Topological phase transitions in $Bi_{1-x}Sb_x$ alloys and composition dependence of the position of the heavy-hole band

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The valence band in $Bi_{1-x}Sb_x$ alloys ($0 \leqslant x \leqslant 0.15$) has been studied by means of a Lifshitz phase transition. The energy position of the edge of the heavy-hole band is found as a function of the composition: $E_\Sigma = 259x - 70$ meV, where the energy is measured from the middle of the gap at the L point.

The valence band of $Bi_{1-x}Sb_x$ ($0 \leqslant x \leqslant 0.2$) alloys is complicated, containing a light-hole band L and heavy-hole bands T and Σ. Doping the alloy $Bi_{1-x}Sb_x$ with an acceptor impurity can cause the Fermi level to touch the heavy-hole band Σ. In this case, according to Lifshitz,[1] the change in the topology of the Fermi surface should give rise to distinctive features in transport phenomena. Near Lifshitz phase transitions, the kinetic coefficients have a square-root singularity $\sim |Z|^{1/2}$, where the parameter $Z = E - E_c$ is a measure of the proximity to the transition point (E_c is the critical value of the Fermi energy of the carriers). An exceptional case is the thermal emf, which should have an infinite singularity, $\sim |Z|^{-1/2}$. The behavior of the thermal emf and of the resistivity has been studied in detail theoretically for metal alloys near phase transitions.

In the present study we have taken the new approach of utilizing the Lifshitz phase transition as a method for determining the energy positions of the heavy holes as functions of the composition for the case of $Bi_{1-x}Sb_x$ alloys. Since the thermal emf is the property which is most sensitive to the phase transition, we have focused on the temperature and concentration dependence of the thermal emf. We studied both semimetal and semiconducting alloys $Bi_{1-x}Sb_x$ ($0 \leqslant x \leqslant 0.15$).

Figure 1 shows the experimental temperature dependence of the thermal emf for the alloys $Bi_{1-x}Sb_x$ ($0 \leqslant x \leqslant 0.15$). The amount of dopant in these alloys was chosen to cause the Fermi level to touch the floor of the heavy-hole band Σ. In this case, a new scattering channel—interband scattering—comes into play for the electron system, and, according to Lifshitz, the thermal emf has an anomalous singularity. This singularity was analyzed in detail in Ref. 3 for $Bi_{1-x}Sb_x$ ($0.12 \leqslant x \leqslant 0.14$) alloys. It follows from the experimental results (Fig. 1a) that the anomaly appears in the thermal emf (the sign changes from positive to negative) for the p-type semiconducting alloys ($0.7 < x < 0.15$) at $T > 4$ K and is seen equally well for samples with different crystallographic orientations. The singularity which arises in the resistivity for the semiconducting alloys at the Lifshitz phase transition, on the other hand, is observed both above $T = 4$ K and below $T = 1.3$ K. This observation means that the light holes of band L can be scattered into the heavy-hole band Σ at such low temperatures only in

