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Translated by J. G. Adashko

Investigation of the zero-gap state induced by a magnetic field in bismuth-antimony alloys

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(Submitted December 31, 1975)
Zh. Eksp. Teor. Fiz. 70, 2296–2317 (June 1976)

The character of the band motion induced by a magnetic field H is investigated in $Bi_{1-x}Sb_x$ alloys in which the spectrum structure has been changed from a direct to inverted one by a hydrostatic pressure p. The measurements are carried out for alloys with a broad range of concentrations $6.6 \leq x \leq 13$ at.%; in fields H up to 65 kOe and at p up to 15 kbar. It is found that the transition to the zero-gap state induced by the magnetic field occurs only in the inverted region of the alloy spectrum for $p > p_i$. The surface of the zero-gap state in the physical parameter space (composition–pressure–magnetic field) is plotted for $Bi_{1-x}Sb_x$ alloys. By extrapolation it is found that the surface is bounded by parameter values such that $x \lesssim 40$ at.%, $p \lesssim 35$ kbar, and $H \lesssim 1500$ kOe. The directions and velocities of the mutual motion of the L and T bands for the direct and inverted alloy spectra are determined. It is found that transition to the zero-gap state induced by a magnetic field results in the isotropization of the transverse relaxation time of the L carriers.

PACS numbers: 71.30.Kt

INTRODUCTION

A study of a new state of matter, intermediate between that of a metal and an insulator, named the zero-gap (gapless) state (ZGS), has attracted much interest in recent years. A characteristic feature of the ZGS is the absence of a direct gap ε_g in the energy spectrum. This gives rise to a number of unusual properties that cause the matter in the ZGS to differ qualitatively from a metal or an insulator.

The ZGS is the result of high symmetry of the crystal lattice. This situation is realized in gray tin (α-Sn) and also in HgTe, HgSe, HgS, Cd_3As_2, and some other compounds, which have been named natural zero-gap semiconductors. A theory of the ZGS, with a detailed analysis of the crystal symmetry at which this state can arise, was developed by Abrikosov and Beneslavskiĭ.[1]

In addition to the natural zero-gap semiconductors, a rather large class of substances is known in which vanishing of the direct gap ε_g and the transition to the ZGS take place as a result of changes in different physical parameters such as the alloy composition, temperature, pressure, and magnetic field.[2] It is particularly interesting to investigate this case inasmuch as by gradually varying the external action it is possible to observe in succession the restructuring of the energy spectrum of the initial matter as it goes over into the ZGS. At the present time, continuous transitions into the ZGS, induced by external action, have been frequently observed and investigated in solid-solution systems such as $Cd_xHg_{1-x}Te$, $Cd_xHg_{1-x}Se$, $Pb_{1-x}Sn_xTe$, $Pb_{1-x}Sn_xSe$, $Bi_{1-x}Sb_x$ etc. Transitions of these alloys in ZGS as a result of the changes in the composition or pressure have revealed an abrupt decrease in the effective masses and an increase in the carrier mobilities,[3,4] as well as anomalies connected with impurity states.[5]

Among the transitions to the ZGS induced by changes of various external parameters, the least investigated at present are transitions due to the action of a strong magnetic field. These transitions have definite features that distinguish them qualitatively from the transitions to the ZGS caused by changes of other physical parameters. The point is that in a strong magnetic field the electron system in the initial material becomes quasi-one-dimensional and polarized. The end points of the conduction band and of the valence band are determined in this case by the Landau levels corresponding to the quantum numbers $n = 0$ (the levels 0^- and 0^+). The electrons and holes at these levels have oppositely directed spins.

The carriers retain with three degrees of freedom and remain unpolarized following other types of action on the energy spectrum of the material (for example, changes in the alloy composition or hydrostatic compression). Therefore the transitions to the ZGS under the influence of a magnetic field can be regarded as a different class that calls for a special theoretical and

experimental study.

The formation of ZGS under the influence of a magnetic field is a consequence of the mutual approach of the boundaries of the valence band and the conduction band, resulting from the quantization of the electron energy in the magnetic field. Until recently it was customarily assumed that the approach of the bands in the magnetic field is feasible in principle only in the case when the spin splitting of the Landau levels, at least in one of the bands, exceeds the orbital splitting $\hbar\omega_c$ ($\omega_c = eH/mc$ is the cyclotron frequency).

