Conductivity inversion and anomalously high hole mobility in a gapless semiconductor resulting from a uniaxial strain

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A transition from an n-type to a p-type conductivity due to a uniaxial strain has been detected in a gapless semiconductor. Formed due to a uniaxial strain, the lateral extrema of the valence band trap the holes with small effective masses, causing the hole mobility to be comparable to the electron mobility.

The band degeneracy in gapless semiconductors with an inverted band structure accounts for several peculiarities in their physical properties. In particular, because of the high mobility of electrons and the existence of acceptor resonance states in the conduction band even when $N_A > N_D$ (N_A and N_D are the acceptor and donor densities), a gapless semiconductor has an electronic conductivity even at low temperatures.

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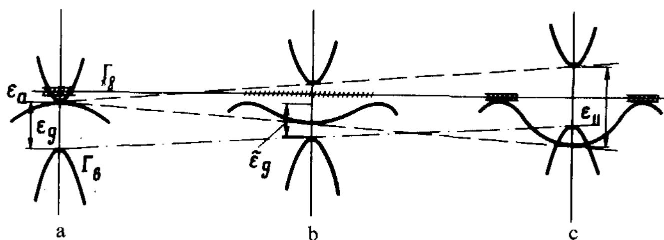

FIG. 1. Experimental arrangement showing a structural change in the energy band of a gapless semiconductor caused by a uniaxial strain (liquid-helium temperature). (a) No strain; (b) intermediate strain; (c) intensive strain.

Imposition of external perturbations changes its energy spectrum, which causes it to change its characteristics dramatically. Hydrostatic compression[1,2] causes an inversion of the terms Γ_8 and Γ_6, which leads to a gapless semiconductor-ordinary semiconductor transition. Application of a strong magnetic field induces an energy gap.[3] The effect of a uniaxial strain on a gapless semiconductor was studied in α-Sn in Ref. 4 and in HgTe in Ref. 5. The results of these experiments were interpreted in Ref. 6 in terms of the formation of an energy gap due to the lifting of the degeneracy of the Γ_8 term by lowering the symmetry of the crystal lattice. However, the structural changes of the valence band and the role of the acceptor resonance states due to a uniaxial strain have not been studied.

In the present letter we show that a uniaxial strain of a gapless semiconductor causes a transition from an n-type to a p-type conductivity in which the band structure is changed. In a highly strained crystal the conductivity is determined by the free holes. The mobility of these holes increases considerably in this case, since the holes with small effective masses are trapped in the lateral edges (extrema) of the valence band which are formed as a result of the strain (Fig. 1c). If an n-type conductivity changes to a p-type conductivity (intermediate strain) as the acceptor states enter the pressure-induced energy gap (Fig. 1b) and the electrons are frozen out, then the charge transfer will be determined by the impurity states.

We have studied the compound $Hg_{1-x}Cd_xTe$ of the submetallic phase with the chemical composition $x = 0.157$ and $x = 0.135$ ($\epsilon_g = -13 \pm 5$ meV and $\epsilon_g = -54 \pm 5$ meV, respectively). The composition of the compound was determined to within 0.3% with an x-ray microanalyzer. The device for uniaxial compression was immersed along with the sample into a helium cryostat, allowing us to measure the electric and galvanomagnetic characteristics of the crystal under a uniaxial compression $P \leq 3.5$ kbar in the temperature range 1.7–77 K.

Figure 2 shows the resistivity ρ for the longitudinal current ($\mathbf{J} \| \mathbf{P}$) and the Hall coefficient R_X plotted as a function of the uniaxial strain for a sample with $x = 0.157$. We see that at $P \simeq 2$ kbar the $\rho(P)$ curves peaks sharply and the sign of $R_X(P)$ changes. Notice that both curves are symmetric. We used the values ρ and R_X on the wings of the curves to calculate the current-carrier densities [$(3.83 \pm 0.04) \times 10^{14}$ cm^{-3} at $P = 0$ and $(5.98 \pm 0.04) \times 10^{14}$ cm^{-3} at $P = 3.25$ kbar] and mobilities [$(3.90 \pm 0.06 \times 10^5$ cm^2/(V · s) and $(1.32 \pm 0.06) \times 10^{-5}$ cm^2/(V · s)]. Reversal of the sign of $R_X(P)$ indi-

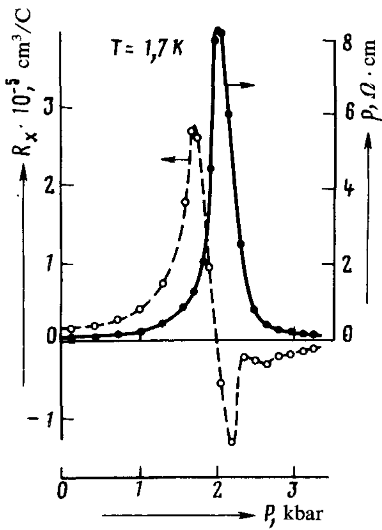

FIG. 2. A change in ρ and R_X produced as a result of a uniaxial strain P‖[110].

cates that in the region of maximum strain the conductivity is determined by the free holes, whose mobility and hence the effective mass are on the order of the mobility and mass of the electrons. In the absence of a strain, however, we usually have $\mu_n/\mu_p \sim 10^2$.

