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AND DIELECTRIC LOSSES IN CRYSTALS
WITH DIPOLE-IMPURITIES**

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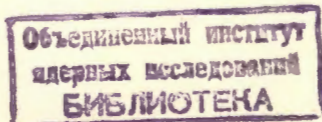
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**FREE-CARRIER ABSORPTION
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Поглощение свободными носителями и диэлектрические потери в кристаллах при рассеянии на диполях

В однозонном изотропном приближении метода эффективной массы и борновском приближении для рассеяния вычислены высокочастотная электропроводность, диэлектрические потери и оптическое поглощение свободными носителями тока в кристаллах, когда механизм рассеяния связан с экранированными электрическими диполями. В данной работе показано, что в некоторых случаях рассеяние на примесных дипольных центрах может быть существенным и даже более эффективным для диэлектрических потерь и поглощения света свободными носителями, нежели другие механизмы рассеяния.

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Dimitrov H.D.

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Free-Carrier Absorption and Dielectric Losses in Crystals with Dipole-Impurities

In the one-band isotropic effective-mass approximation and the second Born approximation of the scattering the high-frequency electrical conductivity, dielectric losses and free-carrier absorption in crystals are calculated when the scattering mechanism is connected with the screened electrical dipoles. As in the case of low-frequency conductivity it is shown that in some cases the scattering from dipole impurity centres may be essential and even more effective for the free-carrier absorption and dielectric losses than the other scattering mechanisms.

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I. INTRODUCTION

In our previous paper^{/1/} it was shown that in some cases the scattering mechanism of current-carriers from randomly distributed electric dipole centres in solids is found to be particularly essential and even more effective than the other scattering mechanisms. This effect is considerable at low temperatures, great effective mass of current-carriers and, naturally, at great values of the electric dipole moment and of the concentration of the dipole impurity centres. Moreover, the relative contribution in the scattering from electric dipole centres with respect to the one from the Coulomb centres (for equal concentrations) grows with increasing concentration of the current-carriers because of their weaker screening effect in the case of dipole centres and it is possible for the former to be significant at the room-temperatures. Impurities and defects in the crystals which practically could scatter the current-carriers at static point (ideal) electric dipoles are, for instance, the neutral associations by opposite-charged atom defects (ions)^{/2-5/} the dipole vacancies in ion crystals, or, when instead of two neighbouring opposite-charged to the same degree ions, one has, in such crystals, neutral atom-impurities, the impurity molecules with a substantial electric dipole moment in some molecular crystals, etc. (See, for instance, ^{/6-8/}). A number of electric properties of semiconductors, semimetals and metals could be related to such a kind of impurities and defects, e.g., electric conductivity, coefficient of light absorption in the infrared range, and so on.

The free-carrier optical absorption in semiconductors or metals, when the scatterers in solids are phonons or ionized impurity centres, has been calculated by various authors ^{/9-17/}.

The present paper aims at calculating the coefficients of light absorption and the dielectric losses in crystalline solids due to the scattering of the quasi-free current-carriers from electric dipole impurity centres. Besides, similar to paper /1/, it is considered that the lattice deformation, connected with the presence of these centres, is small so that its additional effect on the scattering could be neglected. The calculations are carried out in the approximation of the effective mass method by a simple law of dispersion of current-carriers (electrons and holes), the interaction of the latter with every separate electric dipole centre being described by a screening potential obtained in the Febye-Huckel approximation paper /1/. It is assumed that the distribution of the dipole centres in the volume of the crystal is random and not with a very great average concentration so that the scattering from each centre should practically occur independently of the others, while the distribution over orientation does not depend on the position in the volume and could be arbitrarily given. Final results are obtained in the case of equally oriented dipole centres and when all possible orientations of the latter are of equal probability. The scattering amplitudes are calculated in the Born approximation. It is assumed that the absorbed light is monochromatic with frequency much larger than the characteristic value of the frequency of the current-carriers collision. It is also reckoned that the influence of the spatial dispersion of the electric field of the light wave is inessential and can be neglected.

