calculated[8-10] that the "surface energy" is ~1 $\times 10^{-4}$ erg cm^{-2} and that the "surface region" extends over a scale of ~50 Å. The average energy of an electron-hole pair in the surface region should then be higher than that in the deeper region of the drop by ~0.7 meV. Such an excess in energy may account for the above mentioned discrepancy between the values determined by different experimental methods.

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Resonant Scattering of Electrons in Mercury Telluride

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(Received 13 June 1974)

Resonant scattering of electrons on optical phonons in inverted band structure is considered. It is proved that in intrinsic samples transition of the electrons from the conduction band to the valence band with simultaneous emission of optical phonons can cause a minimum of the conductivity. Such a scattering process explains the anomalous behavior of conductivity versus temperature in mercury telluride in the 30–50 K range.

Mercury telluride belongs to the class of symmetry-induced zero-gap semiconductors. In such semiconductors a minimum of the conduction band and a maximum of the valence band are degenerate at the Γ point. Wave functions of the conduction and valence bands are mainly of the p type, similar to the wave functions of the valence band in an uninverted band structure.

The results of measurements of galvanomagnetic phenomena in HgTe pointed out that in the temperature dependence of conductivity two kinds of anomalies are observed.[1-3] A high-temperature anomaly was observed in the range 30–50 K. In the same range of temperatures a weak anomaly of the Hall constant is reported.[1,2] The existing interpretations of this anomaly are based on a hypothesis of resonant acceptor states, degenerate with the conduction band. In this Letter a new explanation of the anomalous behavior of conductivity is proposed. I suggest that resonant scattering of electrons by optical phonons can cause nonmonotonic behavior of the conductivity as a function of temperature. It is obvious that in intrinsic samples of HgTe there are unoccupied electron states in the valence band. These states are concentrated at the top of this band (see Fig. 1). Thus transitions from conduction to valence band with simultaneous emission of the longitudinal optical phonon are possible. This means that when $\epsilon_m + \hbar\omega_0 = \epsilon_F$, where ϵ_m is

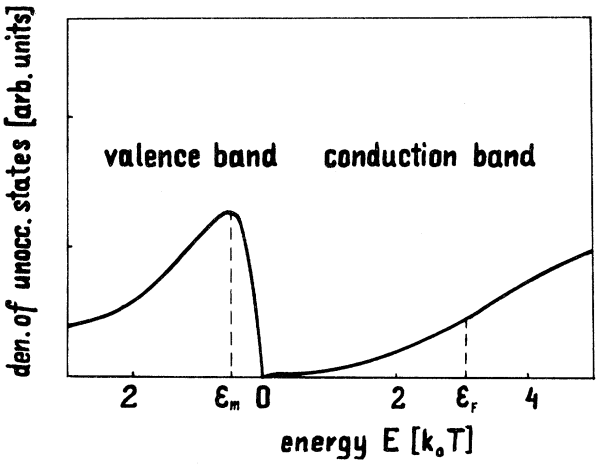

FIG. 1. Density of unoccupied electron states as a function of the energy in a semiconductor with an inverted band structure. ϵ_F is the energy of Fermi level.

the energy corresponding to the maximum density of unoccupied states in the valence band (see Fig. 1) then, because of the type of scattering considered, there is a conductivity minimum.

The calculation of the conductivity was based on some assumptions: (1) I have assumed that both conduction and valence bands are spherical and parabolic with the effective masses m_c and m_v, respectively,

$$\epsilon_c = \hbar^2 k^2/2m_c, \quad \epsilon_v = -(\hbar^2 k^2/2m_v).$$

In the range of the electron energy considered this assumption seems to be a good approximation. (2) Because of the high effective mass of holes, their influence on conductivity was omitted. (3) In partially ionic crystals the electron–optical-phonon interaction is realized in two different ways. Electrons may be coupled to the longitudinal optical phonons by means of polarization associated with the motion of the ions. This type of interaction is called polar optical (PO). On the other hand, electrons can interact with optical phonons through the optical deformation potential. This interaction is denoted by NPO. In these calculations it is assumed that it is possible to define NPO scattering by means of a deformation potential constant E_{NPO}.[4]

