

REFLECTANCE OF ALLOYED SEMICONDUCTORS IN THE INFRARED REGION

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The reflectance of semiconductors is calculated on the basis of the model of free electrons (holes) interacting with "randomly" distributed scattering centers. The parameters of the scattering mechanism are introduced into the theory phenomenologically. An explicit expression for the conductivity of the system is obtained for any frequency of the external field.

1. INTRODUCTION

THE optical properties of alloyed semiconductors in the infrared region of the spectrum lying beyond the edge of the main absorption band (on the side of longer wavelengths) are due essentially to the behavior of the system of free carriers in the external field. Nonselective absorption observed in this region is attributed to the intraband transitions of electrons in the conduction band and of holes in the valence band.

Measurements of the reflectance R

$$R = \frac{(n-1)^2 + \kappa^2}{(n+1)^2 + \kappa^2} \quad (1)$$

where n and κ are respectively the refractive index and the absorption coefficient, point to the presence of a minimum in this region. With increasing free-carrier density, this minimum shifts towards longer wavelengths^[1]. By measuring the frequency at which the minimum of the reflectance takes place it is possible to calculate the effective mass of the free carriers^[2].

The optical coefficients n and κ are determined by the relation

$$n + i\kappa = \left[\epsilon + i \frac{4\pi}{\omega} \sigma(\omega) \right]^{1/2}. \quad (2)$$

Here ϵ is the dielectric constant of the medium, measured at very high frequencies, without allowance for the contribution of the free carriers, ω is the angular frequency of the external field, and $\sigma(\omega)$ is the conductivity.

Thus, a determination of these coefficients involves calculation of the conductivity as a function of the frequency. In practical calculations it is customary to introduce the assumption of the existence of a frequency-independent relaxation time, which in the case of the "plasma" model leads to the classical expression

$$\sigma(\omega) = \frac{e^2 n_e \tau}{m} \frac{1}{1 - i\omega\tau}, \quad (3)$$

where e , n_e , and m are respectively the charge, density, and effective mass of the free carriers. It is well known, however, that this expression for the conductivity still does not explain the optical properties of the materials in the spectral region under consideration, and it is customary to introduce into consideration extraneous factors, such as the interaction between the radiation and the lattice, the influence of induced interband transitions, etc. However, disregarding the influence of these factors and investigating the optical properties of the system of free carriers in itself, the validity of the assumed independence of the relaxation

time of the frequency is more than just doubtful. This is also indicated by measurements of the reflectance of pure metals^[3], where the free-electron model is a good approximation. The authors of that paper believe that the decrease of reflectance observed in the infrared region is due to the frequency dependence of the relaxation time of the system.

In the present paper we present a calculation of the electric conductivity of a system of free carriers interacting with "randomly" arranged scattering centers. The potential of the scatterers, which may be, for example, impurities or inhomogeneities of the crystal structure, are introduced into the theory phenomenologically, by "joining together" at the low-frequency limit ($\omega\tau \ll 1$) the obtained expression for the conductivity with the dc conductivity $\sigma = e^2 n_e \tau / m$. This could be done by assuming that the scatterers have a short-range potential. The latter assumption is perfectly valid, if account is taken of the screening of the scattering centers. We note, however, that the dc relaxation time which enters in our expression for the conductivity is only a phenomenological parameter. Nowhere do we assume that the relaxation time is independent of the frequency, as is done in the classical theory.

We assume that the carrier mean free path is much smaller than the depth of penetration of the field, and calculate the response of the system to external radiation in the long-wave limit. Thus, in spite of the fact that we are considering a rather wide range of frequencies, for which $\omega\tau \ll 1$ in the low-frequency region and $\omega\tau \gg 1$ in the high-frequency region, the periodic external field

$$E(\mathbf{r}, t) = E e^{-i\omega t} \quad (4)$$

is assumed by us to be homogeneous in space.

The present model has been considered in many papers. So far, however, the solution of the problem was confined to two limiting cases of low and very high frequencies. A distinguishing feature of our approach is the possibility of obtaining results for the entire spectrum, including frequencies for which $\omega\tau \sim 1$.