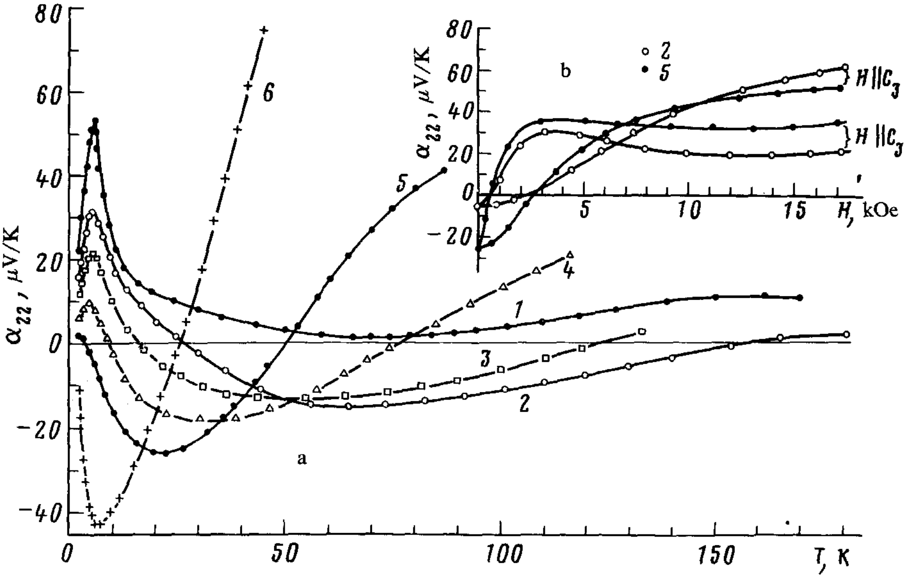

FIG. 1. a: Temperature dependence of the thermal emf $\alpha_{22}(\nabla T\|C_1)$ for samples of the alloy $Bi_{1-x}Sb_x$ ($0 \leqslant x \leqslant 0.12$). 1—$BiSn_{0.24}$; 2—$BiSn_{0.3}$; 3—$Bi_{0.99}Sb_{0.01}$; 4—$Bi_{0.95}Sb_{0.05}$; 5—$Bi_{0.92}Sb_{0.08}$; 6—$Bi_{0.88}Sb_{0.12}$. b: The thermal emf α_{22} as a function of the magnetic field for several samples. 2—$BiSn_{0.3}$ at $T = 34$ K; 5—$Bi_{0.92}Sb_{0.08}$ at $T = 20$ K.

an interaction with point defects, which in single crystals of the $Bi_{1-x}Sb_x$ alloy are isovalent antimony atoms.[3] The phonons which have been identified in bismuth, and which may be responsible for the interband scattering, are excited at[4] ~40 K and are essentially absent at liquid-helium temperatures. For bismuth, the anomaly in the thermal emf is observed at $T > 25$ K (Fig. 1a), while the singularity in the resistivity arises at $T > 20$ K. It can therefore be suggested that phonons are responsible for the interband scattering in bismuth. The magnitude of the effect depends on the state density in the new band, as follows from Refs. 1–3. Independent measurements[5] show that the mass of the state density of valence band Σ is large, $\sim 0.9m_0$. Further evidence for this conclusion comes from the small change in the density of the light holes of band L when the alloy is doped with an acceptor impurity after the Fermi level touches the Σ band. It follows from Fig. 1a that the temperature interval in which the anomalous thermal emf is seen becomes narrower as the alloy composition changes, while the depth of the anomaly increases. The thermal emf in the alloys is determined by light holes from band L (Refs. 3 and 6), primarily because the Fermi level of the light holes (L), which follows the edge of band Σ, decreases as the composition changes, as we will show below, and it moves into the energy gap sooner as the temperature is changed. The depth of the anomaly in the thermal emf from the measurements of $\alpha(T)$ is larger for the semiconducting alloys, since the ratio of the effective masses of the L and Σ bands (m_Σ/m_L) is also larger for them. The effect of interband scattering ($L \rightleftarrows \Sigma$) is also determined by the ratio of the effective masses of the carriers of the different groups.[7] For the light holes of band L, the effective mass at the Fermi level depends on the energy because of the strong deviation from a parabolic situation. The thermal emf in a classically strong magnetic field does not depend on the mechanism for the scattering of the charge carriers, so that an anomaly of the thermal emf is not seen experimentally in a magnetic field (Fig. 1b).

The energy position of the edge of band Σ is determined by the following approach. In those cases in which the Fermi level touches the bottom of the Σ band, the distance between the edges of bands L and Σ is determined from the Fermi energy of the light holes (L), on the basis of the quantum oscillations in the kinetic coefficients. We make use of the relationship between the minimum cross section of the Fermi surface of the L holes, S^y_{min}, and the parameters of the simplified McClure spectrum Q_{ii}, the Fermi energy E_{FL}, and the energy gap E_{gL} (Refs. 8 and 9),