For the investigation of the ZGS induced by a magnetic field, great interest attaches to $Bi_{1-x}Sb_x$ alloys, since the problem of the inversion of the two close bands in a magnetic field has so far been solved theoretically only for substances with a spectrum of the Bi type.[6,7] Thus, an experimental study of the motion of the band boundaries in a magnetic field for $Bi_{1-x}Sb_x$ alloys yields data that can be directly compared with theoretical calculations, and by the same token can be used both for further refinement of our notions concerning the band structure of the alloys and for further development of the theory of their energy spectrum. In addition, in view of the progress in the technology of producing $Bi_{1-x}Sb_x$ single crystals, it is possible at present to obtain samples with impurity carrier densities less than 10^{14} cm^{-3} and with a sufficiently large mean free path at low temperatures, i.e., samples of high degree of purity and perfection, and this makes the system $Bi_{1-x}Sb_x$ preferable to most semimetallic and semiconducting binary and ternary compounds and alloys.

The assumption that a ZGS can be produced in a magnetic field was first used to explain the anomalous minima on the longitudinal-magnetoresistance curves observed in the investigation of semiconducting $Bi_{1-x}Sb_x$ alloys in pulsed magnetic fields of intensity up to 500 kOe at helium temperatures.[8] However, appreciable experimental difficulties connected with measurements in short-period pulsed fields did not permit the authors of [8] to carry out a detailed investigation in a wide range of temperatures and to corroborate experimentally the assumption made.

The transition of the $Bi_{1-x}Sb_x$ into the ZGS under the influence of a constant magnetic field was first observed by us in[9] in which simultaneous action of a magnetic field and of hydrostatic compression was used to alter the parameters of the spectrum. In the present paper, the method of combined action of a magnetic field and of pressure was used for a detailed investigation of the band motion and of transitions to the zero-gap state for a large number of semiconducting $Bi_{1-x}Sb_x$ alloys with concentrations in the interval $6.6 \leq x \leq 13$ at.%. Particular attention is paid to the fact that the use of pressure as an additional parameter makes it possible not only to change the value of the direct gap ε_g, but also to change the sequence of the terms L_a and L_s, which determine the boundaries of the conduction and valence bands in the energy spectrum of the alloys.[10] This makes it possible to investigate the motion of the band boundaries in a magnetic field both in the case of the direct spectrum and in the case of the spectrum inverted with the aid of pressure.

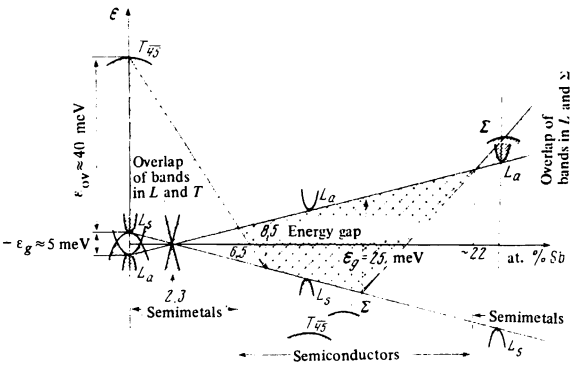

FIG. 1. Restructuring of the energy spectrum of $Bi_{1-x}Sb_x$ alloys in the Sb concentration interval $0 \leq x \leq 24$ at.% at $H = 0$ and $p = 1$ bar. The inverted spectrum of pure Bi at the points L at $x = 0$ is shown schematically. It constitutes two overlapping parabolas for a momentum direction along the elongation of the equal-energy surface; on their vertices are shown the parabolas corresponding to the perpendicular momentum direction.

The components of the galvanomagnetic tensor were measured at a magnetic-field orientation of intensity up to 65 kOe along the binary (C_1) and bisector (C_2) axes of the crystal at a pressure p from 15 kbar at temperatures $T = 1.8$–250 °K. The case when H is oriented along the trigonal axis (C_3) of the crystal, when semiconductor–metal transitions are observed in strong fields,[11,12] has specific distinguishing features connected with the onset of exciton phases[13] and is not considered in this paper.

