSION BY A DIFFRACTED ELECTRON

We shall designate by $\psi(\mathbf{r},\mathbf{R})$ the wave function of an electron undergoing diffraction in a crystal with a lattice that produces a potential $U_L(\mathbf{r})$, and interacting with electrons of the solid that produce a potential $U_e(\mathbf{r},\mathbf{R})$ and are able to participate in plasma oscillations. Here $\mathbf{R}$ is the set of position vectors of the particles in the crystal and $\mathbf{r}$ is the position of the fast electron. The wave function $\psi(\mathbf{r},\mathbf{R})$ is governed by the Schrödinger equation

$$\Delta\psi(\mathbf{r},\mathbf{R})+\frac{2m}{\hbar}[E-U_L(\mathbf{r})-U_e(\mathbf{r},\mathbf{R})-U_c(\mathbf{R})]\psi(\mathbf{r},\mathbf{R})=0. \tag{1}$$

Here the Laplacian operator Δ contains the second derivatives with respect to all components of the variables $\mathbf{r}$ and $\mathbf{R}$. The quantity $U_c(\mathbf{R})$ is the energy of interaction of all the particles of the crystal.

We shall assume that the energy of the fast electron is such that the space-time sequence of events has the following form: first the fast electron incident on the single crystal goes into a diffracted-electron state, and then during diffraction it emits a plasmon. The fast electron which is thus inelastically scattered can then either pass through the crystal (if the crystal is thin) and be detected as an electron that has lost a characteristic amount of energy, or else (if the crystal is thick) it can undergo incoherent scattering through a large angle and leave the crystal through the same surface that it entered. The fate of the electrons that have lost energy greater than the plasmon energy $\hbar\omega_p$ is not tracked and in the present case these electrons are not detected.

We assume that the fast electron incident on the crystal has such an energy and direction of motion that it is in a state close to an exact state of reflection with respect to a system of planes perpendicular to the crystal surface so that Laue diffraction takes place.

The fact that the plasmon is emitted by an electron for which the diffraction field can be considered to have already been formed means that the mean free path l_{pl} of the fast electron with respect to bulk plasmon emission is greater than the extinction length of the wave field. Using in the calculations the expression for l_{pl}

$$l_{pl}\approx\hbar v^2/e^2\omega_p\ln\frac{v}{v_F}, \tag{2}$$

which is valid for the motion of an electron in a homogeneous isotropic electron gas (here v is the velocity of the fast electron, v_F is the velocity of an electron at the Fermi surface, and ω_p is the plasma frequency), and keeping in mind that the extinction length of the wave field of a fast electron in an exact reflecting situation is

$$\xi_g=\hbar v/U_g, \tag{3}$$

(where U_g is the Fourier transform of the potential U_L and corresponds to the reciprocal lattice vector $\mathbf{g}$) we find that the condition $l_{pl}\gg\xi_g$ leads to the inequality

$$\left(\frac{U_g}{\hbar\omega_p}\right)\left(\frac{\hbar v}{e^2}\right)\Big/\ln\frac{v}{v_F}\gg1, \tag{4}$$

which gives a lower bound to the energy of a fast electron for which the theory developed below is valid. From (4) it follows that the energy of the fast electron must at least exceed 10 keV.

Condition (4) allows the wave function $\psi(\mathbf{r},\mathbf{R})$ at a distance of the order l_{pl} below the surface of the crystal to be written in the form

$$\psi(\mathbf{r},\mathbf{R})=\psi_D(\mathbf{r})\Phi_i(\mathbf{R})+\delta\psi(\mathbf{r},\mathbf{R}), \tag{5}$$

with

$$\delta\psi(\mathbf{r},\mathbf{R})\ll\psi_D(\mathbf{r})\Phi_i(\mathbf{R}). \tag{6}$$

The quantity $\psi_D(\mathbf{r})$ in (5) and (6) is the wave function of the diffracted electron without allowance for its interaction with the electrons of the single crystal that are able to take part in the plasma oscillations, $\Phi_i(\mathbf{R})$ is the wave function of the initial state of the electrons in the crystal, and $\delta\psi(\mathbf{r},\mathbf{R})$ accounts for the interaction of the fast electron with the electron subsystem in which the plasmons can be excited in the crystal.

The function $\psi_D(\mathbf{r})\Phi_i(\mathbf{R})$ satisfies the equation

$$\Delta(\psi_D\Phi_i)+\frac{2m}{\hbar^2}[E-U_L(\mathbf{r})-U_c(\mathbf{R})]\psi_D\Phi_i=0. \tag{7}$$

Substituting (5) into (1) and neglecting the terms containing $U_e\delta\psi$ (the latter is of second order in the interaction of the fast electron with the plasmon) and $U_L\delta\psi$ (it describes the diffraction of an electron that has emitted a plasmon and is therefore with high probability no longer coherent with the system of planes considered), and taking into account (7), we obtain an equation for $\delta\psi(\mathbf{r},\mathbf{R})$:

$$\Delta\delta\psi(\mathbf{r},\mathbf{R})+\frac{2m}{\hbar^2}[E-U_c(\mathbf{R})]\delta\psi(\mathbf{r},\mathbf{R})=\frac{2m}{\hbar^2}U_e\psi_D(\mathbf{r})\Phi_i(\mathbf{R}).$$

We now multiply both sides of this equation on the left by $\Phi_f^*(\mathbf{R})$, the complex conjugate of the wave function of the final state of the electrons in the crystal, integrate with respect to $\mathbf{R}$ and thus obtain

$$\Delta_r\psi_{pl}(\mathbf{r},f)+\int d\mathbf{R}\Phi_f^*(\mathbf{R})\Delta_{\mathbf{R}}\delta\psi(\mathbf{r},\mathbf{R})$$
$$+\frac{2m}{\hbar^2}\int d\mathbf{R}\Phi_f^*(\mathbf{R})[E-U_c(\mathbf{R})]\delta\psi(\mathbf{r},\mathbf{R})$$
$$=\frac{2m}{\hbar^2}\psi_D(\mathbf{r})\int d\mathbf{R}\,\Phi_f^*(\mathbf{R})U_e(\mathbf{r},\mathbf{R})\Phi_i(\mathbf{R}). \tag{8}$$

The symbols $\Delta_{\mathbf{r}}$ and $\Delta_{\mathbf{R}}$ stand for the terms of the total Laplacian operator that operate on the variables $\mathbf{r}$ and $\mathbf{R}$, respectively. The quantity

$$\psi_{pl}(\mathbf{r},f)=\int d\mathbf{R}\,\Phi_f^*(\mathbf{R})\delta\psi(\mathbf{r},\mathbf{R})$$

is the probability amplitude of finding the fast electron at the point $\mathbf{r}$ and the electron subsystem of the crystal in the state f. Subsequently, in the calculation of the cross section for inelastic scattering of a fast electron we shall sum over the indices of all the final states f. For the present, however, we shall take f to be fixed. When the fast electron leaves the crystal and the interaction between the fast particle and the crystal becomes negligibly small, the function $\psi_{pl}(\mathbf{r},f)$ can be considered the wave function of a fast scattered particle which has excited the fth state of the crystal, i.e., it has excited a plasmon in the crystal.

