I-V characteristic for electrons with narrow, allowed bands at low temperatures

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The *I-V* characteristic $j(E)$ for electrons with narrow, allowed bands at low temperatures is calculated by solving the Fokker-Planck equations. The characteristic maximum is observed in the $j(E)$ dependence.

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The experimental studies of electron mobility in molecular crystals[1] in a strong electric field showed the need for a theoretical analysis of the kinetics of electrons with narrow, allowed bands. In this paper we calculated the mobility of an electron that interacts with acoustic phonons at a temperature $T \ll \omega_D$ (ω_D is the Debye frequency of phonons) and an arbitrary electric field E. We assumed that the width of the allowed band is $M \ll \omega_D$.

As is well known from the theory of small-radius polarons[2] in narrow-band systems, the linear electron-phonon interaction with respect to the displacements turns out to be strongly suppressed proportionally to the small parameter $M/\omega_D \ll 1$. Under these conditions the quadratic interaction, which does not have such a small parameter, plays the dominant role. This was also mentioned in Rashba's paper[7] in connection with the kinetics of molecular excitons. The Hamiltonian of the quadratic interaction has the form

$$H_{int} = \frac{1}{N} \sum_{q_1, q_2, n} \psi_n^+ \psi_n \gamma_{q_1 q_2} e^{in(q_1 + q_2)} (b_{q_1} + b_{-q_1}^+)(b_{q_2} + b_{-q_2}^+). \tag{1}$$

The interaction constant for the acoustic phonons is $\gamma_{q_1 q_2} = C_2 (q_1 q_2)^{1/2} / M_1 s$, where C_2 is the corresponding deformation potential, M_1 is the mass of a unit cell, and s is the velocity of sound. Below we shall examine a simple cubic lattice with a period $a = 1$. Since $M \ll \omega_D$, the electron velocity v is small compared with s, and therefore the one-phonon and two-phonon emission and absorption processes are forbidden by the conservation law. Thus, at low temperatures there is only Compton scattering of phonons by an electron, which corresponds to the terms such as $b_{q_1}^+ b_{q_2}$ in the Hamiltonian (1). A comparison of the corresponding scattering probability with the contribution from linear interaction shows that the quadratic electron-phonon interaction dominates in narrow-band systems if $MC_1^2 / C_2 \omega_D \ll 1$, where C_1 is the deformation potential for the linear interaction.

At low temperatures $T \ll \omega_D$ the scattering probability of an electron is small and its mobility is described by the kinetic equation. If the conditions $T \ll \omega_D$ and $M \ll \omega_D$

are satisfied, then the thermal momenta of phonons $q \sim T/s$ will be small compared with the electron momentum p. Therefore, the collision integral can be expanded in $q/p \ll 1$, and the kinetic equation becomes the Fokker-Planck equation.[3] This equation for the examined system assumes the form

$$\mathbf{E}\, e\, \frac{\partial}{\partial \mathbf{p}} f = \frac{\partial}{\partial \mathbf{p}} \left(A f + B \frac{\partial}{\partial \mathbf{p}} f \right), \tag{2}$$

where e is the electron charge and the values A_α and B are determined by the relations

$$B = \frac{(2\pi)^5}{60} \omega_D q_D^8 \left(\frac{C_2}{M_1 s^2} \right)^2 \left(\frac{T}{\omega_D} \right)^9, \quad A_\alpha = \frac{1}{T} v_\alpha B, \quad \alpha = x, y, z. \tag{3}$$

Here $q_D = \omega_D/s$ is the Debye momentum of the phonons and v_α is the electron velocity. The distribution function $f(\mathbf{p})$ must satisfy the periodic boundary conditions and the normalization condition.

