INVESTIGATION OF GAPLESS STATES IN BISMUTH-ANTIMONY ALLOYS UNDER PRESSURE

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The transition to a gapless state (GS) under a pressure up to 15 kbar is investigated between 1.9 and 4.2°K in single-crystal samples of $Bi_{1-x}Sb_x$ alloys with X = 0.070 and 0.071 in a magnetic field H up to 74 kOe directed along the binary and trigonal axes of the crystals. For this purpose the longitudinal and transverse magnetoresistances are measured for consecutive "semiconductor-metal" and "metal-semiconductor" transitions to the right and left of the band inversion points in L for $p = p_i$. Shubnikov-de Haas oscillations are observed in the metallic state arising in a certain pressure range $p_1 \leq p \leq p_2$ ($0 < p_1 < p_i$; $p_2 > p_i$). The pressure dependences of the cross sections of the extremal electron S^e and hole S^h parts of the Fermi surface and of the cyclotron electron masses m^e are obtained. The realignment of the energy spectrum on going to the GS, wherein the direct gap ϵ_g in L vanishes, is analyzed. It is found that upon inversion the bands approach each other at a rate which is ~1.7 times greater than the rate at which they move apart. This phenomenon is ascribed to mutual deformation of the extrema and "entanglement" of the La and Ls terms when $p > p_i$. It is shown that on going to the GS the electron "ellipsoid" contracts to a narrow "needle" and the anisotropy of the conduction band in L increases without limit. This indicates that the Lax-Golin model is inapplicable to large cross sections of the electron part of the Fermi surface.

INTRODUCTION

SEMICONDUCTORS with narrow forbidden bands, research on which has greatly expanded in recent years, are of great interest as new engineering materials and as objects for the study of new physical phenomena. A special class among them is made up of substances in which a gapless state (GS), intermediate between metallic and semiconducting, is observed. In this state, at a certain point of the space of the momenta $k = k_0$, the bottom of the conduction band coincides in energy with the top of the valence band. The strong interaction produced between the bands in the "singular" region near $k = k_0$ leads to the appearance of new properties possessed by neither metals nor semiconductors[1].

As shown by Abrikosov and Beneslavskii[1], the vanishing of a direct gap in a semiconductor is due to the very high symmetry of the crystal, and therefore is quite rarely observed under natural conditions. The GS can also occur at Brillouin-zone points where the level degeneracy is not connected with high symmetry, but is the result of adjustment of the parameters of the energy spectrum with the aid of some external action (for example magnetic field or pressure).

Among substances known to recent date, a natural GS exists in gray tin[2] and also in the solid-solutions $Cd_xHg_{1-x}Te$[3], $Pb_{1-x}Sn_xSe$[4], and $Pb_{1-x}Sn_xTe$[5] at definite concentrations of the components. However, the energy spectrum of the indicated substances has not been sufficiently well studied, and the available data were obtained at temperatures T higher than 12°K (most of the data pertain to $T \geq 77$°K). The smallest values of the direct gap ϵ_g that have been reliably measured in the indicated solid solutions as their compositions were varied were not less than 50 meV. Thus, both the character of the continuous transition to the GS, and the properties of the substance in this state have hardly been investigated as yet.

In connection with the problem of investigating the intermediate state between metals and dielectrics, particular interest attaches, from our point of view, to the solid solutions $Bi_{1-x}Sb_x$. The character of the variation of their energy spectrum (see, for example,[6-12]) is illustrated in Fig. 1.

The direct gap ϵ_g in $Bi_{1-x}Sb_x$ alloys, which separates the bottom of the conduction band from the top of the valence band at the point L (terms L_S and L_a for Bi[13]), equal to ~15 meV at x = 0, decreases rapidly with increasing Sb concentration, and vanishes at $x \approx 0.04$. At this point, the terms L_S and L_a become inverted and again diverge. The gap ϵ_g then increases

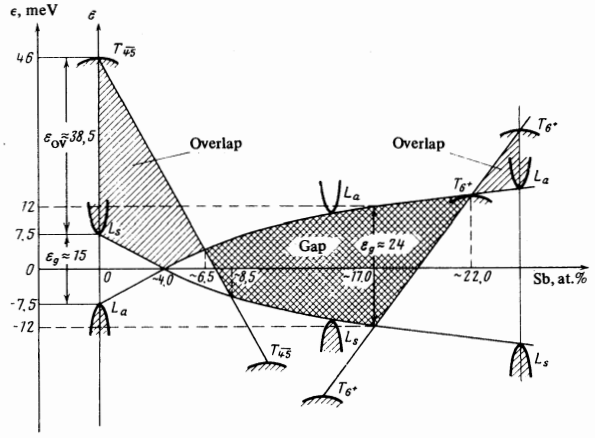

FIG. 1. Variation of the energy spectrum of $Bi_{1-x}Sb_x$ alloys with increasing Sb concentration in the interval $0 \leq x < 0.25$. The region of semiconducting alloys is cross hatched.

monotonically to a value ~100 meV for Sb(x = 1.0). The GS is realized at $x \approx 0.04$.

A direct study of both the transition to the GS with changing Sb concentration and of the GS itself at $x \approx 0.04$ in $Bi_{1-x}Sb_x$ alloys is made difficult by the presence of the large band overlap ϵ_{ov} in L and T (at $x \approx 0.04$ we have $\epsilon_{ov} \approx 20$ meV), as a result of which the characteristic properties of the GS, connected with the relatively small group of electrons in the "singular" region near $k = k_0$, are masked by the presence of a large number of electrons at the Fermi level. In these alloys, however, it is also possible to obtain a GS by altering the spectrum by means of external physical actions. It was observed recently that the semiconducting $Bi_{1-x}Sb_x$ alloys can go over into the GS under the influence of a strong magnetic field H[11] and a pressure p[8,12]. A distinguishing feature of the GS in a magnetic field is that it occurs in a one-dimensional carrier gas.

The approach, inversion, and subsequent divergence of the terms L_a and L_s in $Bi_{1-x}Sb_x$ alloys under pressure (at H = 0) occurs at $x > 0.04$ and is accompanied by a sharp increase of the electron mobility near $\epsilon_g \approx 0$, thus pointing to a strong decrease of the effective electron mass as $\epsilon_g \to 0$. Unfortunately, the data of[10,12], obtained by galvanomagnetic measurements in weak fields, do not yield sufficiently complete information concerning either the transition to the GS or the state with $\epsilon_g = 0$ itself. It is therefore of interest to employ resonant (oscillatory) methods for the study of the transition to the GS.

