CURRENT-VOLTAGE CHARACTERISTIC OF A SEMICONDUCTOR WITH AN ELECTRON-PHONON COUPLING PROPORTIONAL TO THE APPLIED FIELD

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The kinetic equation is solved and the mobility of carriers in a semiconductor is calculated with account of a new type of electron-phonon interaction, which is proportional to the applied field.[1] Other well-known carrier scattering mechanisms are also considered. The latter are predominant in weak external fields, and this leads to Ohm's law. In crystals with a very large dielectric constant (on the order of several thousand) the aforementioned new type of interaction becomes dominant when the field increases. Consequently the current passes through a maximum and then begins to decrease.

IN a recent paper[1] one of us has introduced an electron-phonon coupling arising in an applied electric field $\mathbf{E}$ as a result of dependence of the dielectric constant ϵ on the deformation of the medium. In crystals with very large dielectric constants such a coupling may dominate over the deformation potential, and even over the piezo-electric electron-phonon coupling.

In an isotropic medium the dependence of ϵ on the deformation has the form

$$\varepsilon_{ik} = \varepsilon_0(\delta_{ik} - g_1\delta_{ik}\,\mathrm{div}\,\mathbf{u} - g_2 u_{ik}), \qquad (1)$$

where $\mathbf{u}(\mathbf{r})$ and $u_{ik}(\mathbf{r})$ are the deformation vector and tensor, g_1 and g_2 are numerical coefficients, and ϵ_0 is the permittivity of the undeformed medium. If a potential difference with average gradient $\mathbf{E}$ is applied to a deformed medium, then the total electric field effectively acting on the conduction electron is $\mathbf{E} - \nabla\varphi$, where $\varphi(\mathbf{r})$ is the potential of the inhomogeneous field component connected with the dependence of ϵ on the coordinates, and is given by[1]

$$\Delta\varphi = -(g_1 + g_2/2)(\mathbf{E}\nabla)(\nabla\mathbf{u}) - (\mathbf{E}\Delta\mathbf{u})g_2/2. \qquad (2)$$

In [1] the interaction $\varphi[\mathbf{r}, \mathbf{u}]$ was taken into account in the theory of amplification and generation of ultrasonic waves in a crystal. In the present work, however, it is regarded in calculations of the mobility, as a carrier scattering mechanism,

alongside the deformation potential and other scattering mechanisms.

Let us consider a simple conduction band with an isotropic square dependence of the electron energy $\mathscr{E}$ on its quasimomentum $\mathbf{k}$. In the effective-mass approximation the wave functions of the conduction electron are

$$\psi_k(\mathbf{r}) = \frac{1}{\sqrt{V}}e^{i\mathbf{k}\mathbf{r}}. \qquad (A)$$

The probability (per unit time) of electron scattering due to the interaction φ and followed by the absorption (+) or emission (−) of one acoustic longitudinal phonon is

$$W_\parallel{}^{\pm}(\mathbf{k}, \mathbf{q}) = \frac{\pi e^2 (g_1 + g_2)^2 E^2}{MNs_\parallel q}$$
$$\times \cos^2\alpha \cdot \delta(\mathscr{E}_{\mathbf{k}\pm\mathbf{q}} - \mathscr{E}_{\mathbf{k}} \mp \hbar s_\parallel q)\begin{Bmatrix} N_{\mathbf{q}\parallel} \\ N_{-\mathbf{q}\parallel} + 1 \end{Bmatrix}. \qquad (3)$$

Here $\mathbf{k}$ $\mathbf{k}' = \mathbf{k} \pm \mathbf{q}$ are the quasimomenta of the initial and final electron states, $\mathbf{q}$ is the wave vector of the phonon, M is the mass of the crystal unit cell, N is the number of unit cells in the basic region of the cyclicity of V, $s_\parallel$ is the longitudinal sound velocity, $N_{\mathbf{q}\parallel}$ is the number of phonons prior to scattering, and α is the angle between $\mathbf{q}$ and $\mathbf{E}$.