Let us transform as follows the term in (8) involving $\Delta_{\mathbf{R}}$:

$$\int d\mathbf{R}\,\Phi_f^*(\mathbf{R})\Delta_{\mathbf{R}}\delta\psi(\mathbf{r},\mathbf{R})=\Sigma_n\int d\mathbf{R}\,\Phi_f^*(\mathbf{R})\Delta_{\mathbf{R}}\Phi_n(\mathbf{R})\psi_{pl}(\mathbf{r},n)$$
$$=-\frac{2m}{\hbar^2}\sum_n\psi_{pl}(\mathbf{r},n)\int d\mathbf{R}\Phi_f^*(\mathbf{R})[\varepsilon_n-U_c(\mathbf{R})]\Phi_n(\mathbf{R}). \tag{9}$$

Here we have used an expansion of the function $\delta\psi(\mathbf{r},\mathbf{R})$ in a complete set of orthonormal functions $\Phi_n(\mathbf{R})$ describing the various states of the crystal

$$\delta\psi(\mathbf{r},\mathbf{R})=\sum_n\psi_{pl}(\mathbf{r},n)\Phi_n(\mathbf{R}),$$

and used the equation

$$\Delta_{\mathbf{R}}\Phi_n(\mathbf{R})=-\frac{2m}{\hbar^2}[\varepsilon_n-U_c(\mathbf{R})]\Phi_n(\mathbf{R}).$$

Here the quantity ε_n is the energy of the crystal in the nth excited state. Substituting (9) into (8) we obtain an equation for $\psi_{pl}(\mathbf{r},f)$:

$$\Delta_r\psi_{pl}(\mathbf{r},f)+\frac{2m}{\hbar^2}(E-\varepsilon_f)\psi_{pl}(\mathbf{r},f)=\frac{2m}{\hbar^2}\psi_D(\mathbf{r})T(\mathbf{r},i\to f), \tag{10}$$

in which

$$T(\mathbf{r},i\to f)=\int d\mathbf{R}\,\Phi_f^*(\mathbf{R})U_e(\mathbf{r},\mathbf{R})\Phi_i(\mathbf{R}). \tag{11}$$

The solution of Eq. (10) has the form

$$\psi_{pl}(\mathbf{r},f)=\frac{2m}{\hbar^2}\int d\mathbf{r}_1\,G_0(\mathbf{r}-\mathbf{r}_1,E_f=E-\varepsilon_f)T(\mathbf{r}_1,i\to f)\psi_D(\mathbf{r}_1), \tag{12}$$

where the Green's function is

$$G_0(\mathbf{r}-\mathbf{r}_1,\ E_f)=-\exp(i|k'|\,|\mathbf{r}-\mathbf{r}_1|)/4\pi|\mathbf{r}-\mathbf{r}_1|, \tag{13}$$

and

$$k'=\left[\frac{2m}{\hbar^2}(E-\varepsilon_f)\right]^{1/2}$$

is the modulus of the wave vector of the scattered electron.

The asymptotic form of the solution (12) is

$$\psi_{pl}(\mathbf{r},f)=-\frac{m}{2\pi\hbar^2}\frac{e^{ik'r}}{r}\int d\mathbf{r}_1e^{-i\mathbf{k}'\mathbf{r}_1}T(\mathbf{r}_1,i\to f)\psi_D(\mathbf{r}_1),$$

so that the electron differential scattering cross section, summed over all the final states of the crystal, can be written in the form

$$d\sigma=-\frac{m^2}{4\pi^2\hbar^4}\sum_f\left|\int d\mathbf{r}\,e^{-i\mathbf{k}'\mathbf{r}}T(\mathbf{r},i\to f)\psi_D(\mathbf{r})\right|^2d\Omega. \tag{14}$$

In the subsequent discussion we shall be especially interested in the total cross section for scattering with the emission of a plasmon; this corresponds to double integration over the angles that determine by the direction of the vector $\mathbf{k}'$. This double integral is conveniently written in the form of a fourfold integral. The reduction of a double to a triple integral in the calculation of the total scattering cross section and the advantage of this procedure have been discussed in Ref. 34. This procedure corresponds to the replacement

$$d\Omega\to\left[\delta(\hbar\omega-\varepsilon_f)/m\hbar\left(k^2-\frac{2m\omega}{\hbar}\right)^{1/2}\right]$$
$$\times\delta\left(\frac{E_{\mathbf{p}}-E_{\mathbf{p}-\mathbf{Q}}}{\hbar}-\omega\right)d\omega\,d^3Q. \tag{15}$$

In this formula $\mathbf{Q}$ is the transferred momentum, E_p is the energy of the electron incident on the crystal, $\hbar\omega=\varepsilon$ is the energy transferred to the electrons of the medium, and $\mathbf{p}=\hbar\mathbf{k}$ is the momentum of the incident electron.

Keeping in mind (15), we note that the following summation over f enters into (14):

$$\sum_f \left| \int d\mathbf{r}\, e^{-i\mathbf{k}'\mathbf{r}} T(\mathbf{r}, i\to f)\psi_D(\mathbf{r}) \right|^2 \delta(\hbar\omega-\varepsilon_f)$$

$$= \int d\mathbf{r} \int d\mathbf{r}' e^{i\mathbf{k}'(\mathbf{r}'-\mathbf{r})}\psi_D(\mathbf{r})\psi_D^*(\mathbf{r}') \sum_f \langle \Phi_f | U_e(\mathbf{r},\mathbf{R}) | \Phi_i\rangle$$

$$\times \langle \Phi_i | U_e(\mathbf{r}',\mathbf{R}) | \Phi_f\rangle \delta(\hbar\omega-\varepsilon_f). \tag{16}$$