II. CALCULATION OF HIGH-FREQUENCY ELECTRONIC CONDUCTIVITY

Now we will calculate the high-frequency electric conductivity tensor $\hat{\sigma}(\omega)$ which is related to the scattering of a definite type of quasi-free current-carriers (conductivity electrons or holes) in crystalline solids. The external electric field (of the electromagnetic wave falling on the solids) is assumed to be weak and depend simple-periodically on the time with circular frequency

ω so that the one-zone approximation should hold and the inequalities

$$1 \ll \omega \tau_{\mu}(\omega), \quad \mu = 1, 2, 3, \quad (1)$$

should be satisfied, where $\tau_{\mu}(\omega)$ is the μ -th main tensor value of the average transport relaxation time. The tensor is related to the electroconductivity tensor by means of the relation

$$\sigma(\omega) \tau(\omega) = \tau(\omega) \sigma(\omega) = \frac{n e^2}{m \omega^2} \hat{I}, \quad (2)$$

where n is the average current-carriers concentration, e and m are the absolute values of the electric charge and the effective mass of one current-carrier, respectively, while \hat{I} is the unit tensor.

Under these conditions and those presented in the Introduction the real components of the electroconductivity tensor $\sigma_{\mu\nu}(\omega)$ ($\mu, \nu = 1, 2, 3$) for an arbitrary type of scattering centres can be written as follows :

$$\sigma_{\mu\nu}(\omega) = \frac{e^2 k_0 T}{8 \pi^3 h^4 \omega^3} [S_{\mu\nu}^{(+)}(\omega) - S_{\mu\nu}^{(-)}(\omega)], \quad (3)$$

where k_0 is the Boltzmann constant, T is the absolute temperature, while the quantities $S_{\mu\nu}^{(\pm)}(\omega)$ are determined by the formula

$$S_{\mu\nu}^{(\pm)}(\omega) = \int_0^{\infty} d\xi n_0(\xi) \Lambda_{\mu\nu}^{(\pm)}(\xi; \omega). \quad (4)$$

Here

$$n_0(\xi) = [1 + \exp(\xi - x_F)]^{-1} \quad (5)$$

is the Fermi-Dirac distribution function for the current-carriers, and besides, the energy ϵ of each of them and the chemical potential ζ are connected with ξ and x_F , respectively, according to the equalities

$$\epsilon = k_0 T \xi; \quad \zeta = k_0 T x_F, \quad (6)$$

while the functions $\Lambda_{\mu\nu}^{(\pm)}(\xi, \omega)$ are given by the expressions

$$\Lambda_{\mu\nu}^{(\pm)}(\xi; \omega) = \theta(\xi \pm \omega_T) \int_{p_1^{\pm}}^{p_2^{\pm}} dp p^2 K_{\mu\nu}(p), \quad (7)$$

where $\theta(x)$ is the step function,

$$\theta(x) = \begin{cases} 0 & \text{when } x < 0, \\ 1 & \text{when } 0 < x; \end{cases}$$

$$p_1^{\pm} = \pm \frac{\sqrt{2mk_0 T}}{h} (\sqrt{\xi \pm \omega_T} - \sqrt{\xi}), \quad (8)$$

$$p_2^{\pm} = \pm \frac{\sqrt{2mk_0 T}}{h} (\sqrt{\xi \pm \omega_T} + \sqrt{\xi});$$

$$K_{\mu\nu}(p) = \frac{1}{4\pi} \int_0^{2\pi} d\alpha \int_0^{\pi} d\beta \sin\beta \frac{p_{\mu} p_{\nu}}{p^2} Q(\vec{p}); \quad (9)$$

\vec{p} is the wave vector with the Cartesian rectangular coordinates

$$\vec{p} = (p \cos\alpha \sin\beta, p \sin\alpha \sin\beta, p \cos\beta) \quad (10)$$

and

$$\omega_T = \frac{h\omega}{k_0 T}. \quad (11)$$

In the general case the quantity $Q(\vec{p})$ in (9) is defined by the formula

$$Q(\vec{p}) = Ne^2 \int_0^{2\pi} d\psi \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta P_0(\psi, \phi, \theta) |V(\vec{p} \cdot \hat{A}(\psi, \phi, \theta))|^2, \quad (12)$$

where N is the average concentration of the scattering centres; $P_0(\psi, \phi, \theta)$ is the distribution function of the centres over orientation (ψ, ϕ, θ are the Euler angles), for which naturally one has

$$\int_0^{2\pi} d\psi \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta P_0(\psi, \phi, \theta) = 1;$$