The probability (per second) of scattering by transverse phonons is obtained from Eq. (3) by means of the substitution

$$g_1 + g_2 \to g_2/2, \qquad s_\parallel \to s_\perp, \qquad \cos^2\alpha \to \sin^2\alpha.$$

Assume that the temperature is not too low and the average thermal energy of the conduction electron is much larger than the phonon energy. Then $|\mathbf{k}'| \approx |\mathbf{k}|$, and

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1)In a inhomogeneously deformed medium, bunching of the electronic space-charge arises and forms a field $\mathbf{E}_\rho$. This field has been taken into account in [1] where it had the same order of magnitude as $\nabla\varphi$. In the present work, however, we neglect the field $\mathbf{E}_\rho$ when considering thermal phonons.

$$\delta(\mathscr{E}_{\mathbf{k}\pm\mathbf{q}} - \mathscr{E}_{\mathbf{k}} \mp \hbar s_{\parallel}q) \approx \delta(\mathscr{E}_{\mathbf{k}\pm\mathbf{q}} - \mathscr{E}_{\mathbf{k}})$$

$$= \frac{m^{*}}{\hbar^{2}kq}\,\delta\left(\frac{q}{2k} \pm \cos\vartheta\right), \qquad (4)$$

where $\mathscr{E}_{\mathbf{k}} = \hbar k^{2}/2m^{*}$, and ϑ is the angle between $\mathbf{k}$ and $\mathbf{q}$.

Besides the scattering due to the potential φ, we take account of scattering due to the deformation potential and to the interaction with the optical phonons. It is easy to show that the squared modulus of the matrix element of the scattering by these three mechanisms simply equals the sum of the squared moduli of the matrix elements of scattering by each of the mechanisms separately. This is because the matrix element of φ is real, and the matrix element of the deformation potential is pure imaginary; however, the scattering involving acoustic and optical phonons is alternative. Thus the scattering probabilities of all three types simply sum up.

If we write the kinetic equation for a spatially uniform semiconductor and homogeneous applied field $\mathbf{E}$, and represent the distribution function by

$$f(\mathbf{k}) = f_{0}(\mathscr{E}) + f_{1}(\mathbf{k}) + \dots, \quad f_{1} \ll f_{0}, \qquad (5)$$

where f_{0} is of zeroth order of smallness and $\mathbf{E}$ and f_{1} are of the first order, then we obtain from the kinetic equation

$$f_{1} = -\tau(\mathbf{k})\frac{e\hbar}{m^{*}}\frac{df_{0}}{d\mathscr{E}}(\mathbf{k}\mathbf{E}). \qquad (6)$$

Here the relaxation time $\tau(\mathbf{k})$ is introduced through the collision term by the equation

$$(\partial f / \partial t)_{\text{coll}} = -f_{1}/\tau.$$

Using Eq. (6) for $\tau(\mathbf{k})$ we obtain the integral equation

$$\frac{1}{\tau(\mathbf{k})} = \sum_{\mathbf{k}'} W(\mathbf{k},\mathbf{k}')\left[1 - \frac{\tau(\mathbf{k}')}{\tau(\mathbf{k})}\frac{\mathbf{k}'\mathbf{E}}{\mathbf{k}\mathbf{E}}\right]. \qquad (7)$$

Here $W(\mathbf{k},\mathbf{k}')$ is the total probability of carrier scattering by all three mechanisms.

When the scattering angle enters in $W(\mathbf{k},\mathbf{k}')$ only via the argument of the δ-function, Eq. (7) has an obvious solution of the type $\tau = \tau(|\mathbf{k}|)$. This is the case, for example, in scattering by the deformation potential and optical vibrations. However in Eq. (3) the situation is different because of the factor $\cos^{2}\alpha$, which depends on the scattering angle; therefore τ should depend also on the direction of $\mathbf{k}$.

We solve the integral equation (7) by an iteration method, substituting the approximate expression $\tau(\mathbf{k})$ in the right-hand side and finding from it the next approximation for $\tau(\mathbf{k})$. By choosing

$\tau = \tau(|\mathbf{k}|)$ as the initial approximation, we obtain in the next one

$$\frac{1}{\tau(\mathbf{k})} = \sum_{\mathbf{k}'} W(\mathbf{k},\mathbf{k}')\left(1 - \frac{\mathbf{k}'\mathbf{E}}{\mathbf{k}\mathbf{E}}\right). \qquad (8)$$

In the future we limit ourselves to this approximation, but we perform one more iteration to estimate its error. We consider the most adverse case when the scattering by the potential φ predominates, i.e., the anisotropy of the function $\tau(\mathbf{k})$ is maximal. The error of the quantity (8) proves to be alternating and not to exceed 3% in amplitude.