ENERGY SPECTRUM OF $Bi_{1-x}Sb_x$ ALLOYS

The character of the variation of the energy spectrum in $Bi_{1-x}Sb_x$ alloys with increasing Sb concentration was investigated in a large number of papers (see, e.g.,[4,14]). The results of the latest investigations of the structure of the spectrum of these alloys are in general in sufficiently good agreement with one another and indicate that inversion of two close bands (terms L_a and L_s), located at the points L of the Brillouin zone,[15] takes place in the series of solid solutions $Bi_{1-x}Sb_x$, at a certain Sb concentration $x_i \lesssim 2.3$ at.%, (Fig. 1). In alloys with Sb concentration $x < 2.3$ at.% and in pure Bi, the band spectrum at the points L is apparently inverted. The theory of the direct and inverted spectra for a semimetal of the Bi type was developed by Abrikosov.[16]

At $x > x_i$, the terms L_a and L_s diverge, in the first approximation linearly at a relative rate $\partial\varepsilon_g/\partial x = 2.0 \pm 0.3$ meV/at.%. The term T_{45}, which determines the ceiling of the valence band of Bi and of semimetallic $Bi_{1-x}Sb_x$ alloys, drops downward in energy with increasing Sb concentration, and at $x = 6.5 \pm 0.5$ at.% the overlap ε_{ov} of the bands in L and T vanishes. At this value of the Sb concentration, the alloys change from the semimetallic to the semiconducting state with the minimum indirect gap between the terms L_a and T_{45}.

In the concentration region $8.5 \lesssim x \lesssim 15$ at.% Sb, the minimum gap in the spectrum of the alloys turns out to be the direct gap ε_g. At $x > 15$ at.%, the minimum gap is again the indirect gap between the terms L_a, and apparently between the terms at the points Σ, which rise upward from the interior of the valence band with increasing Sb concentration in the plasma. The terms Σ and L_a overlap at $x \approx 22$ at.%, and the alloys change from the semiconducting to the semimetallic state with a gradually increasing overlap of the bands and an increasing direct gap ε_g in L. Nothing is known at present concerning the character of the hole equal-energy surfaces that are produced in this case. In the described picture of the restructuring of the $Bi_{1-x}Sb_x$ alloy spectrum, least accurately determined is the value x_i of the Sb concentration at which inversion of the terms L_a and L_s takes place. It was shown in[15] that x_i does not seem to exceed 2.3 at.%.

It must be emphasized that the question of the position of the inversion point is of fundamental importance, inasmuch as at $x_i > 0$ the Bi spectrum at the point L is inverted and in this case one must speak not of the value of ε_g of the forbidden band in L, but of the value of the mutual overlap of the bands in L. We note that this representation of the spectrum of the alloys $Bi_{1-x}Sb_x$ and Bi does not agree with the results obtained by others[17,18] in investigations of pure Bi. According to those studies, the spectrum of Bi in L is not inverted, and the width of the forbidden gap ε_g amounts to 15.3 eV[17] or ~ 26 meV.[18] The question of the structure of the L_a and L_s bands of Bi will be considered later on in the discussion of the data of the present study.

Hydrostatic compression makes it possible to alter the structure of the spectrum of $Bi_{1-x}Sb_x$ alloys in a wide range. Under the influence of the pressure, the extremum $T_{\overline{45}}$ moved downward relative to the energy corresponding to the midpoint of the gap between the terms L_a and L_s, at a rate $\partial\varepsilon_T/\partial p \approx 0.25$ meV/kbar.[19] This rate seems to depend very little on the composition of the alloy and remains practically constant in the Sb concentration region up to 20 at.%. The extrema of L_s and L_a at $x > x_i$ approach each other upon compression with relative velocity $\partial\varepsilon_g/\partial p = -(2.5 \pm 0.2)$ meV/kbar (which also depends little on the composition of the alloys at $x < 20$ at.% Sb), so that at $x > x_i$ the pressure leads to the formation of the ZGS at a certain value $p = p_i$ (the gap ε_g vanishes) and to inversion of the positions of the terms L_a and L_s in the region $p > p_i$. The critical pressure corresponding to the formation of the ZGS in the $Bi_{1-x}Sb_x$ alloy depends on the value of the initial gap ε_g at $p = 1$ bar, and consequently on the composition of the alloy.