In the presence of electric field E along the x axis the Boltzmann equation takes the form

$$-\frac{\hbar k_x}{m_c}\left(\frac{\partial f_0}{\partial \epsilon}\right) eE = \left(\frac{\partial f}{\partial t}\right)_{\mathrm{coll}}, \tag{1}$$

where $f_0 = \{\exp[(\epsilon - \epsilon_F)/k_0 T] + 1\}$ is the Fermi-Dirac distribution function and $(\partial f/\partial t)_{\mathrm{coll}}$ is the change in the distribution function due to the scattering. If we put

$$f = f_0 - \frac{\partial f_0}{\partial \epsilon} k_x c(\epsilon),$$

then the collision operator takes the form

$$\left(\frac{\partial f}{\partial t}\right)_{\mathrm{coll}} = \int W(\vec{k}, \vec{k}') \frac{\{1 - f_0(\vec{k}')\}}{\{1 - f_0(\vec{k})\}} \times \frac{\partial f_0}{\partial \epsilon}\{c(\epsilon')k_x' - c(\epsilon)k_x\} d^3k',$$

where $W(\vec{k}, \vec{k}')$ is the probability of transition from the state $\vec{k}$ to the state $\vec{k}'$ in a unit time. The corresponding transition probability for the polar interaction is found to be

$$W(\vec{k}, \vec{k} - \vec{q}) = \frac{\alpha}{\pi}\frac{(\hbar\omega_0)^2}{\hbar p_0}\frac{1}{q^2} \times \delta(\epsilon_v(\vec{k} - \vec{q}) - \epsilon_c(\vec{k}) + \hbar\omega_0) G_{cv}(\gamma)$$

where $p_0 = (2m_c\omega_0/\hbar)^{1/2}$, α is the Fröhlich coupling constant which may be given in terms of the high-frequency and static dielectric constants,

$$\alpha = \frac{e^2}{\hbar}\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0}\right)\left(\frac{m_c}{2\hbar\omega_0}\right)^{1/2},$$

and $G_{cv}(\gamma)$ is the function which determines an overlap of periodic parts of Bloch functions of the conduction and valence bands. Because of the symmetry of these functions $G_{cv}(\gamma)$ takes the form[5]

$$G_{cv}(\gamma) = \tfrac{3}{4}\sin^2\gamma,$$

where γ is the angle between $\vec{k}$ and $\vec{k} - \vec{q}$. For the nonpolar interaction

$$W(\vec{k}, \vec{k} - \vec{q}) = \frac{E_{\mathrm{NPO}}{}^2 \omega_0}{8\pi^2 \rho \mu_l{}^2}\delta(\epsilon_v(\vec{k} - \vec{q}) - \epsilon_c(\vec{k}) + \hbar\omega_0),$$

where ρ is the density of the crystal and μ_l is the longitudinal sound velocity in the crystal.

The scattering process considered is inelastic. Hence a uniquely defined relaxation time does not exist. To solve the Boltzmann equation (1) we use the variational principle.[6,7] In this method the conductivity is expressed by an infinite, rapidly convergent series. Taking into account only the first term of such a series and assuming a strong degeneracy of electron gas, which is equivalent to the relation

$$\left(-\frac{\partial f_0}{\partial \epsilon}\right) = \delta(\epsilon - \epsilon_F),$$

we obtain the following expressions for conductivity. In the case of polar scattering

$$\delta = \frac{4\sqrt{2}}{3\pi^2}\frac{e^2 m_c{}^{1/2}}{\hbar^2 \alpha}\left(\frac{m_c}{m_v}\right)^{3/2}\frac{(k_0 T)^{1/2}\xi^{5/2}(1 + e^z)}{z^{3/2}(z - \xi)^{1/2}\Phi(z, \xi)}, \tag{2}$$

where $z = \hbar\omega_0/k_0 T$, $\xi = \epsilon_F/k_0 T$,

$$\Phi(z, \xi) = 1 - \frac{3}{8s^2}\left(1 + s^2 - \frac{(1 - s^2)}{s}\tanh^{-1}(s)\right) \tag{3}$$