From a Lehmann expansion of the retarded and advanced boson Green's functions[1)]

$$D_R(\mathbf{r},\mathbf{r}',\omega) = \sum_f \left\{ \frac{U_{if}(\mathbf{r}')U_{fi}(\mathbf{r})}{\omega-\varepsilon_f/\hbar - is_0} - \frac{U_{if}(\mathbf{r})U_{fi}(\mathbf{r}')}{\omega+\varepsilon_f/\hbar - is_0} \right\},$$

$$D_A(\mathbf{r},\mathbf{r}',\omega) = \sum_f \left\{ \frac{U_{if}(\mathbf{r}')U_{fi}(\mathbf{r})}{\omega-\varepsilon_f/\hbar + is_0} - \frac{U_{if}(\mathbf{r})U_{fi}(\mathbf{r}')}{\omega+\varepsilon_f/\hbar + is_0} \right\}, \tag{17}$$

it can be seen that the difference of these functions has the form

$$D_R(\mathbf{r},\mathbf{r}',\omega) - D_A(\mathbf{r},\mathbf{r}',\omega) = 2\pi i \sum_f \{\langle \Phi_i | U_e(\mathbf{r}',\mathbf{R}) | \Phi_f\rangle$$

$$\times \langle \Phi_f | U_e(\mathbf{r},\mathbf{R}) | \Phi_i\rangle \delta(\omega-\varepsilon_f/\hbar) - \langle \Phi_i | U_e(\mathbf{r},\mathbf{R}) | \Phi_f\rangle$$

$$\times \langle \Phi_f | U_e(\mathbf{r}',\mathbf{R}) | \Phi_f\rangle \delta(\omega+\varepsilon_f/\hbar)\}. \tag{18}$$

Comparing (16) and (18) we conclude that

$$\sum_f \left| \int d\mathbf{r}\, e^{-i\mathbf{k}'\mathbf{r}} T(\mathbf{r}, i\to f)\psi_D(\mathbf{r}) \right|^2 \delta(\hbar\omega-\varepsilon_f)$$

$$= \int d\mathbf{r} \int d\mathbf{r}'\, e^{i\mathbf{k}'(\mathbf{r}'-\mathbf{r})}\psi_D(\mathbf{r})\psi_D^*(\mathbf{r}') \frac{D_R(\mathbf{r},\mathbf{r}',\omega) - D_A(\mathbf{r},\mathbf{r}',\omega)}{2\pi i\hbar},$$

if the integration over ω on the right hand side of (15) is carried out only for positive values of the frequency. Therefore formula (14) for the differential scattering cross section takes the form

$$d\sigma = -\frac{im}{(2\pi)^3\hbar^5(k^2-2m\omega/\hbar)^{1/2}} \int d\mathbf{r} \int d\mathbf{r}'\, e^{i\mathbf{k}'(\mathbf{r}'-\mathbf{r})}$$

$$\times \psi_D(\mathbf{r})\psi_D^*(\mathbf{r}') [D_R(\mathbf{r},\mathbf{r}',\omega) - D_A(\mathbf{r},\mathbf{r}',\omega)]$$

$$\times \delta(E_\mathbf{p} - E_{\mathbf{p}-\mathbf{Q}} - \hbar\omega)\, d^3Q\, d\omega, \tag{19}$$

where $\mathbf{k}' = \mathbf{k} - \mathbf{Q}/\hbar$ and $\omega > 0$. Therefore, in order to find the cross section for the emission of a plasmon by a diffracted electron it is necessary to know the wave function of the diffracted particle as well as the retarded and advanced Green's functions of the electric field of the electrons in the crystal.

§3. INELASTIC SCATTERING CROSS SECTION UNDER CONDITIONS OF TWO-WAVE DIFFRACTION

The wave function $\psi_D(\mathbf{r})$ of the diffracted particle can be written in the two-wave approximation in the form[10]

$$\psi_D(\boldsymbol{\rho}, z) = e^{i\mathbf{k}\mathbf{r}}[\psi_1(z) + e^{-i\mathbf{g}\boldsymbol{\rho}}\psi_2(z)]. \tag{20}$$

Here $\boldsymbol{\rho}$ and z are the components of $\mathbf{r}$ tangential and normal to the surface of the crystal. The vector $\mathbf{g}$ is a reciprocal lattice vector parallel to the surface. The functions $\psi_1(z)$ and $\psi_2(z)$ have the form

$$\psi_1(z) = \cos^2(\beta/2)\, e^{i\varkappa_1 z} + \sin^2(\beta/2)\, e^{i\varkappa_2 z},$$
$$\psi_2(z) = \sin(\beta/2)\cos(\beta/2)\,[e^{i\varkappa_2 z} - e^{i\varkappa_1 z}], \tag{21}$$

where, neglecting damping of the wave field, we have

$$\varkappa_1 = \frac{1}{2\xi_g}[w - (1+w^2)^{1/2}], \quad \varkappa_2 = \frac{1}{2\xi_g}[w + (1+w^2)^{1/2}]. \tag{22}$$

The quantity w in (22) is a parameter that describes the deviation from the exact reflecting configuration. It is related to another parameter β encountered in the theory of diffraction, and to the parameter s which describes the deviation from reflecting conditions, by the relations $w = \cot\beta$ and $w = s/\Delta k = s\xi_g$. In the exact reflecting configurations $w = 0$ and $\beta = \pi/2$. Neglect of damping of the wave field means that we are dealing either with a thin crystal or a thick crystal in which the finite coherence length is determined mainly by the excitation of electronic states of the crystal. In §4 we shall present additional arguments for the possibility in a certain sense of neglecting the damping of the wave. At present we note that from (22) it follows that $\varkappa_1 < 0$ and $\varkappa_2 > 0$ for all values of the parameter w.

Let us consider the integrals in (19) over the spatial variables. It is convenient to integrate over the coordinates in (19) separately with respect to $\boldsymbol{\rho}$ and $\boldsymbol{\rho}'$ and z and z'. Introducing the notation $\boldsymbol{\rho} - \boldsymbol{\rho}' = \boldsymbol{\rho}_1$ and taking into account (20), we rewrite (19) in the form

$$d\sigma = -\frac{im}{(2\pi)^5\hbar^5(k^2-2m\omega/\hbar)^{1/2}} \int d\mathbf{q} \int dz \int dz' \int d\boldsymbol{\rho} \int d\boldsymbol{\rho}_1$$

$$\times \exp\left[i\frac{Q_z}{\hbar}(z-z') + i\left(\frac{\mathbf{Q}_\parallel}{\hbar} - \mathbf{q}\right)\boldsymbol{\rho}_1 \right]$$

$$\times [\psi_1(z) + e^{-i\mathbf{g}\boldsymbol{\rho}}\psi_2(z)][\psi_1^*(z') + e^{i\mathbf{g}(\boldsymbol{\rho}-\boldsymbol{\rho}_1)}\psi_2^*(z')]$$

$$\times [D_R(z,z',\mathbf{q},\omega) - D_A(z,z',\mathbf{q},\omega)]$$

$$\times \delta(E_\mathbf{p} - E_{\mathbf{p}-\mathbf{Q}} - \hbar\omega)\, d^3Q\, d\omega. \tag{23}$$