According to (8), from the additivity of $W(\mathbf{k},\mathbf{k}')$ for the different scattering mechanisms follows the additivity of the corresponding inverse relaxation times. For the scattering by the potential φ we obtain

$$\frac{1}{\tau_{\varphi}(\mathbf{k})} = \frac{1}{Ak}[3 + \eta - (1 - \eta)\cos^{2}\beta]. \qquad (9)$$

Here β is the angle between $\mathbf{k}$ and $\mathbf{E}$,

$$A = \frac{16\pi\hbar\gamma s_{\parallel}^{2}\alpha}{(g_{1}+g_{2})^{2}e^{2}E^{2}}, \qquad \eta = \left[\frac{g_{2}s_{\parallel}}{2(g_{1}+g_{2})s_{\perp}}\right]^{2}, \qquad (10)$$

$$\alpha = \frac{\hbar^{2}}{2m^{*}k_{0}T},$$

γ is the density of the material, k_{0} is Boltzmann's constant, and T is the temperature of the lattice. For scattering by the deformation potential $V_{d} = b \operatorname{div}\mathbf{u}$ we have

$$1/\tau_{d} = k/B, \qquad B = 2\pi\hbar\gamma s_{\parallel}^{2}\alpha/b^{2} \qquad (11)$$

(see, e.g., [2]).

When electrons interact with the optical vibrations of the crystal, polarons are formed, whose scattering by acoustic vibrations is described by equations that differ from those given above. However, this difference is large only in the case of strongly polar crystals, in which polarons with strong coupling are formed. We will limit ourselves in this paper to weakly polar crystals. In this case[2]

$$\frac{1}{\tau_{p}} = \begin{cases} 1/Ck, & \hbar\omega_{0} \ll k_{0}T \\ 1/C', & \hbar\omega_{0} \gg k_{0}T \end{cases}, \qquad (12)$$

where C and C' are constants, and ω_{0} is the endpoint frequency of the longitudinal optical phonon branch. If there are only two ions in the unit cell, then

$$C = \frac{\mu a^{3}\hbar\omega_{0}^{2}\alpha}{2\pi Z^{2}e^{4}}, \qquad C' = \frac{3\sqrt{2}\,\mu a^{3}(\hbar\omega_{0})^{3/2}}{4\pi Z^{2}e^{4}m^{*1/2}}\exp\left(\frac{\hbar\omega_{0}}{k_{0}T}\right), \qquad (13)$$

where μ is the reduced mass of the two ions, Ze is the effective charge of the ion, and a is the lat-

tice constant (the shortest distance between the unlike ions).

By adding the inverse relaxation times for the three scattering mechanisms, we obtain for the total relaxation time

$$\tau = \frac{Bk}{k^2 + (B/\tau_p)k + F_1 - F_2 \cos^2 \beta},$$

$$F_1 = \frac{B}{A}(3 + \eta), \quad F_2 = \frac{B}{A}(1 - \eta). \quad (14)$$

Let us choose $f_0(\mathscr{E})$ in the form of a Maxwell function

$$f_0 = 4n(\pi a_e)^{3/2} \exp(-a_e k^2), \quad a_e = \hbar^2/2m^* k_0 T_e, \quad (15)$$

where n is the conduction-band electron density, and T_e is the electron temperature, which, generally speaking, does not coincide with the lattice temperature T.[2] Calculating in the usual way the electroconductivity σ and using Eqs. (6), (14), and (15), we obtain

$$\sigma = \frac{2Be^2 n a_e^{5/2}}{\pi^{3/2} m^*} \int_0^\infty k^5 \exp(-a_e k^2) Q(k) dk, \quad (16)$$

$$Q = \frac{2\pi}{F_2}\left(d \ln \frac{d+1}{d-1} - 2\right), \quad d^2 = \frac{k^2 + (B/\tau_p)k + F_1}{F_2}. \quad (17)$$

Before we consider the general case when all three scattering mechanisms act simultaneously, let us consider particular cases in which some of the mechanisms are inessential.

