Lifshitz impurity phase transition in bismuth

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A heavy electron band at the T point has been detected in bismuth on the basis of anomalies in the temperature and concentration dependence of the thermoelectromotive force and the resistivity near the Lifshitz phase transition. The energy gap is found to be $E_{gT} \cong 190$ meV.

The thermoelectromotive force and resistivity of a large number of tellurium-doped bismuth single crystals have been studied over the temperature range 2–300 K. The samples are oriented along the basic crystallographic axes ($\mathbf{j}, \nabla \mathbf{T} \| C_1$ and C_3). The carrier density in the L_s band, determined from the weak-field Hall components $R_{13.2}$ and $R_{31.2}$ at liquid-helium temperatures, is $n_L = 1.8 \times 10^{19}$–1.5×10^{20} cm^{-3}.

Figure 1a shows the temperature dependence of the thermoelectromotive force of six samples with three qualitatively different positions of the chemical potential [Fig. 1(b)]. At low temperatures ($T < 20$ K) the magnitude of the thermoelectromotive force is determined by the phonon-drag component, as was first discovered in Ref. 1. In the region in which the diffusion component is predominant ($T > 40$ K), the thermoelectromotive force is isotropic $\alpha_{22} \cong \alpha_{33}$ (samples 1 and 2). Isotropy of the diffusion component of the thermoelectromotive force of Bi-Te alloys with concentrations $N_{\mathrm{Te}} \geqslant 0.1$ at.% over the temperature interval 80–300 K has been observed previously[2] and attributed to single-band transport. The pronounced anisotropy of the thermoelectromotive force ($\alpha_{33}/\alpha_{22} \cong 2$), which prevails in pure bismuth and which is due to the presence of two nonequivalent carrier groups in the L and T bands, disappears because the doping with the donor tellurium raises the Fermi level. The temperature dependence of the thermoelectromotive force of samples 3–6 is anomalous. At $T > 40$ K we observe a decrease in the thermoelectromotive force, and it even changes sign in samples 5 and 6. After going through a minimum, α tends toward its normal value as the temperature is raised. In the anomalous region, the thermoelectromotive force becomes very anisotropic, as can be seen from the concentration dependence of $\alpha_{22}(n_L)$ and $\alpha_{33}(n_L)$ (Fig. 2). At a sufficiently high electron density, we observe a departure from the anomaly ($n_L > 1.1 \times 10^{20}$ cm^{-3}). The anomaly in the thermoelectromotive force correlates with a sharp increase in the resistivity (Fig. 2). The resistivity anisotropy coefficient $K = \rho_{33}/\rho_{22}$, which differs insignificantly from unity in single-band alloys ($K = 1.03$), increases to $K = 1.3$ at $n_L = 10^{20}$ cm^{-3}.

These features of the kinetic coefficients are evidence that a Lifshitz $2^1/2$ impurity phase transition occurs in the heavily doped Bi-Te alloys.[3] The doping with tellurium raises the Fermi level in the conduction band [Fig. 1(b)], and at a certain critical $E = E_{\mathrm{crit}}$ it touches the bottom of the new band. The kinetic coefficients should have a square-root singularity $Z^{1/2}$ near the phase transition, where $Z = E - E_{\mathrm{crit}}$. An excep-

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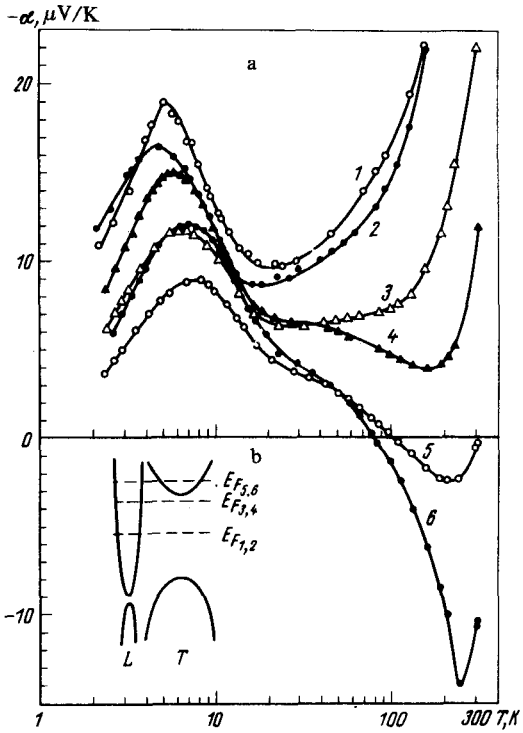