In the case of a one-dimensional electron, Eq. (2) can be easily solved for an arbitrary spectrum $\epsilon(\mathbf{p})$ (as before, the phonon spectrum is assumed to be three dimensional). To do this, it is sufficient to make the substitution $f(\mathbf{p}) = \chi(\mathbf{p}) \exp(-\epsilon(\mathbf{p})/T)$ and perform a Fourier transformation. As a result, the equation for the current $j(E)$ has the form

$$j(E) = Te\, \phi_0 (E/E_0), \quad E_0 = B/e, \quad \phi_0(x) = \phi_1(x)/\phi_2(x), \tag{4}$$

$$\phi_1(x) = \sum_{-\infty}^{\infty} \frac{im}{im - x} A_m B_m^*, \quad \phi_2(x) = \sum_{-\infty}^{\infty} \frac{A_m B_m^*}{im - x}, \tag{5}$$

where A_m and B_m are the Fourier components of $\exp(\epsilon(p)/T)$ and $\exp(-\epsilon(p)/T)$, respectively. If the free electron motion is described by the strong-binding approximation, then $\epsilon(p) = -2M \cos p$ and the values A_m, B_m are defined by the relations

$$A_m = (-1)^m B_m = (-1)^m I_m(\beta), \quad \beta = 2M/T, \tag{6}$$

where I_m are the modified Bessel functions. The plots of the dependence $j(E)/j_0 (j_0 = 2Me)$ for $\beta = 0.2$, 2, and 4 are shown in Fig. 1. This dependence has a characteristic maximum at $E = 1.1\, E_0$. Note that its location is independent of β. In the region $E \ll E_0$, $j(E) \propto E/E_0$. Therefore, the electron mobility μ in weak fields has the form

$$\mu(T) = \frac{T}{eE_0} \frac{I_0^2(\beta) - 1}{I_0^2(\beta)}. \tag{7}$$

at $M \ll T$, $\mu(T) \approx \beta^2 T/2\, eE_0 \propto T^{-10}$. This asymptotic form was obtained by using a different method.[4,5]

In the region $E \gg E_0$, $j(E) \propto E_0/E$. A decrease of $j(E)$ in strong fields results in a negative differential conductivity. The mechanism for the decrease of $j(E)$ in strong

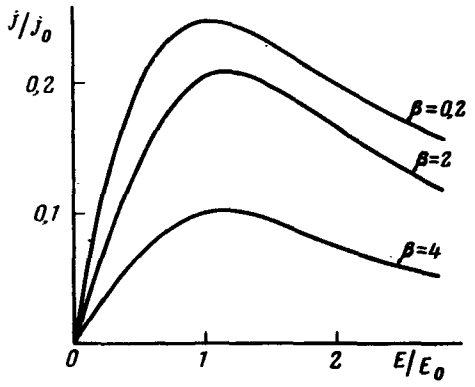

FIG. 1. *I-V* characteristic for $\beta = 0.2$, 2, and 4.

fields is the same as that in Ref. 6. Note that the characteristic field E_0, at which a strong nonlinearity occurs, decreases rapidly with decreasing temperature ($E_0 \propto T^8$). This leads us to believe that a strong nonlinearity can be observed experimentally at temperatures $T \sim 10$ K.

In the strong-binding approximation the electron spectrum in a tetragonal crystal lattice has the form

$$\epsilon(\mathbf{p}) = \sum_{\alpha} \epsilon_{\alpha}(p_{\alpha}). \tag{8}$$

In this case the variables in Eq. (2) are separated and therefore all the results obtained for the one-dimensional problem can be directly extended to systems of any dimension. This makes it possible to use the simple Eqs. (4)–(6) to describe the $j(E)$ dependence in molecular crystals. In this case the current component j_α along the α axis in the field E_α is defined by Eqs. (4) and (5) into which $E = E_\alpha$ and $\epsilon(p) = \epsilon_\alpha(p_\alpha)$ must be substituted. Note that all the obtained results, which are valid for any narrow-band quantum particles, can describe the tunneling of light ions in a crystal lattice.

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