$$S^y_{\rm min} = \pi(E^2 - E^2_{gL}/4)/Q_{11}Q_{33},$$

where $E = E_{FL} + E_{gL}/2, Q_{11}Q_{33} = 0.153 - 0.28x$ for $Bi_{1-x}Sb_x$ ($0 \leqslant x \leqslant 0.15$) (Ref. 10) and $S^y_{\rm min} = S_{\rm extr}\cos 30° \cos\varphi$. The angle ($\varphi$) at which the ellipsoid is inclined with respect to the basis plane decreases for the alloy $Bi_{1-x}Sb_x$ approximately linearly as a function of the composition, having the value $\varphi = 5°$ for $Bi_{0.88}Sb_{0.12}$ (Refs. 8 and 9). For Bi, on the other hand, we have[11] $\varphi = 6°21'$. The extreme cross section of the Fermi surface of the L holes is found from the period of the quantum oscillations of the magnetoresistance and the thermal emf in the case $\mathbf{H} \| C_2$: $S_{\rm extr} = eh/[c\Delta(1/H)]$. In those cases in which the Fermi level is in the Σ band, the distance between the edges of the L and Σ bands is found as $E_{FL} - E_{F\Sigma}$. The Fermi energy E_{FL} is found from the quantum oscillations, while the heavy-hole energy $E_{F\Sigma}$ is found from the density p_Σ and the state-density mass $m_{d\Sigma} = 0.9m_0$ (Ref. 5) in the isotropic approximation: $E_{F\Sigma} = \hbar^2(3\pi^2 p_\Sigma)^{2/3}/(2m_{d\Sigma})$. The hole density is $p_\Sigma = \Sigma p_i - (p_L + p_T)$.

1. The density of light holes, p_L, with the Fermi energy E_{FL} is found from the McClure dispersion relation:

$$p_L = \frac{2}{(2\pi)^2 Q_{11}Q_{33}}\left[\frac{\alpha_{v22}\alpha_{c22}}{30}K_0^2 + \frac{2}{3}E(E+E_{gL})K_0\right]\Bigg|_{E=E_{FL}},$$

where

$$K_0^2 = \frac{E\alpha_{v22} - (E-E_{gL})\alpha_{c22} - 2Q_{22}^2 + \{[E\alpha_{v22} + (E+E_{gL})\alpha_{c22} + 2Q_{22}^2]^2 - 8E\alpha_{v22}Q_{22}^2\}^{1/2}}{\alpha_{c22}\,\alpha_{v22}}$$

with the spectral parameters from the composition of the alloy[10] $Bi_{1-x}Sb_x$,

$$Q_{11} = 0.451 - 0.85x, \quad Q_{22} = 0.0088 + 0.00126/(x+0.05),$$
$$Q_{33} = 0.34 + 0.015x, \quad \alpha_{c22} = 0.5, \quad \alpha_{v22} = 1.15.$$

2. The hole density p_T is found from the expression for the two-band model:

$$p_T = \frac{1}{3\pi^2}\left\{\frac{m_{dT}(0)E_{gT}}{2\hbar^2}\left[(2E_{FT}/E_{gT}+1)^2-1\right]\right\}^{3/2}$$

with the parameters of the T band,[9] E_{FT}, $m_{dT}(0) = 0.141m_0$, and $E_{gT} = 200$ meV. The Fermi energy E_{FT} is found from the Fermi energy of the light holes, L, and from the known composition dependence of the edge of the T band, described in Ref. 9.

3. The total density of holes Σp_i, is found from the concentration of the tin dopant, C_{Sn} (at. %): $\Sigma p_i = N_A \rho_{Bi-Sb} C_{Sn} \eta/(A_{Bi-Sb}\cdot 100)$, where N_A is Avogadro's number, and (ρ, A) are the density and atomic weight of the alloy $Bi_{1-x}Sb_x$. The recoil coefficient $\eta = 0.3$–0.4 is found for the alloy of the given composition in samples in which only the holes of the L and T bands participate in transport processes; for these holes, the condition of a classically strong field is satisfied, and the total density $(p_L + p_T)$ is found from the Hall effect.

Using this method, we have found the position of the edge of the Σ band as a function of the composition of the alloy $Bi_{1-x}Sb_x$ $(0 \leqslant x \leqslant 0.15)$: $E_\Sigma = 359x - 70$ meV. The energy is measured from the middle of the gap at the L point. This dependence of the edge of the Σ band on the composition at $x > 0.15$ agrees with data in the literature. The Σ band intersects the L_s band at $x \simeq 0.16$ and we have $E_\Sigma = E_{L_s} \simeq 12$ meV; it intersects the T band at $x \simeq 0.12$, and we have $E_\Sigma \simeq 26$ meV.

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