1. Only the scattering by the potential φ and by the polarization oscillations are significant (high-temperature case). In the general equations (16) and (17) we must put $B \to \infty$. Then

$$\sigma_{\varphi p} = \frac{4Ae^2 n}{m^*(1-\eta)(\pi a_e)^{1/2}}\left(d_0 \ln \frac{d_0+1}{d_0-1} - 2\right), \quad (18)$$

$$d_0^2 = \frac{3 + \eta + A/C}{1 - \eta}.$$

When $d_0 \gg 1$ the logarithm can be expanded in powers of d_0^{-1}. This yields

$$\sigma_{\varphi p} \approx \sigma^0 \equiv \frac{8Ae^2 n}{3m^*(3 + \eta + A/C)(\pi a_e)^{1/2}} \quad (19)$$

2. Only the deformation-potential scattering is essential. In the general equations (16) and (17) we should put $A \to \infty$ and $\tau_p \to \infty$. We obtain

$$\sigma_d = \frac{4Be^2 n}{3m^*}\left(\frac{a_e}{\pi}\right)^{1/2} \quad (20)$$

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[2] The field-heated electrons may have a Maxwell distribution, particularly owing to their Coulomb interaction (H-theorem). There exists a carrier-density range in which their Coulomb interaction Maxwellizes f_0 but it can be ignored in Eq. (6) for f_1 [3,4].

Scattering by polarization oscillations in the case of low temperatures and weakly polar crystals is often less important than the other scattering mechanisms, and is therefore not considered here. It can be analyzed with the aid of Eqs. (16) and (17).

Returning to the case of simultaneous action of the three scattering mechanisms (the upper equation in (12) is used for τ_p), we expand Q (Eq. (17)) in powers of d^{-1}, $(F_1/F_2 > 3)$ to obtain

$$\sigma = \frac{4e^2 nA}{(\pi a_e)^{1/2} m^*(3 + \eta + A/C)} \sum_{v=1}^\infty \frac{\Phi_v(x)}{(2v+1)d_0^{2(v-1)}}; \quad (21)$$

$$\Phi_v(x) = \frac{(-1)^{v-1}}{(v-1)!}\left\{\sum_{k=1}^\infty (-1)^k (k-1)!(v-k-1)\right.$$

$$\times (v-k-2)x^{v-k} - (2v-3)x^v - x^{v+1}$$

$$\left. - [x^{v+2} + 2(v-1)x^{v+1} + (v-1)(v-2)x^v]e^x \operatorname{Ei}(-x)\right\},$$

$$x \equiv 2\frac{\sigma_d}{\sigma^0} > 0, \quad \operatorname{Ei}(-x) \equiv -\int_x^\infty \frac{e^{-u}}{u} du. \quad (22)$$

For usual values of the crystal parameters it is sufficient to retain two or three terms in the expansion (21); $\Phi_v(\infty) = 2$.

We have above used the kinetic equation. It is valid when the Heisenberg uncertainty in the kinetic energy $\hbar/\tau$ of the carrier is much less than the kinetic energy $k_0 T$ itself.[5] This inequality is equivalent to requiring that the deBroglie wavelength of the carrier be much shorter than the free path. Unfortunately, this inequality is violated in many real cases. The above results are therefore applicable only to semiconductors with comparatively high mobility, or at sufficiently low temperatures. The applicability range of the theory of scattering by the polarization oscillations of the lattice is especially limited, because in this case the free path is often less than the lattice constant. Therefore it is unjustified to assume that the optic-phonon field is a small perturbation, and it is necessary to proceed to the polaron theory. However the mobility calculation in the polaron theory is complicated, and the approximations of different authors lead to different results. In this case it is better to use experimental data for the mobility due to the interaction with optical vibrations.

With increasing $\epsilon_0 E$ the probability of scattering by the potential φ increases in proportion to $(\epsilon_0 E)^2$, and for large $\epsilon_0 E$ this scattering mechanism begins to dominate. Then the mobility begins to decrease approximately like E^{-2}, i.e., the current-voltage characteristic of the semiconductor begins to fall off. Using the Lorentz-Lorenz

equation to estimate g_1, we obtain $g_1 \approx \epsilon_0/3$ when $\epsilon_0 \gg 1$.[1] The characteristic begins to fall off at practicable values of E if the dielectric constant ϵ_0 is very large (on the order of several thousand). Substances with such ϵ_0 are known (compounds based on barium titanate and lead titanate, rutile, SbSI, etc.).

