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Letters to the Editor

SEMICONDUCTOR-METAL TRANSITION BY RANDOMLY SHIFTED BANDS MODEL

ПЕРЕХОД ПОЛУПРОВОДНИК-МЕТАЛЛ В МОДЕЛИ СО СЛУЧАЙНО СДВИНУТЫМИ ЗОНАМИ

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The semiconductor-metal transition is a well-known experimental fact observed at high temperatures in many liquid semiconductors. The results obtained on some liquid semiconductors (namely on liquid chalcogenides) are summarized in A. A. Andreev's review [1]. The general features of the observed temperature range (including the semiconductor-metal transition region) are as follows:

i) There are no essential differences between the solid noncrystalline semiconductor and its crystalline counterpart. The ln σ vs $1/T$ plot gives a straight line, the slope of which yields the thermal activation energy of el. conductivity. Some deviation from the straight line can be observed at low. temperatures in certain cases. The low-temperature region is discussed in [2, 3] in more detail.

ii) At temperatures above the melting point a gradual increase of the $\sigma(T)$ dependence is observed, from which the increase of thermal activation energy given as $\mathrm{d}(\ln\sigma)/\mathrm{d}\frac{1}{T}$ follows.

iii) At high temperatures, usually about 1000 K and more, the semiconductor-metal transition occurs. The value of el. conductivity is equal to about $10^2-10^3\ \Omega^{-1}\mathrm{cm}^{-1}$.

The conception of localized states in the forbidden band of a liquid semiconductor is a common feature of practically all theories of the semiconductor-metal transition (see, e.g. [1]). The delocalization causes the transition to metallic conductivity. It is, therefore, interesting to show that semiconductor-metal transition can be interpreted (under certain assumptions) also in terms of a randomly shifted bands model, i.e. without the conception of localized states.

Starting from the assumption that the one-particle potential can be written as

$$u(r)=u_k(r)+u_p(r)\,, \tag{1}$$

($u_k(r)$ is a periodical function, $u_p(r)$ is a stationary random function) an original approach to the calculation of the density of states of an electron in a random potential was presented [2]. It was shown that in certain ranges of the dispersion of the random potential η and the correlation length L, the quantum-mechanical corrections can be neglected. The expression for the density of states has then the simple form

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$$g(E)=4\sqrt{\pi\eta}\left(\frac{m}{\hbar^2}\right)^{3/2}\Gamma(3/2)\exp\left\{-\frac{E^2}{4\eta^2}\right\}D_{-3/2}\left(-\frac{E}{\eta}\right), \tag{2}$$

where D_ν — is the function of the parabolic cylinder.

The possibility to neglect the quantum-mechanical corrections led us to develop a quasiclassical model of randomly shifted bands [3]. Within the framework of this model the expression for d.c. electrical conductivity was obtained [3]:

$$\sigma=\frac{32\sqrt{\pi}e^2}{3h^3}\frac{(kT)^2}{\eta}\int_{-\infty}^{\infty}\exp\left\{-1/2\left(\frac{kT}{\eta}\right)^2u^2\right\}\left[\iota_{oe}^c\sqrt{m_e^*}\mathscr{F}_2\left(u-\frac{\Delta E}{2kT}-\frac{\delta E}{kT}\right)+\right.$$
$$\left.+\iota_{op}^c\sqrt{m_p^*}\,\mathscr{F}_2\left(u-\frac{\Delta E}{2kT}+\frac{\delta E}{kT}\right)\right]\mathrm{d}u\,, \tag{3}$$

where ΔE is the band gap of the crystalline counterpart, $\Delta E=E_c-E_v$, ι_{oe} and ι_{op} are the pre-exponential terms of the relaxation constant of the scattering of electrons and holes, respectively, m_e^* and m_p^* are the effective masses and $\mathscr{F}_\nu$ is the Fermi integral. The expression (3) is valid for the scattering on charged centers; not essentially different is the expression for the scattering on phonons [3].