The applicability of the model under consideration to a description of the optical properties of alloyed semiconductors is bounded on the high-frequency side by the main absorption edge. At these frequencies another absorption mechanism begins to prevail, namely interband transitions. Therefore the model of the free carriers is no longer consistent here, although

our calculation is valid within the framework of the model in question even at higher frequencies.

In Sec. 2 we derive a transport equation, on the basis of which we calculate in Sec. 3 the conductivity of the system. Starting from the obtained expression for the conductivity, we calculate, using (2), the reflectance (1). Section 4 is devoted to a discussion of the results.

2. TRANSPORT EQUATION

We consider a model in which the free carriers, which obey Fermi statistics, interact with randomly disposed scattering centers under the influence of an external periodic electric field. The carriers, which can be either electrons or holes, will be referred to for brevity as electrons, and will be assigned a charge e , an effective mass m , and a density n_e . The external electric field $\mathbf{E}(t)$ is by assumption homogeneous in space. The scattering centers are distributed with a density N and have a mass M that exceeds greatly the mass of the electrons ($M \gg m$), and therefore can be regarded as stationary in the time scale of the field variation. Their interaction with the external field will thus be neglected. In view of the fact that the electrons do not interact with one another (or else interact in the Hartree-Fock approximation, which is manifest in their effective mass), it is possible to investigate the response of the system to an external field with the aid of the single-particle density matrix ρ .

The total Hamiltonian of the system consists thus of three parts:

- a) The kinetic energy of the electron

$$H_e = p^2 / 2m, \quad (5)$$

where \mathbf{p} denotes the momentum.

- b) The energy of interaction between the electron and the scattering centers

$$V = \sum_{i=1}^N \varphi(\mathbf{r} - \mathbf{r}_i). \quad (6)$$

Here $\varphi(\mathbf{r} - \mathbf{r}_i)$ is the interaction between the electron whose radius vector is \mathbf{r} , and the i -th scattering center located at the point \mathbf{r}_i . The summation is over all the scatterers $i = 1, \dots, N$.

- c) The energy of interaction with the external electric field

$$H_F = -e\mathbf{E}(t)\mathbf{r}. \quad (7)$$

The method of deriving the transport equation for the system in question was developed by Kohn and Luttinger^[4] who, however, confined themselves to low-frequency external fields ($\omega\tau \ll 1$). Our calculation of the electric conductivity of the system will be based on a transport equation obtained, following their method and generalizing their approach, by one of us earlier^[5]. Using the eigenfunctions of the kinetic energy operator normalized in the volume Ω ($\hbar = 1$)

$$\Psi_p = \frac{1}{\sqrt{\Omega}} e^{i\mathbf{p}\mathbf{r}}, \quad (8)$$

and satisfying the equation

$$H_e \Psi_p = \varepsilon_p \Psi_p \quad (9)$$

with eigenvalues

$$\varepsilon_p = p^2 / 2m, \quad (10)$$

we denote the diagonal elements of the density matrix in this representation by f_p . We now represent the distribution function f_p in the form

$$f_p = f_p^{(0)} + f_p^{(1)}, \quad (11)$$

where the symbol ⁽⁰⁾ denotes terms that do not depend on the field $\mathbf{E}(t)$, and ⁽¹⁾ denotes the terms proportional to the field. We have^[5]

$$\begin{aligned} & -i\omega f_p^{(1)} + e\mathbf{E} \frac{\partial}{\partial \mathbf{p}} f_p^{(0)} \\ = & e \frac{N}{\Omega} \sum'_k |\varphi_k|^2 \left(\frac{1}{\omega_{p+k,p} - \omega - i\eta} + \frac{1}{\omega_{p+k,p} + \omega + i\eta} \right) \mathbf{E} \frac{\partial}{\partial \mathbf{p}} \frac{f_{p+k}^{(0)} - f_p^{(0)}}{\omega_{p+k,p}} \\ & - i \frac{N}{\Omega} \sum'_k |\varphi_k|^2 \left(\frac{1}{\omega_{p+k,p} - \omega - i\eta} - \frac{1}{\omega_{p+k,p} + \omega + i\eta} \right) (f_{p+k}^{(1)} - f_p^{(1)}), \end{aligned} \quad (12)$$