$V(\vec{p})$ is the Fourier component of the potential of one scattering centre which is placed at the origin of the coordinate system with a definite fixed orientation; $\hat{A}(\psi, \phi, \theta)$ is the transformation matrix of rotating of the coordinate system, defined by the Euler angles. One has

$$\vec{p} \cdot \hat{A} = (\vec{p} \cdot \vec{n}, \vec{p} \cdot (\vec{s} \times \vec{n}), \vec{p} \cdot \vec{s}), \quad (13)$$

where

$$\vec{n} = (\cos\psi \cos\phi - \sin\psi \sin\phi \cos\theta, \sin\psi \cos\phi + \cos\psi \sin\phi \cos\theta, \sin\phi \sin\theta),$$

$$\vec{s} = (\sin\psi \sin\theta, -\cos\psi \sin\theta, \cos\theta). \quad (14)$$

In the considered case of scattering electric dipole centres the Debye-Huckel screened potential $V_D(\vec{r})$ of one of these centres placed at the origin of the coordinate system and its Fourier-component $V_D(\vec{p})$ were obtained in paper [1] and are given by the expressions, respectively.

$$V_D(\vec{r}) = \frac{(\vec{q} \cdot \vec{r})}{\epsilon_0 r^3} \left(1 + \frac{r}{\rho_0}\right) \exp\left(-\frac{r}{\rho_0}\right), \quad (15)$$

$$V_D(\vec{p}) = -\frac{4\pi i \rho_0^2}{\epsilon_0} \frac{(\vec{q} \cdot \vec{p})}{1 + \rho_0^2 p^2},$$

where \vec{q} is the electric dipole moment of the centre, ϵ_0 is the dielectric permittivity of the medium, ρ_0 is the Debye-Huckel screening radius, $r = |\vec{r}|$ and $p = |\vec{p}|$. Moreover, when all dipole impurity centres are equally oriented (they are assumed to be directed along the axis Oz) one has

$$P_0(\psi, \phi, \theta) = \frac{1}{\sin\theta} \delta(\psi) \delta(\phi) \delta(\theta), \quad (16)$$

where $\delta(x)$ is the Dirac function, and when all their possible orientations are of equal probability*

* Naturally, our description is approximate, since, in fact, the possible orientations of the defects in crystals always form a discrete set.

$$P_0(\psi, \phi, \theta) = \frac{1}{8\pi^2}. \quad (17)$$

Substituting (16) together with (13)-(15) into (12), one obtains

$$Q(\vec{p}) = \frac{6\pi A p_z^2}{(1 + \rho_0^2 p^2)^2} \quad (18)$$

and, analogously, using (17) one finds (see also ^{/1/})

$$Q(\vec{p}) = \frac{A p^2}{(1 + \rho_0^2 p^2)^2}, \quad (19)$$

where

$$A = \frac{16\pi^2 e^2 q^2 N \rho_0^4}{3\xi_0^2}. \quad (20)$$

For simplicity, here and further on we consider only the case of unipolar electric conductivity* assuming that all dipole impurity centres have equal magnitude of dipole moments $q = |\vec{q}|$. If that does not hold, then in (20) and further on instead of q^2 one should write the average quadratic value $\langle q^2 \rangle$, obtained using a definite known distribution function of the impurity dipoles according to the magnitude of the dipole moment ^{/1/}. It is reckoned that the current-carriers dispersion law has the form

$$\frac{\epsilon_{\vec{k}}}{k} = \frac{\hbar^2 k^2}{2m}$$

(k is the value of the wave-vector \vec{k}).

First consider the case of randomly distributed over orientation dipole impurity centres. Then from (9), (10) and (19) one gets

* In the general case the electric conductivity is a sum of terms of the form (3), each being determined by the corresponding type of current-carriers.

$$K_{\mu\nu}(\vec{p}) = \frac{1}{3} A \delta_{\mu\nu} \frac{p^2}{(1 + \rho_0^2 p^2)^2}, \quad (21)$$

where $\delta_{\mu\nu}$ is the Kronicker symbol,

$$\delta_{\mu\nu} = \begin{cases} 1 & \text{when } \mu = \nu, \\ 0 & \text{when } \mu \neq \nu. \end{cases}$$