Data on the character and on the rates of relative motion of the terms L_a, L_s, and T_{45} (the top of the valence band in T[13]) in $Bi_{1-x}Sb_x$ alloys under pressure[8,10,12] allow us to assume that a transition from the semiconducting state to the metallic state should be observed in the narrow Sb concentration interval $0.065 \lesssim x \lesssim 0.075$ near the inversion point $p = p_i$ at $p = p_1 < p_i$, and an inverse transition at $p = p_2 > p_i$ (Fig. 2). The maximum value of the resultant band overlap ϵ_{ov} corresponds to the pressure $p = p_i$ and can be regulated by varying x. The intrinsic carrier degeneracy that appears in such a transition makes it possible to use oscillatory methods for the study of the GS, without additionally doping the samples with donor or acceptor impurities. The latter is very important, since doping leads to a smearing of the band boundaries, and makes observation of small values of the energy gap difficult.

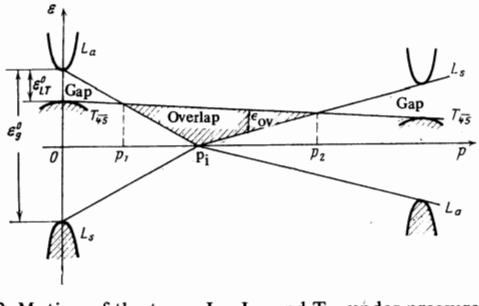

FIG. 2. Motion of the terms L_a, L_s, and $T_{4\bar{5}}$ under pressure for $Bi_{1-x}Sb_x$ alloys ($0.065 \lesssim x \lesssim 0.075$) in the "semiconductor–metal–semiconductor" trnasition near the band inversion point $p = p_i$. The region of existence of the metallic state is $p_1 \leqslant p \leqslant p_2$.

In the present paper we report the results of an investigation of the "semiconductor-metal-semiconductor" transition in accordance with the scheme shown in Fig. 2, for two $Bi_{1-x}Sb_x$ alloys with x = 0.070 and x = 0.071. We measured the longitudinal and transverse magnetoresistance of these alloys under pressures up to 15 kbar in fields up to 75 kOe at temperatures 1.9–4.2°K. Shubnikov-de Haas oscillations were observed in the metallic state that is produced in a definite pressure interval. Plots of the sections of the electron (S^e) and hole (S^e) parts of the Fermi surface were obtained, and also of the cyclotron masses of the electrons and of the holes against the pressure. An analysis of the transition into the state with $\epsilon_g \approx 0$ has been carried out.

The measurements were performed using the apparatus and procedure described in[8]. The magnetoresistance curves were plotted with an x-y recorder with continuous application of the magnetic field. The relative error in the determination of the resistance and of the field did not exceed 2%.

The samples of the $Bi_{1-x}Sb_x$ alloys with x = 0.070 and x = 0.071 were obtained from the laboratory of Professor G. A. Ivanov at the Leningrad State Pedagogical Institute. The alloy compositions were determined with a "Cameka" x-ray microprobe.

MEASUREMENT RESULTS

At normal pressure, the alloys $Bi_{0.930}Sb_{0.070}$ and $Bi_{0.929}Sb_{0.071}$ (henceforth denoted for brevity I and II) are semiconductors with small values of the energy gap ϵ^0_{LT} between the L and T extrema. On the plots of $\ln[\sigma_{22}(T) - \sigma_{22}(0°K)]$ against $1/T$ (σ_{22} is the electric conductivity in the direction of the binary axis C_2 of the crystal), in the temperature interval 1.9–100°K, it is possible to distinguish in the spectrum two linear sections that indicate the presence of two gaps of widely differing magnitude. Since to determine the position of the Fermi level in the forbidden band it is necessary to know the mobility ratios and the state-density masses of the electrons and holes, and also to make use of model representations, the value of the smaller gap ϵ^0_{LT} can be determined quite approximately. It amounts to ~1 meV for both alloy I and alloy II. The direct gap ϵ^0_g is determined in this case with an error on the order of $\sim\epsilon^0_{LT}$ and amounts to ~10 and ~12 meV for alloys I and II respectively.

The resistivities $\rho_{22} = 1/\sigma_{22}$ of the alloys at H = 0 and T = 4.2°K decrease with increasing pressure, go through minima at $p \sim 3.5$ and 3.8 kbar, and then increase. In the region $p > 7$–8 kbar, the growth of ρ_{22} becomes exponentially rapid.

The longitudinal magnetoresistance $\rho_{22}(H)$ current $i \parallel H \parallel C_2$) increases rapidly in the weak fields in the entire pressure range up to 15 kbar, passes through a maximum at a certain value $H = H_m$, and then decreases, passes through a minimum at $H = H_c$, and again increases. In fields $H > H_c$ there is observed an exponential growth of $\rho_{22}(H)$. The maximum and minimum values of the field H_m and H_c depend strongly on the pressure. Inasmuch as the magnetic field was

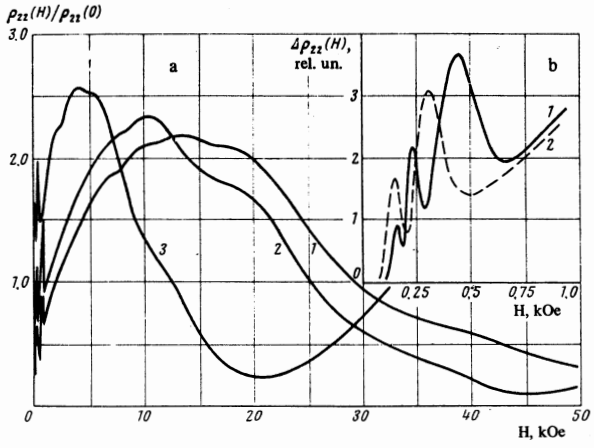

FIG. 3. Plots of the longitudinal magnetoresistance at i||H||C_2 for the alloy $Bi_{0.930}Sb_{0.70}$ in the region of existence of Shubnikov–de Haas oscillations. a–Typical plot: 1–p = 1.8 kbar, 2–p = 2.4 kbar, 3–p = 4.5 kbar (curves 1 and 2 are shifted by an arbitrary amount in the vertical direction); b–initial section of the curves (on an enlarged scale): 1–p = 1.8 kbar, 2–p = 4.5 kbar.