Here $\omega_{p,k} = \varepsilon_p - \varepsilon_k$, and the primed sums do not contain terms with $k = 0$. Since the time dependence of the functions $f^{(1)}$ and $\mathbf{E}(t)$,

$$\mathbf{E}(t) = \mathbf{E} \exp \{-i(\omega + i\eta)t\} \quad (13)$$

(adiabatic application of the external field) is the same, (12) contains the time-independent function $f^{(1)}$ (for convenience we retain for it the same symbol as before), which is proportional to the amplitude of the external electric field \mathbf{E} .

Equation (12) describes the linear response for the system to external fields of any frequency. Its derivation is based on the following two assumptions: a) the off-diagonal elements of the single-particle density matrix are small compared with the diagonal ones; b) the time between two succeeding collisions greatly exceeds the duration of each of the collisions. This transport equation will serve as the starting point for the calculation of the electric conductivity and hence the reflectance of the system.

3. ELECTRIC CONDUCTIVITY

A solution of the transport equation (12) for $f_p^{(1)}$ can be found only in two limiting cases: $\omega\tau \ll 1$ ^[4] and $\omega\tau \gg 1$ ^[5]. However, knowledge of these solution is not sufficient in our case, unfortunately, since the infrared region of interest to us contains frequencies for which the condition $\omega\tau \sim 1$ may be satisfied (the dc relaxation time in a semiconductor varies with the carrier density over a rather broad range). Therefore, being unable to solve Eq. (12) in general form, we proceed to consider its current moment. By the same token, we forgo a determination of the distribution function for the entire frequency spectrum. The latter, in fact, is not our main purpose. We are interested in determining the conductivity at any frequency, for which it is sufficient to find an equation for the current density induced in the system by the external field.

To this end, starting from the definition of the current density \mathbf{j} ,

$$\mathbf{j}(\omega) = \frac{e}{m} \int \frac{d^3p}{(2\pi)^3} \mathbf{p} f_p^{(1)}, \quad (14)$$

we multiply (12) by $e\mathbf{p}/m$ and sum it over the momenta, changing over at the same time from summation to integration in accordance with the scheme

$$\frac{1}{\Omega} \sum_p \rightarrow \int \frac{d^3p}{(2\pi)^3}.$$

The left side of (12), with allowance for the equality

$$\frac{e^2}{m} \int \frac{d^3p}{(2\pi)^3} \mathbf{p} \left(\mathbf{E} \frac{\partial}{\partial \mathbf{p}} \right) f_{\mathbf{p}}^{(0)} = -\frac{e^2 n_e}{m} \mathbf{E}, \quad (15)$$

can be readily transformed, and we obtain

$$\begin{aligned} -i\omega \mathbf{j}(\omega) - \frac{e^2 n_e}{m} \mathbf{E} &= \frac{e^2 N}{m} \int \frac{d^3p}{(2\pi)^3} \mathbf{p} \int \frac{d^3k}{(2\pi)^3} |\varphi_{\mathbf{k}}|^2 \left(\frac{1}{\omega_{\mathbf{p}+\mathbf{k},\mathbf{p}} - \omega - i\eta} \right. \\ &+ \frac{1}{-\omega_{\mathbf{p}+\mathbf{k},\mathbf{p}} + \omega + i\eta} \left. \right) \left(\mathbf{E} \frac{\partial}{\partial \mathbf{p}} \right) \frac{f_{\mathbf{p}+\mathbf{k}}^{(0)} - f_{\mathbf{p}}^{(0)}}{\omega_{\mathbf{p}+\mathbf{k},\mathbf{p}}} - i \frac{eN}{m} \int \frac{d^3p}{(2\pi)^3} \mathbf{p} \int \frac{d^3k}{(2\pi)^3} |\varphi_{\mathbf{k}}|^2 \\ &\times \left(\frac{1}{\omega_{\mathbf{p}+\mathbf{k},\mathbf{p}} - \omega - i\eta} - \frac{1}{\omega_{\mathbf{p}+\mathbf{k},\mathbf{p}} + \omega + i\eta} \right) (f_{\mathbf{p}+\mathbf{k}}^{(1)} - f_{\mathbf{p}}^{(1)}). \quad (16) \end{aligned}$$