The Fourier transforms $D(z,z',\mathbf{q},\omega)$ of the retarded and advanced Green's functions in (23) are defined by the transformation

$$D(\mathbf{r},\mathbf{r}',\omega) = \frac{1}{(2\pi)^2}\int d\mathbf{q}\, e^{-i\mathbf{q}(\boldsymbol{\rho}-\boldsymbol{\rho}')} D(z,z',\mathbf{q},\omega).$$

The integrals over $\boldsymbol{\rho}$ and $\boldsymbol{\rho}_1$ in (23) are now easy to do, and then one can do the integration over $\mathbf{q}$. As a result we obtain the integrated scattering cross section

$$\sigma = -\frac{imS}{(2\pi)^3\hbar^5} \int \frac{d\omega}{(k^2-2m\omega/\hbar)^{1/2}}$$

$$\times \int d\mathbf{Q}_\parallel \int dQ_z\, \delta\left(\hbar\omega - v_z Q_z - \mathbf{v}_\parallel \mathbf{Q}_\parallel + \frac{Q_z^2 + Q_\parallel^2}{2m}\right)$$

$$+ \int dz \int dz' \exp\left[\frac{iQ_z(z-z')}{\hbar}\right]$$

$$\times \left\{ \psi_1(z)\psi_1^*(z') \left[D_R\left(z,z',\frac{\mathbf{Q}_\parallel}{\hbar},\omega\right) \right.\right.$$

$$\left. - D_A\left(z,z',\frac{\mathbf{Q}_\parallel}{\hbar},\omega\right)\right] + \psi_2(z)\psi_2^*(z')$$

$$\left.\times \left[D_R\left(z,z',\frac{\mathbf{Q}_\parallel}{\hbar} - \mathbf{g},\omega\right) - D_A\left(z,z',\frac{\mathbf{Q}_\parallel}{\hbar} - \mathbf{g},\omega\right)\right]\right\}. \tag{24}$$

The quantity S in (24) is the area of the surface of the crystal. The cross terms in ψ_1 and ψ_2 do not contribute to the scattering cross section. The momentum $\mathbf{Q}$ is the momentum transferred to the entire crystal—to the lattice and to the plasmon. The wave vector $\mathbf{g}$ is parallel to the surface, so that the component Q_z of the momentum $\mathbf{Q}$ is imparted only to the electron subsystem. Since the amount of momentum typically transferred to a plasmon during "Čerenkov" generation of the plasmon is in order of magnitude equal to $\hbar\omega_p/v$, while under diffraction conditions, as we shall see below, it can be still smaller, the quantity $Q_z^2/2m$ in the argument of the δ function in (24) can be neglected. In general, the quantity $Q_\parallel^2/2m$ cannot be neglected, since its value can be of the order $\hbar^2 g^2/2m$, i.e., of the same order as the rest of the terms in the argument of the δ function. It can be seen that (24) can be generalized to the case of many-wave diffraction.

Integrating over Q_z in (24) we now obtain

$$\sigma=-\frac{imS}{(2\pi)^3\hbar^3 v_z}\int dz\int dz'\int\frac{d\omega}{(k^2-2m\omega/\hbar)^{1/2}}\int d\mathbf{u}_\parallel\{\psi_1(z)\psi_2^*(z')\times[D_R(z,z'\ \mathbf{u}_\parallel,\omega)-D_A(z,z',\mathbf{u}_\parallel,\omega)]+\psi_2(z)\psi_2^*(z')[D_R(z,z',\mathbf{u}_\parallel-\mathbf{g},\omega)-D_A(z,z',\mathbf{u}_\parallel-\mathbf{g},\omega)]\}\exp\left\{\frac{i(\omega-\mathbf{v}_\parallel\mathbf{u}_\parallel+\hbar^2 u_\parallel^2/2m)(z-z')}{v_z}\right\}. \tag{25}$$

In this formula we have introduced the new quantity $\mathbf{u}_\parallel=\mathbf{Q}_\parallel/\hbar$ in place of $\mathbf{Q}_\parallel$.

The retarded Green's function $D(z,z'z,\mathbf{u},\omega)$, corresponding to a bulk plasmon far from the boundary, can easily be obtained from the last term of formula (3.9) of Ref. 35; this term has the form

$$D_R(z,z',u,\omega)=-\frac{e^2\hbar}{\pi i}\int_{-\infty}^{+\infty}\frac{dk_1\,e^{ik_1z}P(k_1,z')}{(k_1-iu)\,\varepsilon_-(k_1,u,\omega)},\tag{26}$$

where

$$P(k_1,u,\omega,z')=\int_{-\infty}^{+\infty}\frac{dk_2\,e^{ik_2z'}\varepsilon_+(k_2,u,\omega)}{(k_2+iu)\,(k_2-k_1)},$$

and the ratio $\varepsilon_-(k_1)/\varepsilon_+(k_1)=\varepsilon(k_1,u,\omega)$ is a factorization of the dielectric function of an infinite medium in terms of the variable k_1. The function $P(z')$ contains both a spatially oscillating term proportional to $\exp(-ik_1z')$ and exponentially damping terms coming from the pole $k_2=-iu$ and the singularities of the function $\varepsilon_+(k_1)$ in the lower half-plane of the complex variable k_1. The spatially oscillating bulk part of the function $P(k_1,z')$ comes from the pole at $k_1=k_2$. It has the form

$$P_{osc}(k_1,z')=-\frac{2\pi i}{k_1+iu}e^{-ik_1z'}\,\varepsilon_+(k_1,u,\omega).\tag{27}$$

Substituting (27) into (26), we find the retarded Green's function $D_R(z,z',u,\omega)$ for bulk plasmons in an infinite medium:

$$D_R(z,z',u,\omega)=2e^2\hbar\int_{-\infty}^{+\infty}dk_1\frac{e^{ik_1(z-z')}}{(k_1^2+u^2)\,\varepsilon(k_1,u,\omega)}.\tag{28}$$

This Green's function takes into account both time and space dispersion.