Substituting the above expression (21) into (7) and taking into account (8) we find

$$\Lambda_{\mu\nu}^{(\pm)}(\xi; \omega) = \frac{A}{3\rho_0^6} \delta_{\mu\nu} \theta(\xi \pm \omega_T) J^{(\pm)}(\xi; \omega), \quad (22)$$

where

$$J^{(\pm)}(\xi; \omega) = 2\gamma_0 \left[1 + \frac{1}{(1 \pm \gamma_0 \omega_T)^2 + 4\gamma_0 \xi} \right] \sqrt{\xi(\xi \pm \omega_T)} - \ln \left[\frac{1 + \gamma_0(\sqrt{\xi \pm \omega_T} + \sqrt{\xi})^2}{1 + \gamma_0(\sqrt{\xi \pm \omega_T} - \sqrt{\xi})^2} \right], \quad (23)$$

when

$$\gamma_0 = \frac{2m}{\hbar^2} k_0 T \rho_0^2. \quad (24)$$

Obviously, we have

$$J^{(+)}(\xi; \omega) = J^{(-)}(\xi + \omega_T; \omega). \quad (25)$$

Now, from (3) and (4) using (20), (22) and (25) we obtain

$$\sigma_{\mu\nu}(\omega) = \sigma(\omega) \delta_{\mu\nu}, \quad (26)$$

$$\sigma(\omega) = \frac{2e^4 q^2 N k_0 T \rho_0^4}{9\pi \hbar^4 \xi_0^2} \frac{1}{\omega^3} \int_0^\infty d\xi [n_0(\xi) - n_0(\xi + \omega)] J^{(+)}(\xi; \omega). \quad (27)$$

When degeneration of the current-carriers is absent, i.e., when the inequality

$$1 \ll \frac{(mk_0T)^{3/2}}{\pi\sqrt{2\pi}h^3n}$$

holds, from (5), (6), (23) and (27) we find

$$\sigma(\omega) = \sigma^B(\omega) = \frac{32e^4q^2Nn}{9h^3\epsilon_0^2} \left(\frac{2\pi k_0T}{m}\right)^{1/2} \frac{1}{\omega^3} \operatorname{sh} \frac{\omega_T}{2} \times \left\{ e^{-\frac{\omega_T}{2}} (8\gamma_0 \frac{\partial}{\partial a} - 1) J(a, \omega) + \frac{\omega_T}{2} \left[K_1\left(\frac{\omega_T}{2}\right) - \frac{2\gamma_0\omega_T}{1+\gamma_0^2\omega_T^2} K_0\left(\frac{\omega_T}{2}\right) \right] \right\}, \quad (28)$$

where $K_0(x)$ and $K_1(x)$ are the Macdonald functions of order 0 and 1, respectively;

$$J(a, \omega) = \int_0^\infty d\xi \frac{\sqrt{\xi(\xi + \omega_T)}}{a + 4\gamma_0\xi} e^{-\xi}; \quad (29)$$

$$a = (1 + \gamma_0\omega_T)^2. \quad (30)$$

Moreover, the screening radius ρ_0 is determined by the well-known formula

$$\rho_0 = \left(\frac{\epsilon_0 k_0 T}{4\pi e^2 n}\right)^{1/2};$$

the latter, together with (11) and (24) leads to the following expressions for γ_0 and $\gamma_0\omega_T$:

$$\gamma_0 = \frac{m\epsilon_0 k_0^2 T^2}{2\pi h^2 e^2 n}; \quad \gamma_0\omega_T = \frac{m\epsilon_0 k_0 T\omega}{2\pi h e^2 n}.$$

When the inequality

$$4\gamma_0 \ll a \quad (31)$$

holds, as a good approximation for the integral (29) we have

$$J(a, \omega) \cong \frac{1}{a + 3\gamma_0} \frac{\omega_T}{2} e^{-\frac{\omega_T}{2}} K_1\left(\frac{\omega_T}{2}\right). \quad (32)$$

Substituting (32) into (28), we obtain

$$\sigma^B(\omega) = \frac{16e^4q^2Nn}{9h^2\epsilon_0^2} \left(\frac{2\pi}{mk_0T}\right)^{1/2} \frac{1}{\omega^2} \operatorname{sh} \frac{\omega_T}{2} \times \left\{ 1 - \frac{1}{a + 3\gamma_0} - \frac{8\gamma_0}{(a + 3\gamma_0)^2} \left[K_1\left(\frac{\omega_T}{2}\right) - \frac{2\gamma_0\omega_T}{1 + \gamma_0^2\omega_T^2} K_0\left(\frac{\omega_T}{2}\right) \right] \right\}. \quad (33)$$

If, in addition, the inequality $1 \ll \omega_T$ is satisfied, then the formula (33) is approximately written in the form

$$\sigma^B(\omega) = \frac{8\sqrt{2\pi}e^4q^2Nn}{9\epsilon_0^2 m^{1/2} (hc)^{5/2}} \left(1 - \frac{1}{a} - \frac{2\gamma_0\omega_T}{1 + \gamma_0^2\omega_T^2}\right).$$