The second term of the right side of this equation still contains the unknown functions $f_{\mathbf{p}}^{(1)}$. In order to eliminate them both here and in the left side with the aid of (14), and thus obtain an equation for the current, it is necessary to make two assumptions. The first is based on the premise that the scatterers have a short-range potential. It can be concluded hence that its Fourier transform $\varphi_{\mathbf{k}}$ will have a weak dependence on \mathbf{k} . We neglect this dependence and approximate $\varphi_{\mathbf{k}}$ by a certain constant φ_0 . This is equivalent to assuming that the scattering mechanism under consideration represents elastic collisions of electrons with pointlike scatterers (potential represented by a δ -function). Noting, in addition, that in order to determine the current in accord with (14) it is sufficient to know the antisymmetrical part of $f_{\mathbf{p}}^{(1)}$ (with respect to \mathbf{p}), we represent the last term of (16), following simple transformations, in the form

$$i \frac{e}{m} \int \frac{d^3p}{(2\pi)^3} \mathbf{p} f_{\mathbf{p}}^{(1)} I(\varepsilon_{\mathbf{p}}, \omega), \quad (17)$$

where

$$I(\varepsilon_{\mathbf{p}}, \omega) = N |\varphi_0|^2 \int \frac{d^3k}{(2\pi)^3} \left(\frac{1}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{p}} - \omega - i\eta} - \frac{1}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{p}} + \omega + i\eta} \right). \quad (18)$$

Our second assumption is that $I(\varepsilon_{\mathbf{p}}, \omega)$ in the integrand of (17) can be replaced by its value for the Fermi energy $\varepsilon_{\mathbf{F}}$. This is based on the fact that at high frequencies the left side of (12) is a small quantity compared with the right side, and in first approximation we have

$$f_{\mathbf{p}}^{(1)} = -i \frac{e}{\omega} \mathbf{E} \frac{\partial}{\partial \mathbf{p}} f_{\mathbf{p}}^{(0)}. \quad (19)$$

For a Fermi distribution function

$$f_{\mathbf{p}}^{(0)} = \left\{ \exp \left[\frac{1}{k_{\mathbf{B}} T} (\varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{F}}) \right] + 1 \right\}^{-1}, \quad (20)$$

where $k_{\mathbf{B}}$ is Boltzmann's constant, at sufficiently low temperatures (including room temperature, under the condition that $k_{\mathbf{B}} T \ll \varepsilon_{\mathbf{F}}$), expression (19) will contain $\delta(\varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{F}})$. This is also the situation at low frequencies, $\omega \ll \varepsilon_{\mathbf{F}}$, although for an entirely different reason. In this case, owing to the Pauli principle, the dominant contribution to the current induced by the radiation is made by electrons in the immediate vicinity of the Fermi level. Thus, averaging the integral in a definite sense, we obtain for the final form of the term of (17) in question

$$i I(\varepsilon_{\mathbf{F}}, \omega) \mathbf{j}(\omega). \quad (21)$$

Taking into account the assumption made concerning the distribution function (20), i.e., assuming that

$\partial f_{\mathbf{p}}^{(0)} / \partial \varepsilon_{\mathbf{p}} \sim -\delta(\varepsilon_{\mathbf{p}} - \varepsilon_{\mathbf{F}})$, we represent the remaining term of (16) (the first one on the right side), after simple transformations, in the form

$$\frac{e^2 n_e}{m\omega} [I(\varepsilon_{\mathbf{F}}, \omega) + F(\varepsilon_{\mathbf{F}}, \omega)] \mathbf{E}. \quad (22)$$