As an example, let us consider the case when the competing scattering mechanisms are the deformation potential and the potential φ, other mechanisms being inessential. Let $T = T_e = 200°$ K, $\epsilon_0 = 2500$, b = 10 eV, m* equals the free electron mass, $\gamma s_{||}^2 = 2.5 \times 10^{12}$ dyne/cm^2, $g_1 \approx g_2 \approx \epsilon_0/3$, $s_{||}/s_\perp = 2$, and the conduction electron density 10^{15} cm^{-3}. The dependence of the current density J on the applied field E is then represented by a curve a in the figure. The maximum of the curve is at E = 10^5 V/cm.

This curve was calculated from Eqs. (19)–(22), assuming $C \to \infty$. Calculation of the resulting mobility, using Matthiessen's rule

$$\frac{1}{u} = \frac{1}{u_d} + \frac{1}{u_\varphi} \qquad (23)$$

yields a value which differs by 4–5% (even in the region of the maximum of the curve). Matthiessen's rule is exact when: 1) the reciprocal relaxation times are additive, and 2) the ratio of the relaxation times does not depend on the wave vector k. If only the first condition is satisfied, the rule is valid approximately, with an accuracy that is the larger, the weaker the k-dependence of the relaxation-time ratio. To calculate current-voltage characteristics like those shown in the figure we can therefore employ Matthiessen's rule, using the experimental values of the mobility due to all the scattering mechanisms which do not depend upon E, measured at low E. u_φ can be found from Eq. (18) with $C \to \infty$.

At low temperatures the scattering by neutral impurity atoms may turn out to be dominant. The corresponding mobility is[6]

$I \cdot 10^{-3}$ A/cm^3

$E \cdot 10^{-5}$ V/cm
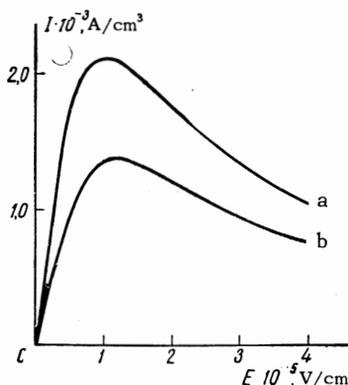
$$u_N = \frac{1}{20} \cdot \frac{m^* e^3}{N \epsilon_0 \hbar^3}. \qquad (24)$$

Here N is the concentration of the neutral impurity atoms. If N = 0.5×10^{16} cm^{-3}, T = 4° K, T_e= 200° K, ϵ_0 = 20000, $\gamma s_{||}^2 = 2.5 \times 10^{12}$ dyne/cm^2, $g_1 = g_2 = \epsilon_0/3$, $s_{||}/s_\perp = 2$, the density of the conduction electrons is n = 10^{15} cm^{-3}, and m* equals the free electron mass, then an account of the scattering by neutral impurities and by the potential φ, using Matthiessen's rule, leads to a current-voltage characteristic represented by curve b on the figure.[3]

In conclusion we note that the kinetic equation is meaningful only if $\hbar e/m^* u \ll (3/2)k_0 T_e$, as mentioned above. The solution of this equation under the assumption $f_1 \ll f_0$, means $uE \ll (3k_0 T_e/m^*)^{1/2}$; the expansion (1) is correct if

$$g_1 \operatorname{div} \mathbf{u} \sim \frac{2g_1}{\pi} \left(\frac{k_0 T}{3\gamma s_{||}^2 \hbar^3} \right)^{1/4} (3m^* k_0 T_e)^{3/4} < 1.$$

Finally, for the competition of the potential φ with other scattering mechanisms, E should not be small. It is difficult to satisfy simultaneously all these inequalities, and in the foregoing numerical examples they are fulfilled without margin. However, the qualitative character of the relations shown in the figure (especially, the presence of a maximum) is subject to no doubt. By using another method to solve the kinetic equation we can get rid of the second inequality. This will broaden the applicability range of the theory and improve the ability to fulfill the other criteria.

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[3]Equations (15)–(22) are correct for any dependence of T_e on E. Unfortunately, this dependence is known only for a few particular cases. If the temperature T_e rises to a value such that the carriers begin to generate optical phonons intensely, further increase of T_e with increasing E is slowed down, and T_e remains nearly constant to a certain critical value of E. Such a case was assumed in the calculation of the curves, each of which corresponds to a fixed T_e.

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