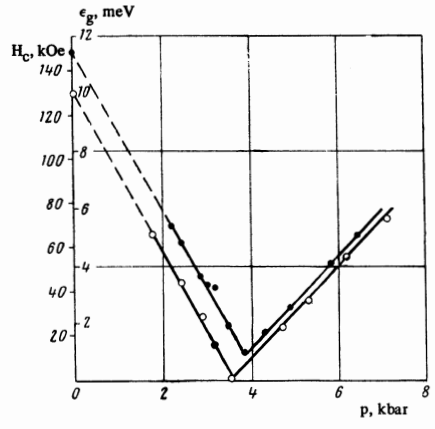

FIG. 5. Dependence of the magnetic field H = H_C at the minimum of ρ_{22}(H) (Figs. 4a and 5), i ∥ H ∥ C_2, and T = 4.2°K and of the corresponding values of the direct energy gap ϵ_g on the pressure for the alloys $Bi_{0.930}Sb_{0.070}$(○) and $Bi_{0.929}Sb_{0.071}$(●).

limited in the measurements to H = 75 kOe, the minimum of ρ_{22}(H) could not be observed at all values of the pressure. The ratio obtained was $\rho_{22}(H = H_m)/\times\rho_{22}(H = 0) \approx 2.0–3.5$ at $H_m > 2$ kOe, and decreased to unity at small values of H_m. The value of $\rho_{22}(H = H_C)/\rho_{22}(H = 0)$ was usually ~0.1–0.2.

Similar magnetoresistance curves ρ_{22}(H) in a field H ∥ C_2 were observed for $Bi_{1-x}Sb_x$ alloys with $0.09 < x < 0.15$ at p = 0 in pulsed magnetic fields up to 500 kOe[11]. The minimum of ρ_{22}(H) on these curves at H = H_C was attributed to the occurrence of a GS (called "quasi-metallic") in the magnetic field.

In the pressure range $1.0 \lesssim p \lesssim 9.5$ (in kilobars), the ρ_{22}(H) curves of alloy I clearly show Shubnikov-de Haas oscillations. Oscillations are observed in alloy II at pressures $0.9 \lesssim p \lesssim 3.1$ and $4.9 \lesssim p \lesssim 9.6$. There were no oscillations in this alloy in the interval $3.2 < p < 4.2$ down to the lowest temperatures. Figure 3a shows plots of ρ_{22} against the field H for alloy I at three values of the pressure from the region where oscillations exist. The presence of oscillations does not change the previously described general character of the magnetoresistance curve. At H ∥ C_2 there are observed oscillations with two essentially different frequencies (in terms of the coordinates $\rho = \rho(H^{-1})$): low frequency (in fields up to 1 kOe) and high frequency (in fields from ~3 to ~30 kOe). The low-frequency oscillations are shown in Fig. 3b on an enlarged scale.

The longitudinal magnetoresistance curves ρ_{22}(H) for alloy II at four values of pressure outside the regions where oscillations exist are shown in Fig. 4. The pressure dependence of the position of the minimum (H = H_C) on the ρ_{22}(H) curves is shown in Fig. 5. The values of H_C at p = 0 for alloys I and II, ~130 and ~150 kOe, respectively, were borrowed from the results of measurements in pulsed magnetic fields[11]. The dependence of H_m on p for each alloy is irregular. In addition to the principal minimum in the pressure region p ~ 3.3–3.8 (kbar), there are observed additional minima at p ~ 0.5 and p ~ 8.4, and also two maxima at p ~ 1.7 and p ~ 6.8. The value of H_C under pressure decreases linearly (Fig. 5), goes through a minimum at p ~ 3.5 and ~3.8 (for alloys I and II, re-

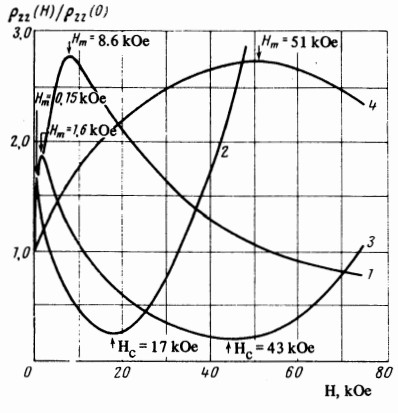

FIG. 4. Typical plots of longitudinal magnetoresistance at i ∥ H ∥ C_2 for the alloy $Bi_{0.929}Sb_{0.071}$ outside the region of existence of Shubnikov–de Haas oscillations: 1–p = 1 bar, 2–p = 3.8 kbar, 3–p = 3.2 kbar, 4–p = 13.4 kbar.

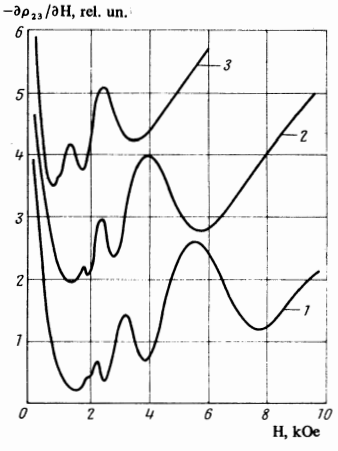

FIG. 6. Typical plot of oscillations of the derivative of the transverse magnetoresistance $-\partial\rho_{23}/\partial H$ at i ∥ C_2 and H ∥ C_3 for the alloy $Bi_{0.930}Sb_{0.070}$: 1–p = 2.1 kbar, 2–p = 2.8 kbar, 3–p = 3.1 kbar.

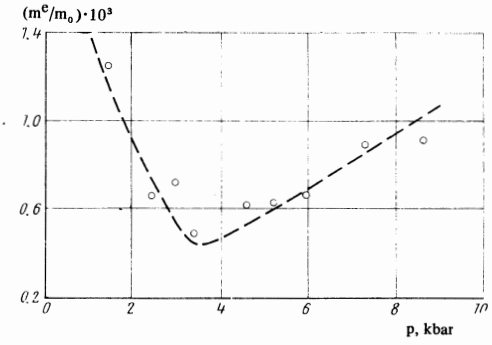

FIG. 7. Pressure dependence of the cyclotron mass of the electrons at $H \parallel C_2$ for the sample $Bi_{0.930}Sb_{0.070}$.

spectively), and then increases linearly at a rate that is slower by an approximate factor 1.7. We note that the smallest values of H_C, H_m, and $\rho_{22}(p)/\rho_{22}(0)$ were observed at approximately the same pressure for each alloy.