The retarded and advanced Green's functions of the electromagnetic wave have arguments of the same form as the function (28) and can, of course, be written in the form of a Lehmann expansion, as was done for the functions $D_R(\mathbf{r},\mathbf{r}',\omega)$ and $D_A(\mathbf{r},\mathbf{r}',\omega)$. From the Lehmann expansion it can be seen that in this as well as in the other case these two functions differ only in the sign in front of the infinitesimally small imaginary correction to the frequency ω. Therefore, taking the damping of the plasmons to be infinitesimally small, we can write

$$\begin{aligned}D_R(z,z',\mathbf{u},\omega)-D_A(z,z',\mathbf{u},\omega)&=2e^2\hbar\int dk_1\frac{e^{ik_1(z-z')}}{(k_1^2+u^2)}\left[\frac{1}{\varepsilon(k_1,u,\omega)}-\frac{1}{\varepsilon^*(k_1,u,\omega)}\right]\\&=4ie^2\hbar\int dk_1\,e^{ik_1(z-z')}\frac{1}{(k_1^2+u^2)}\,\mathrm{Im}\frac{1}{\varepsilon(k_1,u,\omega)}.\end{aligned}\tag{29}$$

Substituting (29) into (25) and introducing the new variable $\mathbf{u}_1=\mathbf{u}-\mathbf{g}$, and designating the volume element $d\mathbf{k}_1d\mathbf{u}_1$ in wave vector space by the symbol $d\mathbf{K}$, we can write the inelastic scattering cross section σ in the form

$$\sigma=\frac{S}{2\pi^3a_Bv_z}\int dz\int dz'\int\frac{d\omega}{(k^2-2m\omega/\hbar)^{1/2}}\int\frac{dK}{K^2}\times\exp\left[i\frac{\omega-\mathbf{vK}}{v_z}(z-z')\right]\times\left\{\psi_1(z)\psi_1^*(z')+\psi_2(z)\psi_2^*(z')\times\exp\left[-i\frac{(\mathbf{vg}-\hbar g^2/2m)}{v_z}(z-z')\right]\right\}\mathrm{Im}\frac{1}{\varepsilon(K,\omega)}.\tag{30}$$

In this formula, $a_B=\hbar^2/me^2$. Let us now take the integrals over z and z'. Keeping in mind (21) we can see that in (30) there appear integrals, over the variable z, of the form

$$\int dz\,\psi_1(z)\exp\left[i\frac{(\omega-\mathbf{vK})}{v_z}z\right]=2\pi\left\{\cos^2\frac{\beta}{2}\delta\left(\varkappa_1+\frac{\omega-\mathbf{vK}}{v_z}\right)+\sin^2\frac{\beta}{2}\delta\left(\varkappa_2+\frac{\omega-\mathbf{vK}}{v_z}\right)\right\}.\tag{31}$$

Therefore the double integral in (30) over the variables z and z', containing the functions ψ_1 and ψ_1^* in the integrand can be written as

$$\left|\int dz\,\psi_1(z)\exp\left[i\frac{(\omega-\mathbf{vK})}{v_z}z\right]\right|^2=2\pi L\left[\cos^4\frac{\beta}{2}\delta\left(\varkappa_1+\frac{\omega-\mathbf{vK}}{v_z}\right)+\sin^4\frac{\beta}{2}\delta\left(\varkappa_2+\frac{\omega-\mathbf{vK}}{v_z}\right)\right].\tag{32}$$

Here L is the thickness of the crystal. Similarly, we can calculate the double integral over z and z' of the part of the integrand containing the function ψ_2. Substituting the value obtained for the integrals into (30), we find that the scattering cross section can be written in the form

$$\sigma=\frac{V}{\pi^2a_B}\int\frac{d\omega}{(k^2-2m\omega/\hbar)^{1/2}}\int\frac{dK}{K^2}$$

$$\times\left\{\cos^4\frac{\beta}{2}\delta(\omega+\varkappa_1v_z-\mathbf{vK})+\sin^4\frac{\beta}{2}\delta(\omega+\varkappa_2v_z-\mathbf{vK})\right.$$

$$+\sin^2\frac{\beta}{2}\cos^2\frac{\beta}{2}\left[\delta\left(\omega+\varkappa_2v_z-\mathbf{v}(\mathbf{K}+\mathbf{g})+\frac{\hbar g^2}{2m}\right)\right.$$

$$\left.\left.+\delta\left(\omega+\varkappa_1v_z-\mathbf{v}(\mathbf{K}+\mathbf{g})+\frac{\hbar g^2}{2mv}\right)\right]\right\}\mathrm{Im}\,\frac{1}{\varepsilon(K,\omega)}. \qquad (33)$$

Here $V=SL$ is the volume of the crystal.

We now introduce the angle ϑ, defined by the relation $\mathbf{v}\cdot\mathbf{g}=vg\cos(\pi/2-\vartheta)$. The expression $\mathbf{v}\cdot\mathbf{g}-\hbar^2g/2m$ that is contained in the argument of the last two delta functions in (33) can be expressed in terms of the angle ϑ defined above

$$\mathbf{vg}-\frac{\hbar g^2}{2m}=vg\left(\sin\vartheta-\frac{\hbar g}{2mv}\right)=vg(\sin\vartheta-\sin\vartheta_B),$$

where $\vartheta_B=\hbar g/2mv$ is the Bragg angle. Since both ϑ_B and the deviation $\Delta\vartheta=\vartheta-\vartheta_B$ from the Bragg angle are much less than unity, we have $\sin\vartheta-\sin\vartheta_B\approx\Delta\vartheta$ and

$$\mathbf{vg}-\hbar g^2/2m=vg\Delta\vartheta=vs=wU_g/\hbar=vw/\xi_g.$$

Therefore

$$\mathbf{vg}-\hbar g^2/2m=(\varkappa_1+\varkappa_2)v_z. \qquad (34)$$

In the derivation of (34) it was taken into account that v and v_z differ by an amount the order of $U_g/4mv\ll v$. Taking into account (34) and integrating over the angle variables in $\mathbf{K}$-space we obtain

$$\sigma=\frac{2V}{\pi a_B}\int\frac{d\omega}{(k^2-2m\omega/\hbar)^{1/2}}\int\frac{dK}{K}$$

$$\times\left\{\cos^4\frac{\beta}{2}\theta\left(K-\frac{|\omega+\varkappa_1v_z|}{v}\right)\right.$$

$$+\sin^4\frac{\beta}{2}\theta\left(K-\frac{\omega+\varkappa_2v_z}{v}\right)$$

$$+\sin^2\frac{\beta}{2}\cos^2\frac{\beta}{2}\left[\theta\left(K-\frac{\omega-\varkappa_1v_z}{v}\right)\right.$$

$$\left.\left.+\theta\left(K-\frac{|\omega-\varkappa_2v_z|}{v}\right)\right]\right\}\mathrm{Im}\,\frac{1}{\varepsilon(K,\omega)}. \qquad (35)$$

The θ-functions appear in (35) because the cosine of the angle between the vectors $\mathbf{v}$ and $\mathbf{K}$ must lie in the range -1 to $+1$. We also took it into account that the conditions $\varkappa_1<0$ and $\varkappa_2>0$ always hold.