In the case opposite to (31), i.e., when $a \ll 4\gamma_0$, and moreover the condition $\omega_T \ll 1$ is satisfied; for the integral (29) we can write

$$J(a, \omega) \cong \frac{1}{4\gamma_0}.$$

Then from (28) we approximately find

$$\sigma^B(\omega) \cong \frac{16e^4q^2Nn}{9h^2\epsilon_0^2} \left(\frac{2\pi}{\pi k_0T}\right)^{1/2} \frac{\xi}{\omega^2}. \quad (34)$$

Thus, for scattering from dipole centres and the Boltzmann statistics of current-carriers the dependence of the electric conductivity on the frequency ω of the external electric field in general is by the law ω^{-2} , when $h\omega/k_0T \ll 1$, and by the law $\omega^{-5/2}$, when $1 \ll h\omega/k_0T$.

Here we shall note that the high-frequency electric conductivity corresponding to (28) for the scattering

from the screened Coulomb centres (with charges $\pm Ze$) can be written in a similar form, namely,

$$\sigma_I^B(\omega) = \frac{8Z^2 e^6 Nn}{3h\epsilon_0^2 m} \left(\frac{2\pi}{mk_0 T}\right)^{1/2} \frac{1}{\omega^3} \frac{\text{sh}\left(\frac{\omega_T}{2}\right)}{1 + \gamma_0^2 \omega_T^2} \times \quad (35)$$

$$\times \left\{ \gamma_0^2 \omega_T^2 K_0\left(\frac{\omega_T}{2}\right) - 4\gamma_0 e^{-\frac{\omega_T}{2}} \left[\gamma_0^2 \omega_T^2 + 2\gamma_0 (1 - \gamma_0^2 \omega_T^2) \frac{\partial}{\partial a} \right] J(a, \omega) \right\},$$

and when $1 \ll \omega_T$ this expression transforms into the result obtained in paper¹⁰. Using the approximation (32) from (35) one obtains

$$\sigma_I^B(\omega) = \frac{8Z^2 e^6 Nn}{3h\epsilon_0^2 m} \left(\frac{2\pi}{mk_0 T}\right)^{1/2} \frac{1}{\omega^3} \text{sh}\left(\frac{\omega_T}{2}\right) \frac{\gamma_0^2 \omega_T^2}{1 + \gamma_0^2 \omega_T^2} \times$$

$$\times \left\{ K_0\left(\frac{\omega_T}{2}\right) - \frac{2}{a + 3\gamma_0} \left[\gamma_0 \omega_T - \frac{2}{\omega_T} \frac{1 - \gamma_0^2 \omega_T^2}{a + 3\gamma_0} \right] K_1\left(\frac{\omega_T}{2}\right) \right\}.$$

If the dipole centres screening is weak and may be neglected ($\rho_0 = \infty$), then the general formula (28) is reduced to

$$\sigma^B(\omega) = \frac{16e^4 q^2 Nn}{9h^2 \epsilon_0^2} \left(\frac{2\pi}{mk_0 T}\right)^{1/2} \frac{1}{\omega^2} \text{sh}\left(\frac{h\omega}{2k_0 T}\right) K_1\left(\frac{h\omega}{k_0 T}\right). \quad (36)$$

Note, that the formula (36) is obtained from the corresponding formula at scattering from the Coulomb centres (which is following from (35) when $\rho_0 = \infty$)^{12,13,18/}

by multiplying $\frac{2mq^2\omega}{3hZ^2 e^2}$ and substituting the function $K_0\left(\frac{\omega_T}{2}\right)$ by $K_1\left(\frac{\omega_T}{2}\right)$. Besides, when $m=10m_0$ (m_0 is the

mass of the free electron), $T = 300^\circ\text{K}$, $q = 6D$, $\omega = 5.10^{14} \text{ rad/s}$, $Z = 1$ and for equal concentrations of the

dipole and Coulomb centres, the electric conductivity at the scattering from dipole centres is only two times smaller than that at scattering from the Coulomb centres.