For a complete calculation of conductivity the shift of the Fermi level E_F

$$\delta E=\frac{\Delta E}{2}-(E_c-E_F)\,,$$

must be known. It can be numerically calculated starting from the electrical neutrality condition $n=p$, consequently from:

$$\int_{-\infty}^{\infty}\exp\left\{-1/2\left(\frac{kT}{\eta}\right)^2u^2\right\}\left\{m_e^{*3/2}\mathscr{F}_{1/2}\left(u-\frac{\Delta E}{2kT}-\frac{\delta E}{kT}\right)-\right.$$
$$\left.-m_p^{*3/2}\mathscr{F}_{1/2}\left(u-\frac{\Delta E}{2kT}+\frac{\delta E}{kT}\right)\right\}\mathrm{d}u=0\,. \tag{4}$$

The expressions given above were numerically calculated using $\Delta E=1$ eV, $m_p^*/m_e^*=3$, $\iota_{oe}^c/\iota_{op}^c=1$. Details of the numerical calculation are presented in [4].

Let us turn our attention to the "ad hoc" chosen temperature dependence of the parameter η (Fig. 1). In the temperature range, in which the material is in the solid state, the arrangement of atoms does not change with temperature. Thus the parameter η can be considered as a constant. On the other hand, changes of a short range order and an increase of the measure of structural disorder are expected above the melting point T_M. This assumption can be supported by the experimental experience from structural measurements [5,6]. In connection with this the temperature dependence $\eta(T)$ at temperatures above T_M is suggested to be an increasing function. On the basis of orientational considerations about the correspondence between the parameter η and the structure [7] it can be shown that the parameter η cannot approach infinity. The value of the parameter η for the case of a real gas, which is (after [7]) $\eta\lesssim 1$, can stay as a limit. Thus at high temperatures (above 1000 K) we expect saturation in the dependence of $\eta(T)$.

The numerical calculation of d.c. conductivity, including the suggested dependence $\eta(T)$ as well as the dependence $\delta E(T)$ (calculated from (4)), are presented in Fig. 1. It can be seen that the obtained dependence ln σ vs $1/T$ posesses all general features which were listed at the beginning of the paper.

Finally we will show the way in which the energy spectrum at the semiconductor-metal transition changes. The density of states, numerically calculated from the expression (2), is presented in Fig. 2. In

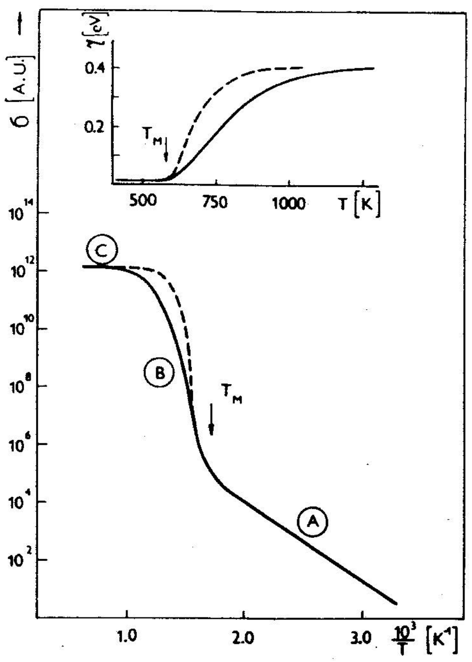

Fig. 1. Numerical calculation of d.c. electrical conductivity (3). In the insert the suggested dependence $\eta(T)$ is presented.

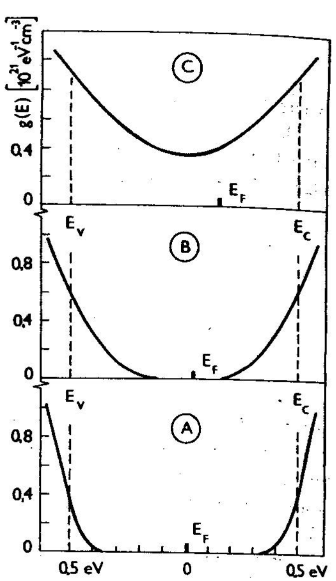

Fig. 2. The evolution of the energy spectrum with increasing temperature. The position of E_F is denoted, too.

the temperature range below T_M (it is denoted as A) one can speak about a forbidden band E_c:E_v. In the latter the nonzero density of states in the gap increases with a temperature above T_M (range B). At high temperatures (range C) it has little meaning to speak about a forbidden gap. The density of states in the gap is comparable with that in the bands. This fact causes that the conduction is metallic in nature.

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