Here

$$F(\varepsilon_{\mathbf{F}}, \omega) = \frac{1}{m\omega} \frac{N}{n_e} \frac{|\varphi_0|^2}{6\pi^4} \int_0^{\infty} dk \cdot k^2 [Q_{\mathbf{k}}(\varepsilon_{\mathbf{F}}, \omega) - Q_{\mathbf{k}}(\varepsilon_{\mathbf{F}}, 0)], \quad (23)$$

where

$$Q_{\mathbf{k}}(\varepsilon_{\mathbf{F}}, \omega) = \int_0^{\infty} dp \cdot p^2 (p^2 + k^2) \frac{f_{\mathbf{k}}^{(0)} - f_{\mathbf{p}}^{(0)}}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{p}} - \omega - i\eta}. \quad (24)$$

(The electron density n_e is connected with the Fermi energy by the relation $n_e = (2m\varepsilon_{\mathbf{F}})^{3/2} / 3\pi^2$.)

Now taking (21) and (22) into consideration, we rewrite (16) in the form

$$-i\omega \mathbf{j}(\omega) - \frac{e^2 n_e}{m} \mathbf{E} = \frac{e^2 n_e}{m\omega} [I(\varepsilon_{\mathbf{F}}, \omega) + F(\varepsilon_{\mathbf{F}}, \omega)] \mathbf{E} + i I(\varepsilon_{\mathbf{F}}, \omega) \mathbf{j}(\omega). \quad (25)$$

This equation makes it possible to express the current induced in the system by the external field in terms of the functions $I(\varepsilon_{\mathbf{F}}, \omega)$ and $F(\varepsilon_{\mathbf{F}}, \omega)$, determined by (18) and (23) respectively. Whence, according to

$$\mathbf{j}(\omega) = \sigma(\omega) \mathbf{E},$$

follows directly an expression for the conductivity

$$\sigma(\omega) = \sigma^{(0)}(\omega) \left[1 + \frac{F(\varepsilon_{\mathbf{F}}, \omega)}{\omega + I(\varepsilon_{\mathbf{F}}, \omega)} \right], \quad (26)$$

where $\sigma^{(0)}(\omega)$ denotes the high-frequency reactance

$$\sigma^{(0)}(\omega) = i e^2 n_e / m\omega. \quad (27)$$

The functions $I(\varepsilon_{\mathbf{F}}, \omega)$ and $F(\varepsilon_{\mathbf{F}}, \omega)$ are complex. To calculate their real and imaginary parts we shall use the formal relation

$$\frac{1}{\omega_{\mathbf{p},\mathbf{p}'} \pm i\eta} = \mathbf{P} \frac{1}{\omega_{\mathbf{p},\mathbf{p}'}} \mp i\pi \delta(\omega_{\mathbf{p},\mathbf{p}'}),$$

where \mathbf{P} means that the integral is taken in the sense of the principal value.

For the first of these functions, (18), this yields

$$\begin{aligned} I(\varepsilon_{\mathbf{F}}, \omega) &= I_1 + iI_2 = N |\varphi_0|^2 \mathbf{P} \int \frac{d^3k}{(2\pi)^3} \left(\frac{1}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{F}} - \omega} - \frac{1}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{F}} + \omega} \right) \\ &+ i\pi N |\varphi_0|^2 \int \frac{d^3k}{(2\pi)^3} [\delta(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{F}} - \omega) + \delta(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{F}} + \omega)]. \quad (28) \end{aligned}$$