MEASUREMENT PROCEDURE. SAMPLES

An investigation of the galvanomagnetic characteristics of $Bi_{1-x}Sb_x$ alloys was carried out in a special cryostat that made possible measurements in magnetic fields up to 65 kOe at pressures up to 20 kbar in the temperature range 1.8–300 °K. The pressure was produced with a booster.[20] The pressure-transmitting medium was a mixture of isopentane and dehydrated transformer oil. The pressure was measured directly at liquid-helium temperature by a contactless method[21] on the basis of the superconducting transition temperature of a tin transducer[22] located in the booster channel alongside the sample.

The booster was centered in a thin-wall cylindrical cell of stainless steel, placed in the internal channel of a superconducting solenoid. In measurements at intermediate temperatures, the cell was evacuated with a carbon sorption pump and the temperature of the booster was varied with the aid of a manganin heater coil wound bifilarly on the booster surface. The temperature was measured with an $Au_{0.99}Fe_{0.01}$—Cu thermocouple, the cold junction of which was placed directly in the high-pressure chamber. The results of measurements in a magnetic field were corrected for the dependence of the thermocouple emf on the field strength.

To exclude the possible influence of thermomagnetic effects, all the measurements were performed with alternating current at the two possible orientations of the magnetic field. The signal picked off the potential electrodes was amplified with a narrow-band amplifier, detected, and fed to the Y coordinate of an x-y recorder. The X-coordinate received a signal proportional to the magnetic field intensity or to the temperature.

For a simultaneous measurement of the four components of the magnetoresistance tensor, three samples were placed in the high-pressure chamber; they were cut from neighboring regions of the ingot, along the crystal axes C_1, C_2, and C_3 by the electric-spark method. The samples were arranged in such a way that the axis C_1 or C_2 of each of them was parallel to the magnetic field. This arrangement of the samples made it possible to measure simultaneously the longitudinal, the two transverse, and the Hall component of the magnetoresistance tensor.

To prepare the samples we used $Bi_{1-x}Sb_x$ alloy ingots specially chosen for their homogeneity, with 12 compositions in the Sb concentration range $6.6 \leq x \leq 13$ at.%. The alloys were obtained from G. A. Ivanov's laboratory of the Leningrad State Pedagogical Institute and from the Metallurgy Institute of the USSR Academy of Sciences. The composition of the alloys and their homogeneity were monitored, with the aid of the "Cameca" x-ray microprobe. According to the Hall measurement data, the concentration of the n- or p-type impurity carriers in the alloys did not exceed 10^{15} cm^{-3} at liquid-helium temperature.

The determination of small and nearly equal gaps in a semiconductor from the temperature dependence of resistance (at $H = 0$) usually entails great difficulties. The task is simplified in measurements in strong fields corresponding to the ultraquantum region. On the basis of the data of Fenton *et al.*[12], the longitudinal magnetoresistance ρ^{-1} for two-gap semiconductors with Bi-type spectra in the low-temperature region, in the ultraquantum limit of magnetic fields, can be written in the form

$$\rho^{-1}=\sigma_0+a_1T^n\exp(-\varepsilon_g/2kT) \quad \text{at} \quad \varepsilon_g<\varepsilon_{LT},$$
$$\rho^{-1}=\sigma_0+a_2\exp(-\varepsilon_{LT}/2kT) \quad \text{at} \quad \varepsilon_{LT}<\varepsilon_g. \qquad (1)$$

The exponent n of the pre-exponential factor in the first formula does not exceed 0.75 and decreases with increasing magnetic field. In the ultraquantum limit, the temperature dependence of the pre-exponential factor becomes so weak that the exponential factor can be quite easily separated graphically.

Formulas (1) for ρ^{-1} describe only the region of the intrinsic conductivity and cease to be valid at temperatures below the degeneracy temperature T_{deg}. Unfortunately, as a result of the extremely low mass, the density of states of the carriers in $Bi_{1-x}Sb_x$ alloys, even the purest alloys with $n \sim 10^{14}$ or $p \sim 10^{14}$ cm^{-3}, become degenerate at low temperatures. As a result, for alloys with impurity carrier density $\sim 10^{15}$ cm^{-3} ($T_{deg} \approx 1.5$ °K) the minimum values of the gaps ε_g and ε_{LT} that can be determined from formulas (1) are limited to ~ 0.3 meV.