FIG. 1. a: Temperature dependence of the thermoelectromotive force of tellurium-doped bismuth. Samples 1, 3, 5—α_{22} ($\nabla\mathbf{T}\|C_1$); 2, 4, 6—α_{33} ($\nabla\mathbf{T}\|C_3$). The electron density in the L_s band is (1,2) 1.8×10^{19} cm^{-3}, (3,4) 5.3×10^{19} cm^{-3}, and (5,6) 1.1×10^{20} cm^{-3}. b: Arrangement of the chemical potential with respect to the L and T bands in Bi-Te samples.

tional case is the thermoelectromotive force, $\alpha\sim Z^{-1/2}$. Vaks *et al.*[4] have studied the behavior of the thermoelectromotive force at a phase transition ($Z\to0$) for metals. The anomaly in the thermoelectromotive force is a consequence of a selective scattering of carriers that lie above and below the Fermi level, and it can occur only if the

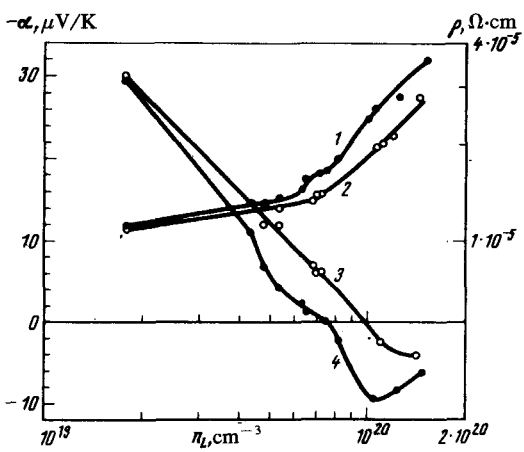

FIG. 2. Components of the resistivity and of the thermoelectromotive force versus the concentration. 1—$\rho_{33}(\mathbf{j}\|C_3)$, 2—$(\rho_{22}(\mathbf{j}\|C_1)$ at $T=4.2$ K; 3—α_{22}; 4—α_{33} at $T=200$ K.

electron gas is strongly degenerate. In our case, this condition is satisfied quite well. A partial lifting of the degeneracy at room temperature leads to a decrease in the anomalous thermoelectromotive force [Fig. 1(a)]. The selectivity of the scattering can also be eliminated by raising the Fermi level above the bottom of the new band; this change corresponds to a departure from the anomaly as the concentration is increased (Fig. 2). The complex structure of the $\alpha(n_L)$ curve may be related to the effect of tellurium impurity states.

An important feature of the phase transition which we have detected is its anisotropy. Analysis of the anisotropic anomalous thermoelectromotive force, the resistivity, and the integral isotropy of the L band unambiguously shows that the condition $\sigma_{33}/\sigma_{22} \ll 1$ holds for the new band. In order to observe the anomaly experimentally, it is necessary to arrange a sufficiently high state density in the new band.[5] Among the bands that lie near the Fermi level,[6] the T band meets these requirements. Calculating $E_{\text{crit}} = f(n_{L_{\text{crit}}})$, we can determine its energy position with respect to the bottom of the L band. The possible position of the electron T band was discussed in the review by Édel'man.[7] The serious discrepancies in the results reported by different investigators for the size of the energy gap at the T point (E_{gT} = 170–740 meV) are linked with the indirect method of determining E_{gT}, from the deviation from a parabolic valence T band. The direct observation of the electron band in our experiments makes it possible to carry out some more reliable quantitative calculations. Using the parameters from Ref. 8 for the L_s band, we find $E_{\text{crit}} \cong 230$ meV. In the rigid-band approximation we then find $E_{gT} \cong 190$ meV.

The method of studying the band structure on the basis of the anomaly in the thermoelectromotive force at the phase transition has proved effective in an interval of temperatures and concentrations which is inaccessible to oscillation methods. Further evidence that this method is of a rather general applicability for studying multiband materials comes from the successful study of the valence band in Bi-Sb alloys.[9]

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