SOLUTION OF THE KINETIC EQUATION

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Abstract

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SOLUTION OF THE KINETIC EQUATION

FOR SEMICONDUCTORS WITH A NARROW CONDUCTION BAND

IN A STRONG ELECTRIC FIELD

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The solution of the kinetic equation for semiconductors with a narrow conduction band in strong electric fields is of interest in connection with the study of the properties of organic crystals, whose band widths at ordinary temperatures, as calculations show (^{1}), are of the order of k_0T. The electrical conductivity in such semiconductors in strong electric fields must have a number of special features. These features are connected primarily with the fact that current carriers located in the lower half of the band have a positive effective mass and behave as electrons, while in the upper half of the band they behave as holes.

As the electric field increases, the energy acquired by an electron between two collisions also increases. The magnitude of the acquired energy is determined by the relaxation time of electron–phonon collisions. For relatively small electric fields, the displacement in the distribution of current carriers in the band, which disturbs its symmetry, is proportional to the field, and in this region the electrical conductivity obeys Ohm' s law. There exists, however, a critical electric field at which the transfer of energy to the lattice becomes too slow and the electrons "heat up." In this case a further increase in the electric-field strength leads to an accumulation of carriers in the upper half of the band, and their distribution again becomes symmetric owing to the narrowness of the bands. The return to symmetry in the carrier distribution at fields exceeding a certain critical value leads to a decrease in the current with increasing field. This result is given in (^{2}), where an asymptotic solution of the kinetic equation for large fields was obtained for a narrow-band model with a truncated quadratic dispersion.

In the present work a solution of the kinetic equation is obtained for crystals with a narrow conduction band under the following assumptions:

1) For the current carriers, a spectrum calculated in the nearest-neighbor approximation is used.

2) It is assumed that the gap Δ between bands is considerably larger than the energy of the electric field

$$eEa \ll \Delta, \tag{1}$$

where a is the distance between nearest neighbors; for this reason interband transitions are excluded from consideration. It should be noted that for organic crystals $\Delta \sim 1$ eV; therefore for them condition (1) is satisfied practically at all fields.

3) It is assumed that the band width W is smaller than the energy of optical photons $\hbar\omega_0$,

$$W < \hbar\omega_0, \tag{2}$$

and therefore interaction with optical vibrations is not considered. In addition, we shall assume that the electric field is not so large as to strongly change the wave function and the spectrum of the carriers in the

zone

$$eEa < W, \tag{3}$$

which for organic semiconductors corresponds to fields $E \lesssim 5 \cdot 10^5$ V/cm.

The solution of the kinetic equation will be obtained for the case of a one-dimensional chain; however, the generalization of this method to the three-dimensional case presents no difficulty.

The spectrum of current carriers for the model of a one-dimensional molecular crystal in the nearest-neighbor approximation has the form

$$\varepsilon(k) = \frac{1}{2}W(1 - \cos ka). \tag{4}$$

Here the band is shifted in such a way that its bottom is at $k = 0$.

The basic scattering mechanism, taking into account assumption (2), is scattering by intermolecular acoustic vibrations. If the nonequilibrium distribution function is sought in the form

$$n_k = n_k^{(0)} + \Delta n_k, \qquad \Delta n_k = n_k^{(0)}\chi v_k, \tag{5}$$

where $n_k^{(0)}$ is the equilibrium distribution function, $\chi(\varepsilon_k)$ is the function to be found, and $v_k = \dfrac{1}{\hbar}\dfrac{\partial\varepsilon(k)}{\partial k}$ is the velocity of the current carriers, then the electron-phonon collision operator can be written as follows

$$(\partial n_k/\partial t)_{\text{st}} = -n_k^{(0)} \chi v_k/\tau. \tag{6}$$

Since in the case of narrow bands the relaxation time τ is a smooth function of the quasimomentum k (^{3}), τ may be regarded as constant. For the change in the number of particles in the state k under the influence of the electric field, we then obtain

$$\left(\frac{\partial n_k}{\partial t}\right)_{\text{field}} = \frac{\partial n_k}{\partial k}\frac{dk}{dt} = -\frac{eE}{k_0 T} n_k^{(0)} \left[v_k + (\chi v_k) v_k - \chi' v_k k_0 T - \chi \hat{m}^{-1} k_0 T\right], \tag{7}$$

where

$$(\hat{m}^{-1})_{ij} = \frac{1}{\hbar^2}\frac{\partial^2 \varepsilon(k)}{\partial k_i \partial k_j}, \qquad \chi' = \frac{\partial \chi(\varepsilon)}{\partial \varepsilon}.$$