To explain the nature of the oscillations of the longitudinal magnetoresistance at $H \parallel C_2$, we also investigated the longitudinal and transverse magnetoresistance in a field H parallel to the trigonal axis C_3. For each alloy, the regions of existence of oscillations at $H \parallel C_2$ and $H \parallel C_3$ are the same. Figure 6 shows the oscillations of $\partial\rho_{23}/\partial H (i \parallel C_2, H \parallel C_3)$ for alloy I at three values of the pressure. In a field $H \parallel C_3$ there are observed oscillations of only one period.

From the temperature dependence of the amplitude of the oscillations of $\rho_{22}(H)$ $(i \parallel H \parallel C_2)$ and $\rho_{33}(H)$ $(i \parallel H \parallel C_3)$, using the formulas of Adams and Holstein[14], we calculated the cyclotron masses of the carriers. The cyclotron masses corresponding to the high-frequency oscillations at $H \parallel C_2$, and also to the oscillations at $H \parallel C_3$, have no functional dependence on p and lie in the respective intervals $(0.15-0.25)m_0$ and $(0.055-0.07)m_0$ (m_0 is the mass of the free electron). The cyclotron masses determined by the low-frequency oscillations at $H \parallel C_2$ are very small $(4\times10^{-4}-1.3\times10^{-3})m_0$ and depend strongly on the pressure (Fig. 7). The character of their variation following compression agrees with the change in the values of ρ_{22}, H_m, and H_C (Fig. 5).

The following should be noted concerning the determination of the carrier cyclotron masses. Formulas for them were obtained in[14] under the condition that the Fermi energy is independent of the magnetic field, and consequently these formulas are valid only for sufficiently large serial numbers of the Landau levels. We succeeded in observing oscillations corresponding to only the zeroth, first, and second Landau levels. In addition, at a small number of oscillation peaks, their amplitude is determined with an error that is the larger the smaller the number of observed peaks. As a result of these two circumstances, the obtained cyclotron masses should be regarded only as estimates.

The extremal sections S of the Fermi surface were determined in the following manner. The usual method[6,8] was used to determine the period of the oscillations in the reciprocal field $\Delta(1/H)$ from the curve of the oscillations with the maximum number of peaks; this period is connected with S by the formula[15]

$$S = eh/c\Delta(1/H), \tag{1}$$

where e is the electron charge, h Planck's constant, and c the velocity of light in vacuum. We then calculated the proportionality coefficient η in the relation

$$S \approx \eta H_0^+, \tag{2}$$

where H_0^+ is the value of the magnetic field corresponding to the 0^+ Landau level (the last oscillation minimum of the magnetoresistance). With decreasing number of oscillation peaks, the value of S was determined from formula (2) under the assumption that η remains constant at a given field orientation. The approximate satisfaction of (2) was verified in[8] for the semimetallic $Bi_{1-x}Sb_x$ alloys in a wide range of Sb concentrations (x) and pressures (p). It was shown that at the same orientation of H the value of η depends very little on the carrier Fermi energy.

The ratio of the extremal cross sections determined from the high-frequency oscillations at $H \parallel C_2$ and the oscillations at $H \parallel C_3$ is independent of the pressure in first approximation, and equals 3.0 ± 0.2. This value coincides with the ratio of the corresponding extremal sections of the hole ellipsoid in T of Bi[6] for the semimetallic $Bi_{1-x}Sb_x$ alloys with $x < 0.065$[8]. The latter circumstance, together with the data on the cycloton masses, makes it possible to assume that the oscillations at $H \parallel C_3$ and the high-frequency oscillations at $H \parallel C_2$ are connected with the holes in T. The values of the cyclotron masses determined from the low-frequency oscillations at $H \parallel C_2$, and also the character of their dependence on the pressure, indicate that these oscillations are connected in turn with the electrons in L. The theoretical analysis presented in the next section provides an additional justification of the last statement.

Thus, the data obtained confirm the correctness of the initial premises (Fig. 2) concerning the character of the pressure-induced "semiconductor–metal–semiconductor" transition in the investigated alloys.

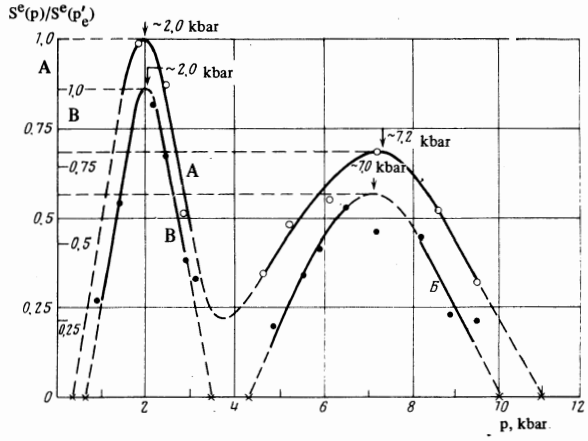

FIG. 8. Pressure dependence of the extremal sections of the electronic equal-energy surfaces at $H \parallel C_2$ for the alloys ○–$Bi_{0.930}Sb_{0.070}$ and ●–$Bi_{0.929}Sb_{0.071}$. The crosses on the abscissa axis denote the pressures at which Shubnikov–de Hass oscillations are not observed.

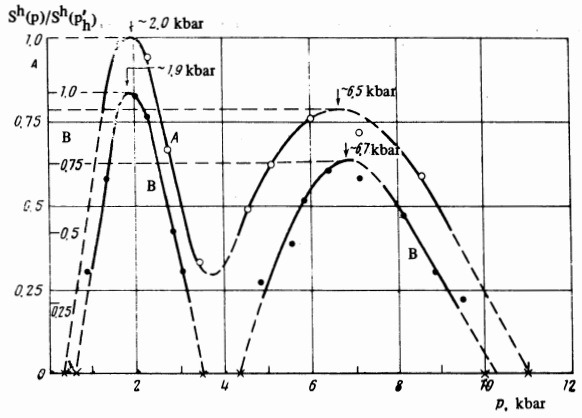

FIG. 9. Pressure dependence of the extremal sections of the hole ellipsoids at $\mathbf{H} \parallel C_2$ for the alloys O–$Bi_{0.930}Sb_{0.07}$ and ●–$Bi_{0.929}Sb_{0.071}$. The crosses on the abscissa axis denote the pressures at which no Shubnikov–de Haas oscillations are observed.