Since we have already assumed infinitesimally small damping of the plasmons, we can write

$$\mathrm{Im}\,\frac{1}{\varepsilon(K,\omega)}=\frac{\pi}{2}\omega_p\delta(\omega-\omega_p)\theta(K_c-K). \qquad (36)$$

Here K_c is the limiting value of the plasmon wave vector at which strong Landau damping begins (in statistically degenerate systems) and the plasmon ceases to exist as a well defined quasiparticle. Substituting (36) into (35), integrating over $\mathbf{K}$, and changing over from the concept of an inelastic scattering cross section σ to the probability W per unit time of a transition we obtain from the usual relation $W=\sigma v/V$

$$W=\frac{\omega_p}{a_B(k^2-2m\omega_p/\hbar)^{1/2}}\left\{\cos^4\frac{\beta}{2}\ln\frac{K_cv}{|\omega_p+\varkappa_1v_z|}\right.$$

$$+\sin^4\frac{\beta}{2}\ln\frac{K_cv}{\omega_p+\varkappa_2v_z}$$

$$\left.+\sin^2\frac{\beta}{2}\cos^2\frac{\beta}{2}\left[\ln\frac{K_cv}{\omega_p-\varkappa_1v_z}+\ln\frac{K_cv}{|\omega_p-\varkappa_2v_z|}\right]\right\}. \qquad (37)$$

Going from σ to W makes sense, since the generation of plasmons occurs in the bulk of the single crystal, far from the surface.

The transition probability (37) can be represented in the form

$$W=W_0F(\beta), \qquad (38)$$

where

$$W_0=\frac{\omega_p}{a_B(k^2-2m\omega_p/\hbar)^{1/2}}\ln\frac{vKc}{\omega_p} \qquad (39)$$

is the probability of plasmon excitation in a homogeneous electron gas and the function $F(\beta)$ describes the orientation effect. Deviation of the function F is different from unity corresponds in fact to existence of an orientation effect.

The form of the function $F(\beta)$ is clear from a comparison of (39) and (37), but to exhibit the physical meaning of these terms, it is helpful to write the function in a special form. To do so we shall transform the expression in the curly brackets in (37) in the following way:

$$\left\{\cos^4\frac{\beta}{2}\ln\frac{K_cv}{|\omega_p+\varkappa_1v_z|}+\sin^4\frac{\beta}{2}\ln\frac{K_cv}{\omega_p+\varkappa_2v_z}\right.$$

$$\left.+\sin^2\frac{\beta}{2}\cos^2\frac{\beta}{2}\left[\ln\frac{K_cv}{\omega_p-\varkappa_1v_z}+\ln\frac{K_cv}{|\omega_p-\varkappa_2v_z|}\right]\right\}=\ln\frac{K_cv}{\omega_p}$$

$$+\cos^2\frac{\beta}{2}\left[\cos^2\frac{\beta}{2}\ln\frac{1}{|1+\varkappa_1v_z/\omega_p|}\right.$$

$$\left.+\sin^2\frac{\beta}{2}\ln\frac{1}{|1-\varkappa_2v_z/\omega_p|}\right]$$

$$-\sin^2\frac{\beta}{2}\left[\sin^2\frac{\beta}{2}\ln\left(1+\frac{\varkappa_2v_z}{\omega_p}\right)+\cos^2\frac{\beta}{2}\ln\left(1-\frac{\varkappa_1v_z}{\omega_p}\right)\right].$$

This allows the quantity $F(\beta)-1$, which describes the orientation effect and vanishes in the case of an isotropic medium, to be written in the form

$$F(\beta)-1=\frac{1}{\ln(vK_c/\omega_p)}\left\{\cos^2\frac{\beta}{2}\left[\cos^2\frac{\beta}{2}\ln\frac{1}{|1+\varkappa_1v_z/\omega_p|}\right.\right.$$

$$\left.+\sin^2\frac{\beta}{2}\ln\frac{1}{|1-\varkappa_2v_z/\omega_p|}\right]$$

$$\left.-\sin^2\frac{\beta}{2}\left[\sin^2\frac{\beta}{2}\ln\left(1+\frac{\varkappa_2v_z}{\omega_p}\right)+\cos^2\frac{\beta}{2}\ln\left(1-\frac{\varkappa_1v_z}{\omega_p}\right)\right]\right\}. \qquad (40)$$

§4. ANALYSIS OF THE EXPRESSION FOR THE PROBABILITY OF INELASTIC SCATTERING OF FAST PARTICLES DURING DIFFRACTION

The most important feature of the function $F(\beta)$, which describes the orientational dependence of the transition probability per unit time, is the presence of logarithms whose arguments and the coefficients depend on the parameter β that characterizes the deviation of the beam of incident particles from the exact reflecting configuration. The function $F(\beta)$ and, even better, the function $F(\beta)-1$, can be conveniently be written so that this dependence becomes explicit. Since

$$\frac{\varkappa_1 v}{\omega_p}=\frac{U_g}{2\hbar\omega_p}[w-(1+w^2)^{1/2}]=-\frac{U_g}{2\hbar\omega_p}\operatorname{tg}\frac{\beta}{2}$$

and

$$\frac{\varkappa_2 v}{\omega_p}=\frac{U_g}{2\hbar\omega_p}\operatorname{ctg}\frac{\beta}{2},$$

the function $F-1$ depends explicitly on β in the following way:

$$F(\beta)-1=\frac{1}{\ln(vK_c/\omega_p)}\left\{\cos^4\frac{\beta}{2}\ln\frac{1}{|1-f_g\operatorname{tg}(\beta/2)|}+\sin^4\frac{\beta}{2}\ln\frac{1}{|1+f_g\operatorname{ctg}(\beta/2)|}+\sin^2\frac{\beta}{2}\cos^2\frac{\beta}{2}\ln\frac{1}{|[1-f_g\operatorname{ctg}(\beta/2)][1+f_g\operatorname{tg}(\beta/2)]|}\right\}. \tag{41}$$