In the region where the resistivity peaks, we see a sharp (nearly exponential) temperature dependence of ρ over the temperature range $T = 1.7$–8 K (Fig. 3) with an

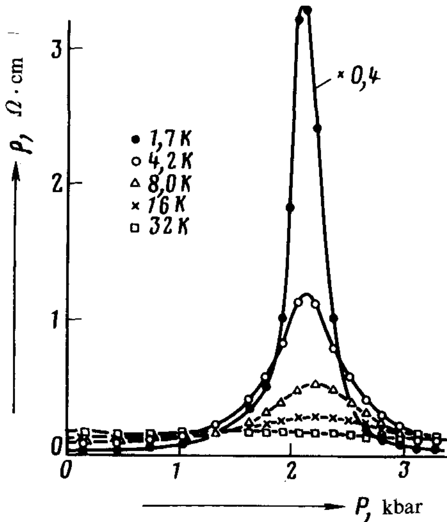

FIG. 3. The temperature dependence of ρ(**P**).

activation energy of 0.25 meV, indicating that we have an extrinsic conductivity in the intermediate-pressure range. Here the freezing-out of the electrons from the conduction band toward the acceptors accounts for the increase in resistivity with increasing P and the reduction of the effective mass and the increase in density of the free holes accounts for the decrease in resistivity. The resistivity decreases because the depth at which the acceptors are embedded decreases relative to the lateral edges of the valence band.[7] We obtained a qualitatively similar result for the composition $x = 0.135$.

The structural change in the energy spectrum of a gapless semiconductor is given by the dispersion equation

$$\frac{k^2}{2m} = \frac{(\xi - \tilde{\epsilon}_g)(\xi^2 - \epsilon_{\parallel}^2/4)}{|\epsilon_g|\left[\xi + \frac{\epsilon_{\parallel}}{2} P_2(\cos\theta)\right]}, \qquad \xi = \epsilon + \frac{k^2}{2m^*}, \tag{1}$$

where ϵ_g is a negative band gap ($\tilde{\epsilon}_g$ is the change in this parameter value for a crystal strained uniaxially along the z axis; see Fig. 1), $\epsilon_{\parallel}$ is the splitting energy of the degenerate Γ_8 term, m are the effective masses of the light subband Γ_8 and of the term Γ_6 in the symmetric-band approximation (with $m^* \to \infty$), m^* is the mass of the heavy holes, $P_2(x) = (3x^2 - 1)/2$, and θ is the angle included between the wave vector $\mathbf{k}$ and the compression direction. Equation (1) was derived for an isotropic Kane model with a large spin-orbit splitting.[6] The pressure-induced gap is governed by the energies ϵ for which the right side of (1) is negative; i.e., the only possible solutions are those with an imaginary value of k. From Eq. (1) we find that the electronic extremum is situated at the point $\mathbf{k} = 0$ and has an energy $\epsilon_{\parallel}/2$. In the symmetric-band approximation, the hole extrema are situated in the limit $k \to \infty$, $\cos\theta = \pm\pi/2$ and have an energy $\epsilon_{\parallel}/4$. Since $1/m^* \neq 0$, these extrema shift toward the finite wave vectors and their energy decreases slightly. The dispersion law near the hole extremum is given by the expression $k_z^2/2m_{\parallel}$ with an effective longitudinal mass

$$\frac{m_{\parallel}}{m} \simeq \sqrt{\frac{m^*}{m}\,\frac{\epsilon_{\parallel}/4 - \tilde{\epsilon}_g}{3|\epsilon_g|}}. \tag{2}$$

The transverse mass arises only when the band-structure anisotropy is considered.

Since the static and elastic strain-energy constants of $Hg_{1-x}Cd_xTe$ change only slightly with the composition, we find $\tilde{\epsilon}_g \simeq -4.13$ meV and $\epsilon_{\parallel} \simeq 49.61$ meV by using the numerical values of Refs. 1, 2, and 5 for $x = 0.157$ at $P = 3.25$ kbar. We infer from these values that the lateral extrema lie above the maximum of the Γ_6 band (although at the point $\mathbf{k} = 0$ the order of the terms Γ_6 and Γ_8 changes; see Fig. 1c). Using the ratio $m^*/m \sim 10^2$, we calculate from Eq. (2) the value $m_{\parallel}/m \simeq 5.50$, in reasonably good agreement with the experimentally obtained mobility ratio $\mu_n/\mu_p \simeq 2.95$.

Consequently, the structural change in the energy spectrum of a gapless semiconductor caused by a uniaxial strain is responsible for the experimentally obtained conductivity inversion and the high mobility of holes.

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