The dependences of the extremal electron and hole sections S^e and S^h in a field $\mathbf{H} \parallel C_2$ on the pressure are shown for alloys I and II in Figs. 8 and 9. In accordance with the character of the realignment of the spectrum of the $Bi_{1-x}Sb_x$ alloys (Fig. 1) and the scheme shown in Fig. 2, the sections S^e and S^h of alloy II are smaller than the corresponding sections of alloy I. The sections S^e and S^h pass twice through a maxima, almost simultaneously for each alloy, at $p' \approx 2.0$ kbar and $p'' \approx 7.0$ kbar. For alloy I at $p \approx 3.5$ kbar, the sections S^e and S^h pass through a minimum. It is seen from Figs. 8 and 9 that

$$S^e(p'') < S^e(p'), \quad S^h(p'') < S^h(p'). \tag{3}$$

The ratios of these quantities for both alloys are

$$S^e(p'')/S^e(p') \approx 0.67, \quad S^h(p'')/S^h(p') \approx 0.77. \tag{4}$$

DISCUSSION OF RESULTS

1. Band Inversion in L Under Pressure

In the present investigation, the change of the direct gap ϵ_g under pressure was determined from the change of the proportional quantity H_c[11,16]. The dependence of H_c on p (Fig. 5) shows that ϵ_g decreases linearly when the alloy goes over into the GS (at $p < p_i$) to an anomalously small value, and then increases linearly (at $p > p_i$) at a lower rate. The ratio of the rates of these changes, determined from the equation

$$\left|\frac{\partial \varepsilon_g}{\partial p}\right|_{p<p_i} \Big/ \left|\frac{\partial \varepsilon_g}{\partial p}\right|_{p>p_i} = \left|\frac{\partial H_c}{\partial p}\right|_{p<p_i} \Big/ \left|\frac{\partial H_c}{\partial p}\right|_{p>p_i}, \tag{5}$$

is the same, with sufficient accuracy, for both alloys and amounts to ~1.7. The absolute values of the rates can be estimated from the values of the gaps ϵ_g^0 at $p = 0$ (~10 and ~12 meV) and the values of p_i (~3.5 and 3.8 kbar, Fig. 5) for each alloy. The estimate yields

$$\left.\frac{\partial \varepsilon_g}{\partial p}\right|_{p<p_i} \approx -3.0\,\frac{\text{MeV}}{\text{kbar}}, \quad \left.\frac{\partial \varepsilon_g}{\partial p}\right|_{p>p_i} \approx +1.8\,\frac{\text{MeV}}{\text{kbar}} \tag{6}$$

The results agree with those of the measurements[8,10,12].

The minimum values of the gaps ϵ_{gmin} at $p = p_i$ on Fig. 5 are apparently connected with the smearing of the band boundaries in L, and amount to ~0.1 and ~1.0 meV for alloys I and II, respectively.

The absence of symmetry in the absolute value of the rate $|\partial\epsilon_g/\partial p|$ relative to the point $p = p_i$ is, in our opinion, additional evidence that band inversion takes place at the point L at this pressure. As shown by Golin[13], in pure Bi and in $Bi_{1-x}Sb_x$ alloys with $x < 0.04$, the bands in L are "pressed" one into the other, and the terms L_s and L_a are "entangled" with each other. This means that the extremum of the conduction band has the symmetry L_s only in the intermediate vicinity of the energy minimum; away from this minimum, the symmetry goes over into L_a. In turn, the extremum of the valence band has the symmetry of L_a near the energy maximum and of L_s far from it. In semimetals of group V (As, Sb, Bi) of the periodic table, such a situation is observed only for Bi, the extrema of which in L are inverted with respect to the analogous extrema of As and Sb. An increase of the Sb impurity in the $Bi_{1-x}Sb_x$ alloys causes the mutual deformation of the bands in L to decrease and to vanish at $x \approx 0.04$. At $x > 0.04$ the terms L_s and L_a "split" and a band symmetry similar to that observed for Sb and As is restored: L_a for the conduction band and L_s for the valence band.

Under the influence of pressure, the bands in L come closer together in the $Bi_{1-x}Sb_{-x}$ alloys at $x > 0.04$. One can expect in this case that the band extrema, which are not deformed at $p < p_i$, will begin to "press" one into the other at $p > p_i$, as a result of which there is produced under pressure (beyond the inversion point) a situation similar to that observed in pure Bi and in $Bi_{1-x}Sb_x$ alloys with $x < 0.04$. The discrepancy between the extrema in the region $p > p_i$ is a consequence of their mutual penetration and deformation (Fig. 10). The latter apparently explains the fact that the bottom of the conduction band moves away from the top of the valence band in this case at a rate $\partial\epsilon_g/\partial p|_{p>p_i}$, which is lower than that at which the nondeformed bands came closer together.

The ratio of the quantities $\partial\epsilon_g/\partial p|_{p<p_i}$ and $\partial H_c/\partial p|_{p<p_i}$ makes it possible to estimate the rate of approach of the bands in L, $\partial\epsilon_g/\partial H|_{H<H_c}$ in L on going over to the GS in a magnetic field $\mathbf{H} \parallel C_2$. In accordance with the data of[11], this rate amounts to approximately −0.08 meV/kOe for $Bi_{1-x}Sb_x$ alloys with $0.065 < x < 0.15$. It determines the difference between

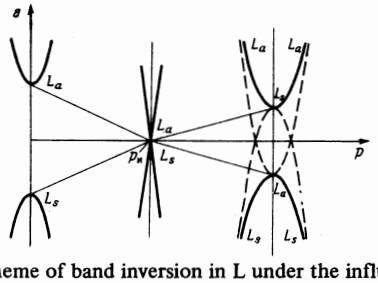

FIG. 10. Scheme of band inversion in L under the influence of pressure in $Bi_{1-x}Sb_x$ alloys with $x > 0.04$. At $p > p_i$, a mutual deformation of the bands and a "mixing" of the symmetries of the terms L_a and L_s takes place.

the values of the spin and orbital splittings in L[11]. If it is assumed, according to Malgrange[17], that the conduction band and the valence band in L are similar and are "mirror reflections" of each other, then for each value of the electron cyclotron mass m_0^e on the bottom of the bands it is possible to estimate from $\partial\epsilon_g/\partial H|_{H<H_c}$ the corresponding value of the electron spin mass on the bottom of the band. Baraff[16] has shown theoretically that the extrema in L of Bi should move together and apart with equal velocities in a magnetic field. Unfortunately, we do not have experimental data on $\partial\epsilon_g/\partial H|_{H>H_c}$ to compare it with $\partial\epsilon_g/\partial H|_{H<H_c}$.