Here the integrands do not depend on the direction of the vector \mathbf{k} , and consequently $d^3k = 4\pi k^2 dk = 4\pi m \sqrt{2m\varepsilon_{\mathbf{k}}} d\varepsilon_{\mathbf{k}}$, introducing the symbol $\gamma = \omega / \varepsilon_{\mathbf{F}}$, and integrating, we obtain for the real part

$$I_1(\varepsilon_{\mathbf{F}}, \omega) = \begin{cases} 0, & \text{if } \gamma \leq 1, \\ Nm_{\mathbf{p}_{\mathbf{F}}} |\varphi_0|^2 \sqrt{\gamma - 1} / 2\pi, & \text{if } \gamma \geq 1, \end{cases} \quad (29)$$

and for the imaginary part

$$I_2(\varepsilon_{\mathbf{F}}, \omega) = \frac{Nm_{\mathbf{p}_{\mathbf{F}}} |\varphi_0|^2}{2\pi} \begin{cases} \sqrt{1+\gamma} + \sqrt{1-\gamma}, & \text{if } \gamma \leq 1, \\ \sqrt{1+\gamma}, & \text{if } \gamma \geq 1. \end{cases} \quad (30)$$

Here $\mathbf{p}_{\mathbf{F}} = \sqrt{2m\varepsilon_{\mathbf{F}}}$ is the momentum corresponding to the Fermi energy.

The function $F(\varepsilon_{\mathbf{F}}, \omega) = F_1 + iF_2$ is calculated in similar fashion. Using the Fermi distribution function (20) at absolute zero, we obtain for the imaginary part

$$F_2(\varepsilon_{\mathbf{F}}, \omega) = -\frac{Nm_{\mathbf{p}_{\mathbf{F}}} |\varphi_0|^2}{3\pi\gamma} \begin{cases} (1+\gamma)^{3/2} - (1-\gamma)^{3/2}, & \text{if } \gamma \leq 1 \\ (1+\gamma)^{3/2}, & \text{if } \gamma \geq 1 \end{cases} \quad (31)$$

To calculate the real part, F_1 , it is best to use the dispersion relation

$$F_1(\epsilon_F, \omega) = \frac{1}{\pi} P \int_{-\infty}^{+\infty} \frac{F_2(\epsilon_F, \omega')}{\omega' - \omega} d\omega', \quad (32)$$

the existence of which can in our case be easily verified by direct substitution. As a result we get

$$F_1(\epsilon_F, \omega) = \begin{cases} 0, & \text{if } \gamma \leq 1, \\ -\frac{2Nmp_F |\varphi_0|^2}{3\pi\gamma} (\gamma - 1)^{3/2}, & \text{if } \gamma \geq 1. \end{cases} \quad (33)$$

The dependence of the conductivity on the frequency is determined by substituting the functions $I(\epsilon_F, \omega)$ and $F(\epsilon_F, \omega)$ in (26). However, as can be readily seen from their explicit expressions, these functions contain $|\varphi_0|^2$, a factor due to the potential of the scatterers. Since the latter is assumed unknown in our analysis, we exclude the latter, comparing the conductivity in the low-frequency limit with the dc conductivity

$$\sigma_0 = e^2 n_e \tau / m. \quad (34)$$

As a result of this we introduce into the theory phenomenologically the quantity τ . However, unlike in the classical analysis, the relaxation time in our case is not assumed to be independent of the frequency. Its dc value, taken from experiment, is introduced here only as a numerical characteristic of the scattering mechanism.

It follows from (30) and (31) that at low frequencies, when $\gamma = \omega/\epsilon_F \rightarrow 0$,

$$I_2(\epsilon_F, 0) = -F_2(\epsilon_F, 0) = Nmp_F |\varphi_0|^2 / \pi. \quad (35)$$

On the other hand, the real parts of these functions, I_1 and F_1 , vanish identically at frequencies $\omega \leq \epsilon_F$. Accordingly, we obtain from (26)

$$\sigma(0) = \frac{e n_e}{m} \frac{\pi}{Nmp_F |\varphi_0|^2}, \quad (36)$$

and the relaxation time, according to (34), is

$$\tau = \pi / Nmp_F |\varphi_0|^2. \quad (37)$$

Finally, substituting the obtained expressions for $I(\epsilon_F, \omega)$ and $F(\epsilon_F, \omega)$ [(29), (30), (31), and (33)] in (26) and introducing the dimensionless parameter $b = \epsilon_F \tau$, we obtain for the real and imaginary parts of the conductivity $\sigma = \sigma_1 + i\sigma_2$ the following expressions:

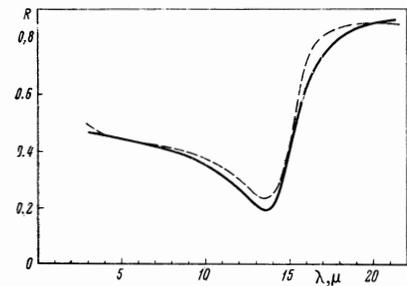
$$\sigma_1(\gamma) = \frac{1}{3\pi} \frac{\omega_p^2}{\gamma \epsilon_F} \begin{cases} \frac{b[(1+\gamma)^{3/2} - (1-\gamma)^{3/2}]}{(2b\gamma)^2 + (\sqrt{1+\gamma} + \sqrt{1-\gamma})^2}, & \text{if } \gamma \leq 1, \\ \frac{1}{2\gamma^2} \frac{\sqrt{\gamma^2 - 1} + b\gamma(\gamma+1)^{3/2}}{2b^2\gamma + 2b\sqrt{\gamma-1} + 1}, & \text{if } \gamma \geq 1, \end{cases} \quad (38)$$

$$\sigma_2(\gamma) = \frac{1}{3\pi} \frac{\omega_p^2}{\gamma \epsilon_F} \begin{cases} \frac{3(b\gamma)^2 - 1/2(1 - \sqrt{1-\gamma^2})}{(2b\gamma)^2 + (\sqrt{1+\gamma} + \sqrt{1-\gamma})^2}, & \text{if } \gamma \leq 1, \\ \frac{3}{4} \left[1 - \frac{2}{3\gamma^2} \frac{b\gamma(\gamma-1)^{3/2} + (\gamma^2+1)}{2b^2\gamma + 2b\sqrt{\gamma-1} + 1} \right], & \text{if } \gamma \geq 1, \end{cases} \quad (39)$$

where $\omega_p^2 = 4\pi e^2 n_e / m$ is the plasma frequency. The parameter b also takes into account the temperature dependence of the conductivity.

In the low-frequency limit, $\gamma = \omega/\epsilon_F \ll 1$, under the condition $b = \epsilon_F \tau \gg 1$ (which incidentally is satisfied in the majority of the practical cases), the conductivity obtained by us coincides with the classical expression (3). This can be verified by expanding the corresponding expressions (38) and (39) in powers of γ and discarding terms of order higher than the second in this expansion.

Reflectance of Single-crystal Bi_2Se_3 . The solid line is the result of the theoretical calculation, and the dashed line is the experimental curve.



4. DISCUSSION OF THE RESULTS

Comparison of the reflectance calculated by us with the experimental data is shown in the figure. The experimental curve (dashed line) is taken from^[1] and represents the reflectance of single-crystal Bi_2Se_3 at 300°K. Using the parameters given their for the material (carrier density $n_e = 2 \times 10^{19} \text{ cm}^{-3}$ and mobility $\mu = 720 \text{ cm}^2/\text{V-sec}$), we calculate our parameter $b = \epsilon_F \tau$. The relaxation time contained in it is determined from the relation

$$\mu = n_e \tau.$$

For the effective mass we assumed a value $m = 0.125m_0$, where m_0 is the mass of the free electron, in lieu of the value $m = (0.10 \pm 0.01)m_0$, which is determined in^[1] on the basis of the classical theory. Having thus determined the parameter b , we calculate from (38) and (39) the complex conductivity and find with the reflectance (1) the aid of (2).

The model considered by us is a rather crude approximation of reality. However, as can be verified from the results, it provides a fairly good qualitative description of the observed phenomena.

The minimum of the reflectance is located in the vicinity of the frequency corresponding to the energy of the Fermi level of a system of free carriers. The decrease of the concentration of the latter leads to a lowering of this level, which causes a shift of the minimum towards lower frequencies, in full agreement with experiment. In metals, where the Fermi level lies beyond the edge of the main absorption band, the observed decrease of the reflectance^[3] is apparently only part of the total picture described here.

In conclusion, it is our pleasant duty to thank Joseph Regev for help with the numerical calculations.

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