Here $f_g=U_g/2\hbar\omega_p$. This parameter depends on the nature of the single crystal. For some typical crystals $f_g<1$, but the case $f_g\gtrsim 1$ is apparently also realistic. In experimental investigations the quantity w is used more frequently instead of β as the parameter that takes into account the deviation from the exact reflecting condition. In this case the function $F-1$ takes on the form

$$F(w)-1=\frac{1}{4(1+w^2)\ln(vK_c/\omega_p)}\times\left\{[w+(1+w^2)^{1/2}]^2\ln\frac{1}{|1+f_g[w-(1+w^2)^{1/2}]|}+[w-(1+w^2)^{1/2}]^2\ln\frac{1}{|1+f_g[w+(1+w^2)^{1/2}]|}+\ln\frac{1}{|\{1-f_g[w+(1+w^2)^{1/2}]\}\{1-f_g[w-(1+w^2)^{1/2}]\}|}\right\}. \tag{42}$$

In order to understand better the physics of the orientation dependence of the scattering cross section, let us consider formula (35). The θ-functions in (35) determine the minimal wave vector that the emitted plasmons can have. Since $\varkappa_1<0$, the first term in (35) corresponds to the generation of plasmons with wave vector $K_{\min}<\omega_p/v$. The same applies to the last term in (35) (because of the condition $\varkappa_2>0$). From energy-momentum conservation in an isotropic medium it follows that in the "Čerenkov" generation of plasmons, only such plasmons for which the wave vector is greater than or equal to ω_p/v can be emitted.

The fact that formula (35) describes the generation of long-wavelength plasmons cannot be explained simply by the deviation of the magnitudes of the wave vectors $\mathbf{k}^{(1,2)}$ of the plane waves that comprise the function ψ_D from the wave vector $\mathbf{k}$ of a fast particle of the same energy in an isotropic medium. This latter circumstance could lead to a situation where the minimal wave vector of a plasmon generated by a fast particle in a state described by each of the above-mentioned plane waves would not be equal to ω_p/v. In this case

$$K_{min}\geqslant\frac{\omega_p}{v^{(1,2)}}=\frac{\omega_p}{v\left\{1+\dfrac{\hbar}{2mv\xi_g}[w\pm(1+w^2)^{1/2}]\right\}}=\frac{\omega_p}{v}-\frac{\hbar\omega_p}{4E_p\xi_g}[w\pm(1+w^2)^{1/2}].$$

The presence of the small factor $\hbar\omega_p/E_p$ in front of the function $[w\pm(1+w^2)^{1/2}]/4\xi_g$ in this formula means that $K_{\min}$ is essentially unchanged as a result of simply a renormalization of the wave vector of the fast particle in the anisotropic medium.

The substantial change of $K_{\min}$ compared to ω_p/v, which follows from (35) and which leads to the emission of long-wavelength plasmons with $K<\omega_p/v$, is due to a phenomenon that might be called plasmon bremsstrahlung in an anisotropic medium. This phenomenon is associated with the exchange of momentum between the crystal lattice and the fast particle that generates the plasmon. That part of the function $F(w)$ which is due to bremsstrahlung of a longitudinal electromagnetic wave has the form

$$F_{brems}(w)=\frac{1}{\ln(vK_c/\omega_p)}\left\{\cos^4\frac{\beta}{2}\int_0^{\omega_p/v}\frac{dK}{K}\theta\left(K-\left|\varkappa_1+\frac{\omega_p}{v}\right|\right)+\sin^2\frac{\beta}{2}\cos^2\frac{\beta}{2}\int_0^{\omega_p/v}\frac{dK}{K}\theta\left(K-\left|\varkappa_2-\frac{\omega_p}{v}\right|\right)\right\}$$
$$=\frac{[w+(1+w^2)^{1/2}]^2}{4(1+w^2)\ln(vK_c/\omega_p)}\left\{\frac{[w+(1+w^2)^{1/2}]^2}{4(1+w^2)}\theta[1-|1+f_g(w-(1+w^2)^{1/2})|]\ln\frac{1}{|1+f_g(w-(1+w^2)^{1/2}]|}+\frac{[w-(1+w^2)^{1/2}]^2}{4(1+w^2)}\times\theta\{1-|1-f_g[w+(1+w^2)^{1/2}]|\}\ln\frac{1}{|1-f_g[w+(1+w^2)^{1/2}]|}\right\}. \tag{43}$$

The concept we have introduced of bremsstrahlung of a longitudinal electromagnetic wave the term "bremsstrahlung" stands for generation of plasmons with wave vectors from $K_{\min}$ to ω_p/v. The existence of a lattice also has an influence on the emission of plasmons with $K>\omega_p/v$, which in principle can be generated by the "Čerenkov" mechanism also in the absence of a lattice. The total difference between the corresponding part of the scattering cross section and that due to the "Čerenkov" mechanism we shall call the density effect. In this definition, the density effect can, depending on the nature of the interaction between the fast particle and the lattice, lead not only to a decrease but also to an increase in the probability of emitting a plasmon of a given wavelength. We shall see below that the sign of the density effect actually depends on the value of the parameter of deviation from the exact reflecting configuration.

The presence of the logarithms in (40) and (42) leads to a logarithmic divergence in the inelastic scattering cross section for $\varkappa_1 = -\omega_p/v$ and $\varkappa_2 = \omega_p/v$. This divergence is due precisely to the possibility of generation of very long wavelength plasmons at the corresponding values of β (or w). This resonance due to bremsstrahlung of plasmons, in the integrated inelastic scattering cross section can be called plasmon-diffraction resonance. From (41), (42) or (43) it can be seen that the condition $\varkappa_1 = -\omega_p/v$ is satisfied for

$$\beta=2\,\mathrm{arctg}\,(1/f_g).$$

Since $w = \cot\beta$, the condition for the existence of a resonance takes the form

$$w=\mathrm{ctg}\left(2\,\mathrm{arctg}\frac{1}{f_g}\right)=\frac{f_g^2-1}{2f_g}=\frac{U_g}{4\hbar\omega_p}-\frac{\hbar\omega_p}{U_g}. \tag{44}$$

Similarly, we obtain $\varkappa_2 = \omega_p/v$ for $\beta = 2\arctan(1/f_g)$, or

$$w=\mathrm{ctg}\left(2\,\mathrm{arcctg}\frac{1}{f_g}\right)=\frac{f_g}{2}\left(\frac{1}{f_g^2}-1\right)=\frac{\hbar\omega_p}{U_g}-\frac{U_g}{4\hbar\omega_p}. \tag{45}$$

The function $\cos^4(\beta/2)$ in front of the corresponding logarithm is, in case (45), equal to

$$\frac{f_g^4}{(1+f_g^2)^2}=\frac{U_g^4}{(U_g^2+4\hbar^2\omega_p^2)^2}. \tag{46}$$

The quantity $\sin^2(\beta/2)\cos^2(\beta/2)$ at resonance (44) is equal to

$$4U_g^2(\hbar\omega_p)^2/(U_g^2+4\hbar^2\omega_p^2)^2. \tag{47}$$

The ratio of (46) to (47) is $(U_g/2\hbar\omega_p)^2$. Therefore the value of the quantity f_g^2 is determined by which of the two scattering cross section resonances is more pronounced. This same quantity also determines the position of the resonance on the w axis. The positions of the two resonances are symmetric relative to the exact reflecting configuration. However, an asymmetry in the line shapes of these two resonances is due to the fact that, as can be seen from the formulas that have been derived, plasmons can be emitted in these two cases by an electron that is predominantly either in a wave of type I or in a wave of type II. Usually a wave of type II interacts with the lattice more strongly than a wave of type I on account of the known localization of these waves; this enhances both the bremsstrahlung of plasmons and the density effect in the emission of plasmons.

