Electrical conductivity anomalies in a quasi-one-dimensional crystal due to interference of two mechanisms of electron-phonon interaction

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A a quasi-one-dimensional model of a crystal, in which for specific states of the charge carriers, two mechanisms of electron-phonon interaction weaken one another, is examined. As a result, the system has an anomalously large conductivity with an anomalous temperature dependence.

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In this paper we consider the calculation of the electrical conductivity of a molecular crystal by taking into account simultaneously two major mechanisms for interaction of electrons with the lattice vibrations due to fluctuations resulting from intermolecular vibrations of the resonance integrals and the polarization energy of the molecules surrounding the conduction electrons. We shall restrict ourselves to temperatures exceeding the maximum temperature T_C of the phase transition.[1] It is known that above T_C there is a certain temperature range (sufficiently broad for a weak coupling between the one-dimensional filaments) in which, to describe the properties of a quasi-one-dimensional system, we can assume that it is possible to consider the filaments are uncoupled. Thus, we have a one-dimensional model of a crystal. In addition, we shall assume that the impurity concentration is small enough so that $\tau_{ph} \ll \tau_i$ (τ_i and τ_{ph} are the scattering times of an electron by impurities and phonons), and the conductivity σ can be determined from the kinetic equation.[2]

Using the band scheme in the strong coupling and nearest-neighbor approximations, we represent the matrix element of the electron-phonon interaction $A(k, q)$ in the form:

$$A(k, q) = 2i\omega'(2NM\omega_q)^{-1/2}\,[\gamma \sin q a + \sin ka - \sin(k-q, a)]. \qquad (1)$$

Here $\gamma = 2e^2a_0/a_5w'$, e is the electron charge, a is the lattice constant, a_0 and M are the average polarizability and mass of the molecule, N is the number of molecules in the main region of the crystal, w and w', respectively, are the resonance integral between the nearest neighbors and its derivative with respect to the intermolecular distance, k and q are the one-dimensional quasi momenta of the electron and phonon with the energies $\epsilon(k) = -2w \cos ka$ and $\omega_q = 2v_s a^{-1} |\sin qa/2|$, and v_s is the speed of sound.

Analogous Hamiltonian, written in the nodal representation, was used in Ref. 3 in calculating the carrier mobility in anthracene. If the parameter $\gamma \gg 1$, then the first mechanism of the electron-phonon interaction, which is associated with the fluctuations of the polarization energy, is predominant in the Hamiltonian. An analogous situation occurs, for example, in the case of small-radius polarons. If $\gamma \ll 1$, then the second mechanism, which is associated with the fluctuations of the resonance inte-

grals, is predominant. This case has been examined, for example, in Ref. 4. We shall examine the case $\gamma \approx 1$. The interference effects between the two electron-phonon interaction mechanisms mentioned above become important in the Hamiltonian. We shall limit ourselves to intermediate temperatures in order to study the elastic scattering processes of electrons by phonons. It follows from the energy-conservation law that $q = 2k$ is large. Moreover, as seen in Eq. (1), the probability of electron back scattering is zero for values of k determined from the relation $\cos ka = -\gamma^{-1}$. This means that the electron waves corresponding to these states propagate without (or nearly without) scattering. We examine a semiconductor with a p-band conductivity. The conditions for occurrence of anomalies in the temperature dependence of σ in this case are much better as comparison with the s band, since the compensation for the scattering mechanisms is for the states with a small k. We use the kinetic equation to estimate σ. For a nondegenerate hole gas at intermediate temperatures ($k_0 T \gg v_s a^{-1}$), we obtain:

$$\sigma = \frac{e^2 n M v_s w^3}{\pi (k_0 T)^2 \gamma^3 w'^2 I_0(\mu)} \{(1-\gamma+\gamma/\mu)\exp(-\mu) - (1+\gamma+\gamma/\mu)\exp\mu + \exp(\mu/\gamma)[2-\mu(\gamma^2-1)/\gamma][Ei(-\mu(1+\gamma)/\gamma) - Ei(-\mu(1-\gamma)/\gamma)]\}, \quad (2)$$

where n is the concentration of holes, $Ei(x)$ is the integral exponential function, $\mu = 2w/k_0 T$, and $I_0(\mu)$ is the Bessel function of an imaginary argument. In the limiting case of a broad conduction band and $\gamma \ll 1$, the usual temperature dependence $\sigma \sim T^{-1/2}$ follows from Eq. (2). In the general, the dependence of σ on T is more complex and varies significantly as $\gamma \to 1$ (see Fig. 1). At $[\mu(1-\gamma)/\gamma] \ll 1$, it follows from Eq. (2) that

$$\sigma \cong \frac{4e^2 n v_s^2 M w^{7/2}}{\sqrt{\pi} w'^2 \gamma^2 (k_0 T)^{5/2}} \left[\ln \frac{\gamma k_0 T}{2w(1-\gamma)} - C - 1\right], \quad (C = 0{,}577\ldots). \quad (3)$$