2. Rate of Relative Motion of the Term $T_{\bar{45}}$ Under Pressure. Dependence of S^a on p.

The "semiconductor–metal–semiconductor" transition near the inversion point under pressure (see Fig. 2) has been predicted on the basis of the relative rates of motion of the terms L_a, L_S, and $T_{\bar{45}}$ in $Bi_{1-x}Sb_x$ alloys at $x > 0.04$ obtained in[8,10,12]. These data concerning the motion of the term $T_{\bar{45}}$ are based on model concepts and need further confirmation. Let us examine what character of displacement of the $T_{\bar{45}}$ term under pressure follows from the experimental relations obtained in the present paper. To analyze these relations, we introduce the rate $\partial\epsilon_T/\partial p$ of motion $T_{\bar{45}}$ relative to the center of the gap ϵ_g. It follows from[8,10] that $\partial\epsilon_T/\partial p \approx -(0.6-0.8)$ meV/kbar. Let us analyze two possibilities: $\partial\epsilon_T/\partial p < 0$ and $\partial\epsilon_T/\partial p > 0$. The successive transitions on Fig. 2 are possible if the basic condition

$$\varepsilon_{LT}^0 < \varepsilon_g^0/2 \tag{7}$$

is satisfied for the following relations between the rates $\partial\epsilon_g/\partial p$ and $\partial\epsilon_T/\partial p$:

a) For the transition from the superconducting to the metallic state it is necessary to have either $\partial\epsilon_T/\partial p \geq 0$ or $(1/2)|\partial\epsilon_g/\partial p|_{p<\rho} > -\partial\epsilon_T/\partial p > 0$;

b) For the transition from the metallic to the semiconducting state it is necessary to have either $\partial\epsilon_T/\partial p \leq 0$ or $(1/2)|\partial\epsilon_g/\partial p|_{p>p_i} > \partial\epsilon_T/\partial p > 0$.

In the case $\partial\epsilon_T/\partial p < 0$, all the conditions can be unified in the following inequality:

$$\varepsilon_{LT}^0 < \frac{\varepsilon_g^0}{2}\cdot\left(1-\left|\frac{\partial\varepsilon_T}{\partial p}\right|\Big/\frac{1}{2}\left|\frac{\partial\varepsilon_g}{\partial p}\right|_{p<p_i}\right). \tag{8}$$

If inequality (8) is satisfied, then at a certain value of the pressure $p = p_1 < p_i$ there appears a band overlap ϵ_{ov} in L and T, which increases linearly to a maximum $\epsilon_{ov.max}$ corresponding to $p = p_i$, and then decreases linearly and vanishes at $p = p_2 > p_i$. Such an idealized scheme (Fig. 11a) follows from the assumption that the displacement of the terms under pressure has a linear character. It is easy to show that at $\partial\epsilon_T/\partial p < 0$ we have

$$\varepsilon_{ov.max} = \frac{\varepsilon_g^0}{2}\left(1-\left|\frac{\partial\varepsilon_T}{\partial p}\right|\Big/\frac{1}{2}\left|\frac{\partial\varepsilon_g}{\partial p}\right|_{p<p_i}\right) - \varepsilon_{LT}^0. \tag{9}$$

Since the Fermi energy of the electrons ϵ_F^e does not exceed ϵ_{ov}, we have in the entire range of pressures $p_1 \leq p \leq p_2$

$$\varepsilon_F^e < \varepsilon_{ov} \leqslant \varepsilon_{ov}^{max} \tag{10}$$

($\epsilon_F^e = 0$ at $p = p_1, p_2$).

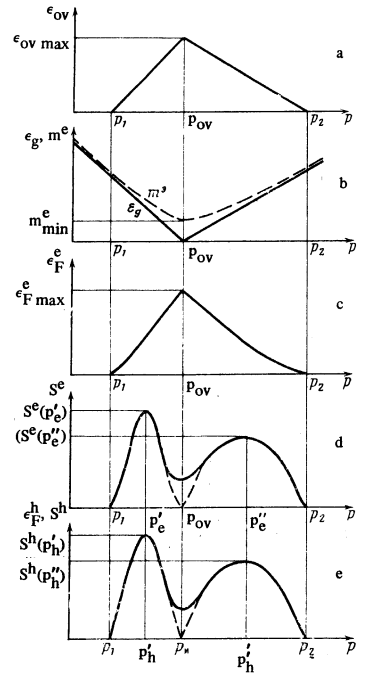

FIG. 11. Qualitative form of the pressure dependences of different parameters of the energy spectrum of $Bi_{1-x}Sb_x$ alloys ($0.065 \lesssim x \lesssim 0.075$) for the "semiconductor–metal–semiconductor" transition near the band inversion point $p = p_i$: a–of the overlap ϵ_{ov} of the bands in L and T, b–of the direct gap ϵ_g in L and of the cyclotron mass m^e of the electrons at the Fermi level, corresponding to the minimum section, c–of the electron Fermi energy ϵ_F^e, d–of the minimum section of the electron Fermi surface S^e, e–of the hole Fermi energy ϵ_F^h and of the extremal section of the hole Fermi surface S^h. In cases d and e, the solid curves correspond to the experimental data and the dashed curves to the quadratic dispersion law for electrons.

In the general case, the dependences of ϵ_{ov} and ϵ_g on p (Figs. 11a and b) can be written in the form

$$\varepsilon_{ov} = \begin{cases} \left[\frac{1}{2}\left|\frac{\partial\varepsilon_g}{\partial p}\right|_{p<p_i} \mp \left|\frac{\partial\varepsilon_T}{\partial p}\right|\right](p-p_1), & p_1 \leqslant p \leqslant p_i, \\ \left[\frac{1}{2}\left|\frac{\partial\varepsilon_g}{\partial p}\right|_{p>p_i} \pm \left|\frac{\partial\varepsilon_T}{\partial p}\right|\right](p_2-p), & p_i \leqslant p \leqslant p_2; \end{cases} \tag{11}$$

$$\varepsilon_g = \begin{cases} \left|\frac{\partial\varepsilon_g}{\partial p}\right|_{p<p_i}(p_i-p), & p \leqslant p_i, \\ \left|\frac{\partial\varepsilon_g}{\partial p}\right|_{p>p_i}(p-p_i), & p \geqslant p_i. \end{cases} \tag{12}$$

The upper and lower signs in (11) pertain to $\partial\epsilon_T/\partial p < 0$ and $\partial\epsilon_T/\partial p > 0$, respectively. The values of p_1 and p_2 are determined from the two equations $\epsilon_{ov} = \epsilon_{ov.max}$, which follow from (11) at $p = p_i$. The unknown quantity $\partial\epsilon_T/\partial p$ can be calculated if the measured extremal sections S^e are expressed in terms of ϵ_{ov}.