From a comparison of (42) and (43) it can be seen that the function $F(w) - 1$ has resonances at the same values of w as the function $F_{\rm brems}(w)$. The form of these functions is given in Fig. 1 for various values of the parameter f_g. It can be seen that the sharpness of the resonance depends on the value of f_g. There is also a tendency towards an increase in the nonresonant part of the plasmon bremsstrahlung with increasing deviation parameter w. For negative w the density effect is dominant everywhere except at the resonance point and supresses the generation of plasmons. Therefore, the peak of the plasmon-diffraction resonance for $w<0$ is very narrow and sharp, almost like a δ function. For positive values of w the density effect can give an additional contribution to W, i.e., the density effect and bremsstrahlung in this case increase the probability of plasmon generation in comparison with the generation that would occur in the case of a homogeneous electron gas.

Let us discuss finally the possibility of experimental observation of the plasmon-diffraction resonance. Since the resonances are rather peaked, their observation requires a definite accuracy in the determination of the mutual orientation of the crystal and the beam of fast particles. We assume that the accuracy of the orientation of the beam relative to the exact resonance configuration is $\pm\Delta w$. We introduce the quantity

$$M=\frac{S_1}{S_1+S_2}=\int\limits_{w_0-\Delta w}^{w_0+\Delta w} dw[F(w)-1]\Big/\int\limits_{w_0-\Delta w}^{w_0+\Delta w} dwF(w), \tag{48}$$

which gives the ratio of the area under the part of the curve

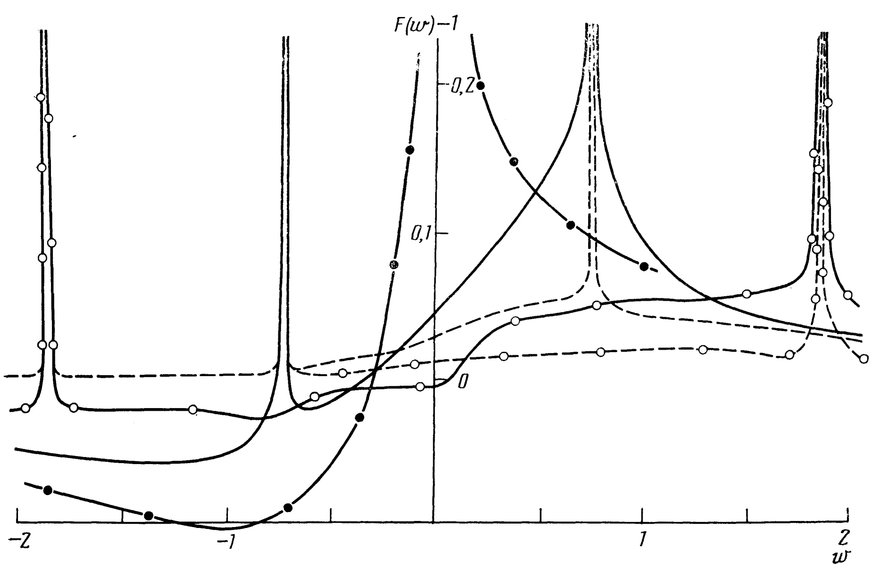

FIG. 1. The quantity $F-1$, as a function of w, the parameter of deviation from exact reflecting configuration, for $E_p = 20$ keV and for various values of the parameter f_g, is shown by the solid line. The solid curve without additional symbols on it corresponds to $f_g = 0.5$. The resonances at $w = \pm 0.75$ correspond to this value of f_g. The resonance at $w = +0.75$ is broad and the resonance at $w = -0.75$ is very peaked. The dashed lines show the function $F_{\rm brems}$ for various f_g. It can be seen that for $f_g = 0.5$ in the region $w \approx -0.75$ the density effect, which inhibits the emission of plasmons, is large. The solid and dashed curves with open points were plotted for $f_g = 0.25$; the solid curve with the black points was plotted for $f_g = 1.0$.

$F(w)$ defined by formula (42), for $F>1$, to the area under the entire curve, i.e., for all values of F. The quantity w_0 in (48) characterizes the exact resonant value of the parameter w. From the definition (48) it follows, in particular, that $S_2=2\Delta w$. It is also clear that if the resonance had an exact δ-function form, then $M\to 1$ as $\Delta w\to 0$. Evaluation of (48) with the use of (42) gives

$$M\approx\left\{1+\frac{\ln(vK_c/\omega_p)}{f_g^2[2+\ln(1/f_g\Delta w)]}\right\}^{-1}. \tag{49}$$

To estimate this expression we use the fact that $\ln(vK_c/\omega_p)\approx 4$. We take the parameter f_g equal to 0.25. By choosing $f_g=0.25$ we have chosen the case of sharp resonances, which in some sense are the most complicated for experimental observation. In this case we have $M=0.111$, i.e., the effect is quite observable for $\Delta w\approx 0.1$. In other words, to observe the effect at the chosen values of v and f_g^2 it is sufficient that w be determined with such accuracy that Δw is between 0.01 and 0.1. As far as we know this accuracy in the determination of Δw, in any case, is within the possibilities of present day experiments.

In conclusion we note that the actual resonances in the scattering cross section obviously will not be infinitely high. In thin crystals their height will be determined by the thickness of the crystal. In thick crystals it will be dependent on the damping of the wave field of the fast particles as they penetrate into the crystal and possibly dependent also on the effect of the orientational dependence of the surface reaction channels on the bulk channel considered in this investigation. This question should be the topic of a separate investigation. We can suppose, however, that since the resonances have a logarithmic, i.e., an integrable, character, and allowance for the finite height of the resonances in the calculation of the integrated scattering cross section will lead to comparatively small corrections.

[1)]In this paper the Fourier transform is defined in the following way:

$$D(\omega)=\int_{-\infty}^{+\infty} D(t)e^{-i\omega t}\,dt.$$

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