In the case of strongly degenerated statistics of current-carriers, i.e., when the inequality

$$1 \ll \frac{\zeta_0}{k_0 T} = \frac{h^2 (3\pi^2 n)^{2/3}}{2mk_0 T} \quad (37)$$

is satisfied (ζ_0 is the value of the chemical potential when $T = 0$), from (5), (6), (23) and (27) we find

$$\sigma(\omega) = \sigma^F(\omega) = \frac{2me^4 q^2 N}{9\pi h^6 \epsilon_0^2} [F(\zeta_0) - \theta(\zeta_0 - h\omega)F(\zeta_0 - h\omega)] \frac{1}{\omega^3}, \quad (38)$$

where

$$F(x) = (3\eta_0 + 2x + h\omega)\sqrt{x(x+h\omega)} + 2\eta_0 xL(x) + \quad (39)$$

$$+ \frac{1}{4} [3\eta_0^2 + (4\eta_0 + h\omega)h\omega] [\mathcal{E}(\eta_0 - h\omega)M(x) - N(x)];$$

$$L(x) = \ln \left[\frac{\eta_0 + (\sqrt{x+h\omega} - \sqrt{x})^2}{\eta_0 + (\sqrt{x+h\omega} + \sqrt{x})^2} \right]; \quad (40)$$

$$M(x) = \ln \left\{ \frac{[(\eta_0 + h\omega)^2 + 4\eta_0 x] h\omega}{|2(|\eta_0^2 - h^2 \omega^2|)\sqrt{x(x+h\omega)} - (\eta_0^2 + h^2 \omega^2)(2x+h\omega) - 2\eta_0 h^2 \omega^2|} \right\}; \quad (41)$$

$$N(x) = \ln \left[1 + \frac{2}{h\omega} (x + \sqrt{x(x+h\omega)}) \right]; \quad (42)$$

$$\eta_0 = \frac{h^2}{2m\rho_0^2}; \quad (43)$$

$$\mathcal{E}(x) = \theta(x) - \theta(-x).$$

As is known, because of (37) ρ_0^2 in (43) is given by the expression

$$\rho_0^2 = \frac{h^2 \epsilon_0}{4me^2} \left(\frac{\pi}{3n}\right)^{1/3}.$$

In the particular case when the additional conditions

$$\zeta_0 \leq \eta_0 \ll h\omega$$

hold, from (38) - (42) approximately we have

$$\sigma^F(\omega) \approx \frac{16me^4 q^2 \zeta_0^{3/2} N}{27h^3 \epsilon_0^2 (h\omega)^{5/2}} \quad (44)$$

We shall note that the high-frequency electric conductivity corresponding to (36) for the scattering from the screened Coulomb centres can be written in the following form

$$\sigma_1^F(\omega) = \frac{2Z^2 e^6 N}{2\pi h^4 \epsilon_0^2 \omega^3} [F_1(\zeta_0) - \theta(\zeta_0 - h\omega) F_1(\zeta_0 - h\omega)],$$

where

$$F_1(x) = -2\sqrt{x(x+h\omega)} - xL(x) - \frac{1}{2}(\eta_0 + h\omega)[\epsilon(\eta_0 - t\omega)M(x) - N(x)].$$

Exactly in the same way one carries out the calculation of the electric conductivity tensor for equally oriented dipole impurity centres. Then, it is easy to see that, using the expressions (18) and (20), from (3) - (10) one obtains*

$$\sigma_{\mu\nu}(\omega) = \frac{6\pi}{5} \sigma(\omega) a_{\mu\nu}^\circ, \quad (45)$$

where $\sigma(\omega)$ is the considered above scalar electric conductivity for randomly distributed over orientation dipole impurity centres, which in the general case is determined by (5), (6), (11), (23), (24) and (27), while $a_{\mu\nu}^\circ$ are tensor elements with values as follows:

$$a_{\mu\nu}^\circ = 0 \quad \text{for } \mu \neq \nu; \quad a_{11}^\circ = a_{22}^\circ = \frac{1}{3} a_{33}^\circ = 1. \quad (46)$$

* In fact the formula (45) is valid in a more general case, when the impurity dipoles can be oriented opposite to each other too.

The result (45) shows that for equal orientation of the dipole centres the high-frequency electric conductivity in the direction perpendicular to the dipole moments is 3.77 times larger and in direction parallel to them 11.3 times larger than the corresponding electric conductivity with randomly distributed over orientation of dipole centres.