We note that in any model of the electron energy spectrum in L, the deviation from quadratic dispersion can be neglected if $\epsilon_F^e < \epsilon_g$ (strictly speaking, if $\epsilon_F^e \ll \epsilon_g$). This inequality is certainly satisfied near p_1 and p_2, where ϵ_F^e is small. It is violated when $p = p_i$ is approached, where $\epsilon_g \approx 0$. Let us calculate the dependence of S^e on p for a quadratic electron dispersion law. The pressure regions in which this condition is satisfied will be defined more accurately below. (The dispersion law of the holes in T is assumed, in accordance with the generally accepted concept, to be

quadratic). The carrier gas in the metallic state is degenerate at helium temperatures (in $Bi_{1-x}Sb_x$ alloys even at the minimum carrier concentration $\sim 10^{14}$ cm^{-3} the degeneracy temperature is $T_{deg} > 30^\circ$K). In this case we can show that

$$\varepsilon_F^e = \frac{m_c^h}{m_c^h + m_c^e}\varepsilon_{ov}, \quad \varepsilon_F^h = \frac{m_c^e}{m_c^h + m_c^e}\varepsilon_{ov} \tag{13}$$

where ϵ_F^h is the Fermi energy of the holes in T, and m_s^e and m_s^h are the state-density masses of the electrons and holes at the Fermi level. The latter quantities are determined by the principal values of the effective electron masses m_1^e, m_2^e, m_3^e and holes masses $M_1^h = M_2^h$, M_3^h at the Fermi level:

$$m_s^e = (9m_1^e m_2^e m_3^e)^{1/3}, \quad m_c^h = ((M_1^h)^2 M_3^h)^{1/3}. \tag{14}$$

Relations (13) are the consequence of the equality of the electron concentration n to the hole concentration p, and also of the condition $\epsilon_F^e + \epsilon_F^h = \epsilon_{ov}$. It follows from the experimental data that at least some of the principal values of m_i^e (i = 1, 2, 3) decrease together with ϵ_g (Fig. 7), whereas M_i^h (i = 1, 2, 3) remain constant. Since we are interested in the process of the transition to the GS, we put for simplicity $m_s^e \ll m_s^h$ and simplify (13):

$$\varepsilon_F^e \approx \varepsilon_{ov}, \quad \varepsilon_F^h \approx (m_c^e/m_c^h)\varepsilon_{ov}. \tag{15}$$

(see Fig. 11c). The extremal cross sections S^e and S^h can therefore be written in the form

$$S^e = 2\pi m^e \varepsilon_F^e \approx 2\pi m^e \varepsilon_{ov}, \quad S^h = 2\pi m^h \varepsilon_F^h \approx 2\pi m_c^e (m^h/m_c^h)\varepsilon_{ov}. \tag{16}$$

where m^h is the cyclotron mass of the holes in T.

In the present investigation we have observed close to minimal sections S^e of the electron ellipsoid ($H \parallel C_2$) and the corresponding cyclotron masses m^e. For the cyclotron masses m_0^e pertaining to this section at the bottom of the band, as follows from[8], Golin's hypothesis[13] $m_0^e \sim \epsilon_g$ holds true. (Favoring this hypothesis is also the sharp increase of the mobility μ_2 of the electrons in the direction of the C_2 axis as $\epsilon_g \to 0$[10,12]). Our experimental data, which are shown in Fig. 7, agree with this assumption.

In our approximation $\epsilon_F^e < \epsilon_g$, the mass m_0^e at the bottom of the band coincides with the mass m^e at the Fermi level. It then follows from (11), (12), and (16) that

$$S \sim \begin{cases} (p-p_1)(p_i-p), & p_1 \leqslant p < p_i \\ (p_2-p)(p-p_i), & p_i < p \leqslant p_2 \end{cases}. \tag{17}$$

In accordance with (17), S^e should pass twice through a maximum at

$$p_e' = \tfrac{1}{2}(p_1 + p_i), \quad p_e'' = \tfrac{1}{2}(p_2 + p_i) \tag{18}$$

and should vanish at $p = p_1$, $p = p_i$, and $p = p_2$ (Fig. 11d). We recall that formulas (15)–(17) given above were obtained for a quadratic dispersion law. Near $p = p_i$, however, it is necessary to take into account the nonparabolicity of the band in L. Consequently, at $\epsilon_F^e \neq 0$ and $\epsilon_g \approx 0$, the mass $m^e \neq 0$ and the cross section S^e at $p = p_i$ does not vanish but passes through a minimum (see Fig. 8 and the solid curve in Fig. 11d). The minimum of S^e is explained by the fact that in spite of the growth of the overlap ϵ_{ov} on approaching $p = p_i$, the density of states of the electrons decreases together with ϵ_g (naturally, the decrease of the density of states is noticeable only near the bottom of the band, i.e., at sufficiently small values of ϵ_F^e). The latter leads to a decrease of the electron concentration n, and consequently also of the section S^e. The extremal hole section S^h also goes through a minimum (Figs. 9 and 11e), since at n = p we have $\epsilon_F^h = \epsilon_{ov} - \epsilon_F^e$, and as $p \to p_i$ we have $\epsilon_F^e \to \epsilon_{ov} - \delta$, and $\epsilon_F^h \to \delta$, where δ is a small quantity.