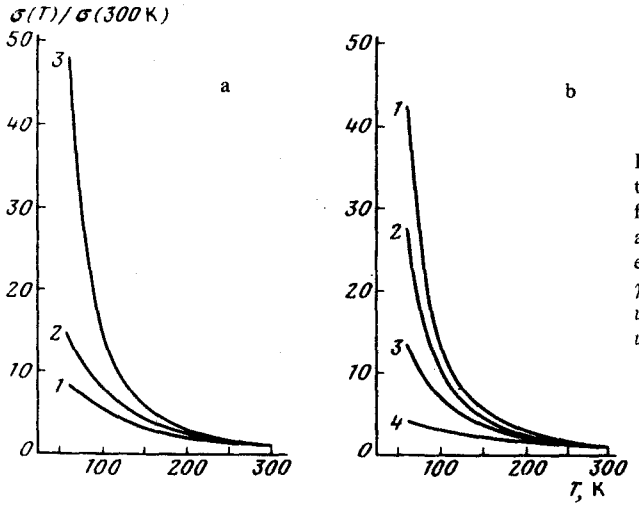

FIG. 1. Temperature dependence of the electrical conductivity calculated from Eq. (2) and reduced to its value at room temperature: (a) $w = 0.013$ eV; 1, $\gamma = 0.1$, 2, $\gamma = 0.5$, 3, $\gamma = 0.999$; (b) 1,2,3, $\gamma = 0.999$, 1, $w = 0.026$ eV, 2, $w = 0.26$ eV, 3, $w = 2.6$ eV, 4, $\gamma = 0.5$, $w = 0.065$ eV.

First, we see that in these materials we can expect anomalously large conductivities as $\gamma \to 1$. Second, the temperature dependence of σ, which is now close to $T^{-5/2}$, varies.

We shall further assume that γ varies with temperature only due to variation of the lattice constant a as a result of thermal broadening of the crystal. In general, this variation, which is attributable to the anharmonicity of the lattice vibrations, is small, and we take it into account only in the expression $(1-\gamma)$ under the logarithm in Eq. (3), since because of it $\gamma \to 1$. We have

$$\gamma = \gamma_0(1 - 5\beta T), \tag{4}$$

where γ_0 is the value of γ at a temperature of absolute zero and β is the linear expansion coefficient.

Suppose the value of γ at room temperature (or higher) is $\lesssim 1$. As T decreases, the value of γ increases according to Eq. (4), and at some temperature T' it reaches unity. Thus, from Eq. (3) we obtain

$$\sigma \cong \frac{4e^2 n v_s^2 M w^{7/2}}{\sqrt{\pi} w'^3 \gamma^2 (k_0 T)^{5/2}} \left[\ln \frac{k_0 T}{10\beta w (T - T')} - C - 1 \right], \tag{5}$$

$$T' = (5\beta)^{-1}(1 - \gamma_0^{-1}). \tag{6}$$

As seen in Eq. (5), σ diverges logarithmically as $T \to T'$.

If the hole gas is degenerate, we obtain for σ

$$\sigma = \frac{e^2 v_s^2 M \epsilon_F w^2 (4w - \epsilon_F)}{\pi w'^2 a (5\beta\gamma_0)^2 (2w - \epsilon_F)^2} \frac{1}{k_0 T (T - T'')^2}, \tag{7}$$

$$T'' = (5\beta)^{-1}[1 - 2w/(\gamma_0(2w - \epsilon_F))], \tag{8}$$

where ϵ_F is the Fermi energy.

Taking into account the impurities or other crystals imperfections, we can see that σ is finite and reaches near T' or T'' a certain maximum which decreases with increasing impurity concentration and may even be completely smeared out. It should be noted, however, that in the immediate vicinity of the maximum the condition $\tau_{ph} \ll \tau_i$ is violated, and a more rigorous treatment is required to calculate σ.[2,5]

Taking into account the weak coupling between the one-dimensional filaments also limits the sharp increase of conductivity, and the strong coupling may completely smear out the maximum of the conductivity. This problem will be examined separately.

Finally, we note that such dependences with a sharp conductivity maximum were indeed observed (see Ref. 4). However, since we do not know the specific values of all

the parameters, we cannot verify the validity of this model. We note that if we assume that $a \sim 4$ Å, the width of the conduction band $\Delta \sim 0.1$ eV, and $w' \sim 2w$ Å^{-1}, then γ reaches unity at $a_0 \sim 1$ Å^3, which is realistic for a_0.

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