Substituting now (6) and (7) into the stationarity condition

$$(\partial n_k/\partial t)_{\text{st}} + (\partial n_k/\partial t)_{\text{field}} = 0,$$

for the spectrum (4) it is not difficult to obtain the basic equation

$$\chi \sin z - \alpha \sin z - \alpha \chi v_0 \sin^2 z + \chi' v_T \sin z + \chi v_T \cos z = 0. \tag{8}$$

Here the notation introduced is

$$v_0 = \frac{Wa}{2\hbar}; \qquad v_T = \frac{k_0 T a}{\hbar}; \qquad z = ka; \qquad \chi = \chi(z); \qquad \chi' = \chi'(z);$$

$$\alpha = \frac{eE\tau}{k_0 T}.$$

By the change of variable $\chi \sin z = u$, equation (8) is reduced to the form

$$u' - \left(\frac{v_0}{v_T}\sin z - \frac{1}{\alpha v_T}\right) u - \frac{\sin z}{v_T} = 0.$$

Its general solution is

$$u(z) = \frac{1}{v_T}\exp\left[-\frac{v_0}{v_T}\cos z - \frac{z}{\alpha v_T}\right]\left\{\int \exp\left[\frac{v_0}{v_T}\cos z + \frac{z}{\alpha v_T}\right]\sin z\, dz +\right.$$

$$+ C \exp\left[-\frac{v_0}{v_T}\cos z - \frac{z}{\alpha v_T}\right]\Bigg\}.$$

Taking into account that

$$n_k^{(0)} = n_0 \exp\left[-\frac{v_0}{v_T}(1-\cos z)\right],$$

we find Δn_k

$$\Delta n_k = n_0 \frac{Wa}{2\hbar}\exp\left[-\frac{v_0}{v_T}\right]\left\{\frac{1}{v_T}\exp\left[-\frac{z}{\alpha v_T}\right]\int \exp\left[\frac{v_0}{v_T}\cos z + \frac{z}{\alpha v_T}\right]dz + \right.$$

$$\left. + C\exp\left[-\frac{z}{\alpha v_T}\right]\right\}. \tag{9}$$

The constant C is determined from the condition of conservation of the number of particles:

$$\sum_k \Delta n_k = 0.$$

Passing here from summation over k to integration, we obtain an equation for determining C

$$\frac{1}{v_T}\int_{-\pi}^{\pi}\exp\left[-\frac{z}{a v_T}\right]dz\int \exp\left[\frac{v_0}{v_T}\cos z + \frac{z}{a v_T}\right]\sin z\,dz + C\int_{-\pi}^{\pi}\exp\left[-\frac{z}{av}\right]dz = 0. \tag{10}$$

Expanding in the first term of (10) the exponential in $\frac{v_0}{v_T}\cos z$, we obtain

$$\int_{-\pi}^{\pi}\exp\left[-\frac{z}{a v_T}\right]dz\int \exp\left[\frac{v_0}{v_T}\cos z + \frac{z}{a v_T}\right]\sin z\,dz =$$

$$= \sum_{p=0}^{\infty}\frac{(v_0/v_T)^{2p}}{(2p)!}\int_{-\pi}^{\pi}\exp\left[-\frac{z}{a v_T}\right]F_{2p}(z)\,dz +$$

$$+ \sum_{p=1}^{\infty}\frac{(v_0/v_T)^{2p-1}}{(2p-1)!}\int_{-\pi}^{\pi}\exp\left[-\frac{z}{a v_T}\right]F_{2p-1}(z)\,dz,$$

where $F_n(z) = \int \exp\left[-\frac{z}{a v_T}\right]\cos^n z\,\sin z\,dz$ has the form (4)

$$F_{2p}(z) = \frac{1}{2p+1}\left\{\exp\left[-\frac{z}{av_T}\right]\cos^{2p+1} z + \frac{1}{av_T}\frac{\exp[z/av_T]}{2^{2p}}\sum_{s=0}^{\infty}\binom{2p+1}{p-s}\times\right.$$

$$\left.\times\left[\left(\frac{1}{av_T}\right)^2 + (2s+1)^2\right]^{-1}\left[\frac{1}{av_T}\cos(2s+1)z + (2s+1)\sin(2s+1)z\right]\right\},$$