Using formulas (11), (12), (16), and (18), we can show that

$$\frac{S_e(p_e'')}{S_e(p_e')} = \left(1 \mp \left|\frac{\partial \varepsilon_T}{\partial p}\right| \Big/ \frac{1}{2}\left|\frac{\partial \varepsilon_g}{\partial p}\right|_{p<p_i}\right) \times \left(1 \pm \left|\frac{\partial \varepsilon_T}{\partial p}\right| \Big/ \frac{1}{2}\left|\frac{\partial \varepsilon_g}{\partial p}\right|_{p>p_i}\right)^{-1}. \tag{19}$$

Here the upper and lower signs also pertain to the cases $\partial\epsilon_T/\partial p < 0$ and $\partial\epsilon_T/\partial p > 0$, respectively. We assume that at $p = p_e'$ and $p = p_e''$ the influence of the nonparabolicity of the electron spectrum is still small. It follows then from (3) and (19) that $\partial\epsilon_T/\partial p < 0$, in accord with the data of[8,10]. The rate $\partial\epsilon_T/\partial p$ can be calculated with the aid of (19) and the data of (4) and (6):

$$\partial\varepsilon_T/\partial p \approx -0.25 \text{ MeV/kbar} \tag{20}$$

Let us estimate the values of ϵ_F^e and ϵ_g at $p = p_e'$ = 2 kbar and $p = p_e'' \approx 7$ kbar in accordance with formulas (11) and (12), using (10), (4), (6) and (20). Numerical calculation shows that for alloys I and II at these pressures the inequality $\epsilon_F^e < \epsilon_g$ is satisfied. Thus, formula (19) is exact (at $\partial\epsilon_T/\partial p < 0$) and does not depend on the concrete model of the energy spectrum of the electrons in L. This allows us to assume that the rate $\partial\epsilon_T/\partial p$ (20) which is obtained from (19) and which agrees in sign with the data of[8,10], but differs noticeably in absolute magnitude, describes more accurately the motion of the term $T_{\bar{4}5}$ during the realignment of the energy spectrum of the $Bi_{1-x}Sb_x$ alloys under pressure.

c. Anisotropy of the Bands in L on Going to the GS

The data considered in the preceding subsection, concerning the proportionality of ϵ_g to the mass at the bottom of the conduction band in L, pertain to a direction along the short axes of the electronic ellipsoid (to the minimal section). All that follows from them is that the two smallest principal values of the effective masses m_{20}^e and m_{30}^e become anomalously small at the bottom of the band as $\epsilon_g \to 0$. The absence of oscillations from the large sections, both for $H \parallel C_2$ and $H \parallel C_3$, owing to the low mobility of the electrons in the direction of the major axes of the ellipsoid, and also owing to the large values of the corresponding cyclotron masses, does not make it possible to obtain direct information concerning the dependence of m_{10}^e on ϵ_g and concerning the change of the anisotropy of the bands in L as $\epsilon_g \to 0$. These dependences are of great importance, however, for the theoretical description of the intermediate state between the metal and the dielectric that is produced

under pressure in the $Bi_{1-x}Sb_x$ alloys, and also for the choice between the models of Lax-Golin[18,13] and Cohen[19] for the electron energy spectrum in L.

Two qualitatively different types of "natural" GS, differing in the form of the electron dispersion law $\epsilon(k)$ in the "singular" region near the "band tangency" point $k = k_0$: are considered in[1]:

1) GS with quadratic dependence of ϵ on k at all directions of the vector k (with none of the principal values of the effective mass m_{i0} (i = 1, 2, 3) equal to zero);

2) GS with a linear dependence of ϵ on k at all directions of the vector k (in this case all $m_{i0} = 0$, i = 1, 2, 3).

When the GS is produced under the influence of external actions, a hybrid type of GS can arise, when the quadratic dependence of ϵ on k, for k lying in a small solid angle along one of the principal directions of the band, combines with a linear dependence in all other directions of k. In this case two principal values m_{i0} vanish as $\epsilon_g \to 0$, whereas the third remains unchanged.

The Lax-Golin model corresponds to formation of a GS of type 2 in $Bi_{1-x}Sb_x$ alloys. The occurrence of a hybrid type of GS indicates that the Cohen model is valid. The choice between these two possibilities can be made by comparing the dependences of S^e and S^h on p. Their difference, as follows from formula (16), results from the difference between the dependences of m^e and m_s^e on p.

If a GS of type 2 is realized, then all $m_{i0}^e \sim \epsilon_g \sim |p - p_i|$ (i = 1, 2, 3). In this case all $m_i^e \sim \epsilon_g \sim |p - p_i|$ (i = 1, 2, 3) when $\epsilon_F^e < \epsilon_g$, and the state-density mass is $m_s^e \sim \epsilon_g \sim |p - p_i|$. It then follows from (16) that S^e and S^h depend in like manner on p and differ only by a constant factor. This causes, in particular, the maxima of S^e and S^h to be observed at identical values of the pressure:

$$p_h' = p_e', \quad p_h'' = p_e'' \tag{21}$$

(p_e' and p_e'' are defined in (18)), and

$$S^h(p_h'') / S^h(p_h') = S^e(p_e'') / S^e(p_e'). \tag{22}$$

When a GS of the hybrid type is produced, it is obvious that $m_s^e \sim \epsilon_g^{2/3} \sim |p - p_i|^{2/3}$. It can be shown in this case that the maxima of S^h should be observed at

$$p_h' = \frac{{}^2/_3 p_1 + p_i}{{}^5/_3}, \quad p_h'' = \frac{{}^2/_3 p_2 + p_i}{{}^5/_3}, \tag{23}$$

i.e., they are shifted somewhat compared with the electronic ones in the direction towards p_i. Then (22) is replaced by

$$S^h(p_h'') / S^h(p_h') = [S^e(p_e'') / S^e(p_e')]^{2/3}. \tag{24}$$

Unfortunately, the accuracy in the determination of the positions of the maxima on Figs. 8 and 9 is insufficient to reveal a difference between formulas (18) and (23). The accuracy in the determination of the ratio of the maximal values of S^e and S^h at the corresponding $p = p'$ and $p = p''$ is much higher. The experimental values of (4) permit a choice between formulas (22) and (24); indeed, the ratios $S^e(p_e'')/S^e(p_e') \approx 0.67$ and $S^h(p_h'')/S^h(p_h') \approx 0.77$ agree well with (24) ($(0.67)^{2/3} \approx 0.765$) and deviates from (22) by approximately 15%.

Thus, we can apparently assume that a hybrid type of GS is observed in $Bi_{1-x}Sb_x$ alloys under pressure. On going over to the GS, the anisotropy of the bands in L increases without limit. If the formation of the GS occurs with a small band overlap in L and T, then the electron "ellipsoid" contracts to a narrow needle. (We note that in Cohen's model the large sections of the electronic Fermi surface in L are not ellipses, but are bounded by fourth-degree curves; it is therefore more correct to call the body bounded by the Fermi surface an ovaloid. Such a character of the energy spectrum of the electrons in L is indicated also in the paper of Abrikosov and Fal'kovskiĭ[20].)

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