In each of the considered cases the conditions (1) are written in the explicit form with the help of the corresponding expressions, obtained for the electric conductivity tensor, and the average transport relaxation time tensor $\hat{\tau}(\omega)$ is determined by the relation (2). Thus, for instance, from (1), (2), (26) and (34) we have

$$1 \ll \frac{9h^2 \epsilon_0^2 \omega}{16e^2 q^2 N} \sqrt{\frac{k_0 T}{2\pi m}},$$

while from (1), (2), (26), (37) and (44) we obtain

$$1 \ll \frac{9h \epsilon_0^2 (h\omega)^{3/2}}{4\pi^2 \sqrt{2m} e^2 q^2 N}.$$

Note also that the carried-out consideration of the impurity centres as point (ideal) dipoles and the Born approximation for the scattering hold when the inequalities (see also /1/)

$$k\delta < 1; \quad \frac{4me\rho_0}{3h^2 \epsilon_0} |\vec{q} \cdot \vec{k}| \left[\frac{1 + (k\rho_0)^2}{1 + (2k\rho_0)^2} \right]^{1/2} \ll 1$$

hold, respectively, where δ is the distance between the centres of the positive and negative electric charges in the dipoles. But one should take into account that a sufficient condition for the applicability of the Born approximation is usually the inequality $1 \ll 2\pi/k r_0$, where r_0 is the distance to which a current-carrier with a characteristic value k of its quasi-wave vector could approach the force in the repulsive field $e|V_D(r)|$.

III. DIELECTRIC LOSSES AND ABSORPTION COEFFICIENTS

Now we will write the formulae for the dielectric losses and the absorption coefficients of electromagnetic waves corresponding to the obtained results for high-frequency electric conductivity at scattering of current-carriers from electric dipole impurity centres. Moreover, we will assume that the dielectric permittivity $\hat{\epsilon}_0$ determined by the lattice mechanisms of polarization is a scalar quantity. Then, the power $W_J(\omega)$ of the dielectric losses in unit volume of the crystal is defined by the formula:

$$W_J(\omega) = \frac{1}{2} \sum_{\mu=1}^3 E_{0\mu}^2 \sigma_{\mu}(\omega) = \frac{\omega}{8\pi} \sum_{\mu=1}^3 E_{0\mu}^2 \hat{\epsilon}_{\mu}(\omega) \operatorname{tg} \delta_{\mu}(\omega), \quad (47)$$

where $E_{0\mu}$ is the projection of the external electric field vector amplitude onto the μ -th main axis of the electric conductivity tensor, $\hat{\epsilon}_{\mu}(\omega)$ and $\sigma_{\mu}(\omega)$ are the corresponding to this axis main values of the tensors of the general dielectric permittivity $\hat{\epsilon}(\omega)$ and electric conductivity $\hat{\sigma}(\omega)$, while

$$\delta_{\mu}(\omega) = \operatorname{arctg} \left[\frac{4\pi}{\omega} \frac{\sigma_{\mu}(\omega)}{\hat{\epsilon}_{\mu}(\omega)} \right]$$

is the angle of dielectric losses.

Further on, we will assume that the dependence of $\hat{\epsilon}_0$ on the frequency ω of the applied electric field is weak and may be neglected. Besides, the effects from the delay of the lattice polarization with respect to the applied electric field can be neglected, assuming them to be inessential.

For the components of the tensor $\hat{\epsilon}(\omega)$ we will have

$$\hat{\epsilon}_{\mu\nu}(\omega) = \hat{\epsilon}_0 \delta_{\mu\nu} + \Delta \hat{\epsilon}_{\mu\nu}(\omega), \quad (48)$$

where $\Delta \hat{\epsilon}_{\mu\nu}(\omega)$ are the components of the electron part of the dielectric permittivity tensor. The latter could easily be written taking account of the current-carriers

scattering from impurity centres in the Born approximation however, in our case, because of (1), the relaxation contribution, predetermined by the impurity dipoles, is inessential and for this reason, it is completely sufficient to write $\Delta \hat{\epsilon}_{\mu\nu}(\omega)$ only for the quasi-free gas of current-carriers,

$$\Delta \hat{\epsilon}_{\mu\nu}(\omega) = -\delta_{\mu\nu} \hat{\epsilon}_0 \frac{\omega_{pe}^2}{\omega^2}, \quad (49)$$

where ω_{pe} is the plasma frequency,

$$\omega_{pe} = \left(\frac{4\pi n e^2}{m \hat{\epsilon}_0} \right)^{1/2}. \quad (50)$$