$$F_{2p-1}(z) = \frac{1}{2p}\left\{-\exp\left[\frac{z}{av_T}\right]\cos^{2p} z + \binom{2p}{p}\frac{\exp[z/av_T]}{2^{2p}}+\right.$$

$$\left.+\frac{1}{av_T}\frac{\exp[z/av_T]}{2^{2p-1}}\sum_{s=1}^{\infty}\binom{2p}{p-s}\left[\left(\frac{1}{av_T}\right)^2 + 4s^2\right]^{-1}\left[\frac{1}{av_T}\cos 2sz + 2s\sin 2sz\right]\right\}.$$

Substituting the expressions found for $F_{2p}(z)$ and $F_{2p-1}(z)$ into the original integral, it is not difficult to see that it is equal to zero. Hence it follows that also $C = 0$.

For the current we then obtain

$$j = \sum_k e\Delta n_k v_k = n_0 e\frac{v_0^2}{v_T}\exp\left[-\frac{v_0}{v_T}\right]\sum_{n=0}^{\infty}\frac{(v_0/v_T)^n}{n!}\int_{-\pi}^{\pi}\exp\left[-\frac{z}{av_T}\right]\sin z\, F_n(z)\, dz.$$

From the form of the functions $F_{2p}(z)$ and $F_{2p-1}(z)$ it follows that only one term, the last one in $F_{2p}(z)$, with $s = 0$, will not vanish after integration. Thus,

$$j = n_0 e\frac{v_0^2}{v_T}\sum_{p=0}^{\infty}\frac{(v_0/v_T)^{2p}}{(2p)!}\frac{1}{2p+1}\frac{1}{av_T}\frac{1}{2^{2p}}\binom{2p+1}{p}\left[\left(\frac{1}{av_T}\right)^2 + 1\right]^{-1}\times$$

$$\times\int_{-\pi}^{\pi}\sin^2 z\, dz\,\exp\left[-\frac{v_0}{v_T}\right] = 2\pi e n_0 v_0\exp\left[-\frac{v_0}{v_T}\right]\frac{a\omega_T}{1+(av_T)^2}I_1\left(\frac{v_0}{v_T}\right).$$

Here $I_1(v_0/v_T)$ is the Bessel function of purely imaginary argument.

Taking now into account that the concentration of carriers in the band is

$$n = \sum_k n_k^{(0)} = n_0 \int_{-\pi}^{\pi} \exp\left[-\frac{v_0}{v_T}(1-\cos z)\right] dz = n_0 \exp\left[-\frac{v_0}{v_T}\right] 2\pi I_0\left(\frac{v_0}{v_T}\right),$$

we obtain the final expression for the current

$$j = ne^2 \frac{Wa^2}{2\hbar^2} \frac{E\tau}{1+\left(\frac{eE\tau a}{\hbar}\right)^2} \frac{I_1(W/2k_0T)}{I_0(W/2k_0T)}. \tag{11}$$

If one plots the dependence of the current density j on E, it will have a maximum at $E = E_{\max}$, where $E_{\max}$ is found from the condition

$$eE_{\max}\tau a/\hbar = 1; \qquad E_{\max} = \hbar/e\tau a, \tag{12}$$

which, for example, for anthracene and naphthalene crystals corresponds to fields $E \sim 3\div 5\cdot 10^4$ V/cm. Of principal interest, of course, is the inverse problem —the determination of the relaxation time from the position of the maximum on the current-voltage characteristic

$$\tau = \hbar/eE_{\max}a.$$

We note that $E_{\max}$ is at least an order of magnitude smaller than the value of the field at which condition (3) is violated. Thus, one may hope for an experimental determination of the relaxation time.

Relation (11) is not difficult to generalize to the case of a three-dimensional rectangular lattice

$$j_\mu = ne^2 \frac{W_\mu a_\mu^2}{2\hbar^2} \frac{E_\mu \tau_\mu}{1+(eE_\mu\tau_\mu a_\mu/\hbar)^2} \frac{I_1(W_\mu/2k_0T)}{I_0(W_\mu/2k_0T)} \quad (\mu = 1,2,3), \tag{13}$$

where τ_μ, W_μ, and a_μ are, respectively, the relaxation time, the band width, and the distance between nearest neighbors in the direction μ.

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Note: Figure translations are in progress. See original paper for figures.