for

$$s = \left(\frac{m_c \xi}{m_v(z - \xi)}\right)^{1/2} < 1.$$

For $s > 1$ the expression for $\Phi(z, \xi)$ can be obtained by replacing $\tanh^{-1}(s)$ with $\coth^{-1}(s)$ in Eq. (3). For NPO scattering

$$\delta = \frac{2}{3\pi}\frac{e^2\hbar\rho\mu_l{}^2 m_c{}^{1/2}}{E_{\mathrm{NPO}}{}^2 (m_v)^{3/2}}\frac{\xi^{3/2}(1 + e^z)}{z(z - \xi)^{1/2}}. \tag{4}$$

For the particular case of HgTe formulas (2) and (4) are graphically represented in Fig. 2. In the calculation, the following parameters for HgTe

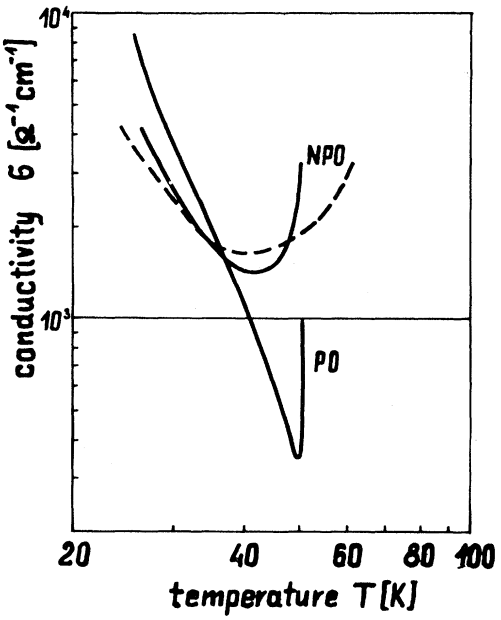

FIG. 2. Nonmonotonic part of conductivity as a function of temperature. The dashed curve represents experimental result.

were used: $m_c = 0.02m_0$, $m_v = 0.5m_0$, $\alpha = 0.1$, $\hbar\omega_0 = 14.1$ meV, $u_l = 2.57 \times 10^5$ cm/sec, $\rho = 8.1$ g/cm^3, and $E_{NPO} = 18$ eV. m_0 is the free-electron mass.

The dashed curve in Fig. 2 corresponds to the nonmonotonic part δ_r of experimental conductivity[1] calculated in the following way. It was assumed that total experimental resistivity ρ_t consists of two parts: ρ_r which is due to the resonant scattering of electrons and ρ_m which results from the elastic nonresonant scattering. ρ_m was obtained by linear graphical interpolation of experimental results.[1] Hence

$$\rho_t = \rho_m + \rho_r$$

or

$$\frac{1}{\sigma_t} = \frac{1}{\sigma_m} + \frac{1}{\sigma_r}.$$

It is seen from Fig. 2 that the minima of theoretical conductivities are, in both cases, very close to the minimum of the nonmonotonic part of experimental conductivity. The deep minimum of PO conductivity results from the strong dependence of this interaction on a phonon wave vector q when q tends to zero and from the strong degeneracy assumption. This last assumption causes both PO and NPO conductivities to tend to infinity when ϵ_F tends to $\hbar\omega_0$.

In the framework of the above approximation a good agreement of the position of nonmonotonic experimental conductivity with theoretical results was obtained. A better fit would be obtained by taking into account the proper degeneracy of electron gas and by adding other scattering mechanisms which are important in the region of temperatures considered.

The proposed scattering mechanism can be observed in intrinsic semiconductors with inverted band structure, only if mobility due to other scattering mechanisms is not too low. Thus it can explain the similar conductivity anomaly observed in HgTe-CdTe[1,8] and HgTe-MnTe[9] mixed crystals.

The author wishes to thank Professor Dr. L. Sosnowski, Professor Dr. J. Kołodziejczak, Dr. R. R. Gałazka, Dr. Grynberg, and Dr. J. Mycielski for helpful discussions.

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