Limiting our investigations to non-magnetic crystals and electromagnetic waves with parallel amplitude and phase planes, for the main coefficients of absorption $a^{(\mu)}(\omega)$ and main (real) refractive indices $n^{(\mu)}(\omega)$, $\mu=1,2,3$, according to classic electrodynamics, we have

$$a^{(\mu)}(\omega) = \frac{2\omega}{c} L_{(-)}^{(\mu)}(\omega); \quad n^{(\mu)}(\omega) = L_{(+)}^{(\mu)}(\omega), \quad (51)$$

where

$$L_{(\pm)}^{(\mu)}(\omega) = \frac{1}{\sqrt{2}} \left\{ \left[\hat{\epsilon}_{\mu}^2(\omega) + \left(\frac{4\pi}{\omega} \sigma_{\mu}(\omega) \right)^2 \right]^{1/2} \pm \hat{\epsilon}_{\mu}(\omega) \right\}^{1/2}, \quad (52)$$

while c is the velocity of light in vacuum.

The formulae (51) and (52) define the propagation velocity $c^{(\mu)}(\omega) = c/n^{(\mu)}(\omega)$ and the absorption coefficient $a^{(\mu)}(\omega)$ of flat monochromatic wave which electric vector oscillates parallel to the μ -th main axis of the electric conductivity tensor, while the normal to the wave front is parallel to one of the other two main axes of this tensor.

In this way, the dielectric losses and coefficients of the electromagnetic wave absorption in the considered cases are obtained from (47), (51) and (52) by substituting (48)-(50) into them and the corresponding expression for the high-frequency electric conductivity.

For optical electromagnetic waves, when the inequalities

$$0 < \epsilon_{\mu}(\omega) \quad \text{and} \quad \frac{4\pi}{\omega} \frac{\sigma_{\mu}(\omega)}{\epsilon_{\mu}(\omega)} \ll 1,$$

are satisfied, from (51) and (52) we have

$$a^{(\mu)}(\omega) \approx \frac{4\pi}{c} \frac{\sigma_{\mu}(\omega)}{\sqrt{\epsilon_{\mu}(\omega)}}; \quad n^{(\mu)}(\omega) \approx \sqrt{\epsilon_{\mu}(\omega)}. \quad (53)$$

Thus, for instance, from (34), (45)-(50) and (53) when $\omega_{pe} \ll \omega$ approximately we find

$$W_J(\omega) = B(E_{01}^2 + E_{02}^2 + 3E_{03}^2) \frac{1}{\omega^2};$$

$$a^{(1)}(\omega) = a^{(2)}(\omega) = \frac{1}{3} a^{(3)}(\omega) = \frac{8B}{c\sqrt{\epsilon_0}\omega^2},$$

while from (44), (47)-(50) and (53)

$$W_J(\omega) = G \frac{E_0^2}{\omega^{5/2}}; \quad a^{(\mu)}(\omega) = a(\omega) = \frac{8\pi G}{c\sqrt{\epsilon_0}\omega^{5/2}},$$

where

$$B = \frac{8\pi e^4 q^2 N_n}{15h^2 \epsilon_0^2} \left(\frac{2\pi}{mk_0 T} \right)^{1/2}; \quad G = \frac{8me^4 q^2 N \zeta^{1/2}}{27h^{11/2} \epsilon_0^2}.$$

In conclusion, let us note that for equality oriented dipole impurity centres the dielectric losses and electromagnetic wave absorption are larger than those for randomly distributed over orientation dipole centres and besides, the absorption is three times larger when the vector of the wave electric field is parallel to the dipole moments compared with the case when it is perpendicular to them.

IV. CONCLUSIONS

In this paper the contributions to the high-frequency electrical conductivity, dielectric losses and free-carrier absorption associated with the scattering from the Debye-Huckel screened dipole impurity centres in crystals are calculated. The consideration is in the one-band isotropic effective-mass approximation and the second-order Born approximation of the scattering. When all the orientations of the impurity dipole moments are realized with equal probability and when they have parallel orientations in the limit cases of the Boltzmann and strongly degenerated statistics presents formulae for the high-frequency electrical conductivity, dielectric losses and absorption coefficients. As on the low-frequency case (see paper /1/) our results here show that the scattering of current-carriers from dipole centres in some cases may be comparable to or even more effective than the other scattering mechanisms. The considered scattering mechanism is found to be particularly essential in some adopted and specially processed materials under relatively low-temperatures and great concentration of current-carriers and frequency of the external electric field. It is possible that the dipole impurity scattering will give us an explanation of impurity effects in crystals.

The corresponding results of the calculation of infrared optical absorption and dielectric losses in n-type germanium and silicon with taking into account the real structure of conduction band will be published additionally.

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