CHARACTER OF DISPLACEMENT OF BAND BOUNDARIES IN SEMICONDUCTING $Bi_{1-x}Sb_x$ ALLOYS UNDER PRESSURE AND IN A MAGNETIC FIELD $H \perp C_3$

1. Experimental results

The results of the measurements of the temperature dependences of the longitudinal magnetoresistances R_{11} and R_{22} ($1 \parallel H \parallel C_1$ and C_2, respectively, where i is the measuring current flowing through the sample) for alloys of different compositions, at various pressures and at various magnetic-field values, can be represented in the form of plots of two types:

1) In the form of families of $\ln R(1/T)$ curves, the parameter of which is the pressure. Each family corresponds to a fixed value of the magnetic field. A typical example of one of these families is shown in Fig. 2.

2) In the form of families of $\ln R(1/T)$ curves, the parameter of which is the magnetic field intensity. Each family corresponds to a definite value of pressure. Typical examples of such families are shown in Figs. 3–5.

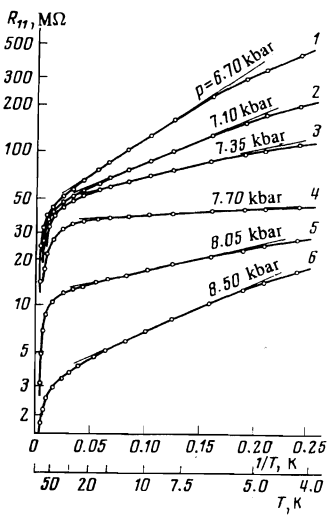

FIG. 2. Dependence of the longitudinal magnetoresistance R_{11} of the alloy $Bi_{0.88}Sb_{0.12}$ on $1/T$ at a fixed magnetic field $H = 8$ kOe ($H \parallel C_1$) at various pressures $p < p_i$ and $p > p_i$ ($p_i = 7.6$ kbar at $H = 8$ kOe). The ordinate scale corresponds to curves 1—3. The scale of curves 4—6 has been decreased, for the sake of clarity, in a ratio 1:1.5, 1:3, and 1:9, respectively.

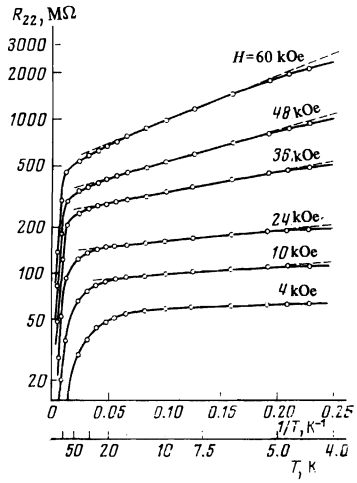

FIG. 3. Dependence of the longitudinal magnetoresistance R_{22} of the alloy $Bi_{0.871}Sb_{0.129}$ on $1/T$ at a pressure $p = 7.8$ kbar $< p_i = 8.25$ kbar and at various values of the magnetic field ($H \parallel C_2$).

On all curves in Figs. 2–5, at low temperatures ($T < 20$–40 °K) and high temperatures ($T > 40$–50 °K), one can clearly observe two linear sections corresponding to two different activation energies, which are determined by the slopes of these sections.

It is convenient to subdivide the semiconductor alloys $Bi_{1-x}Sb_x$ investigated in this study into two composition groups. One group includes alloys with concentrations $x > 8.5$ at.%, in which the indirect gap ε_{LT} goes over into the direct gap ε_g at all values of the pressure and of the magnetic field $H \perp C_3$. The slope of the low-temperature section of the $\ln R(1/T)$ curve determines here the gap ε_g, while the slope of the high-temperature section determines ε_{LT}. The values of the gaps ε_g and ε_{LT} were determined graphically. The difference between the gaps ε_g and ε_{LT} becomes particularly strong near the inversion pressure $p \sim p_i$, where ε_g is very small.

The second group includes the alloys with $6.6 \leq x \leq 8.5$ at.% in which, under normal conditions, the gap ε_{LT} is of the order of or smaller than the gap ε_g. Under pressure, ε_g decreases and vanishes at $p = p_i$. Thus, in each alloy, at $x < 8.5$ at.%, the gaps ε_g and ε_{LT} turn out to be close to each other in a certain pressure region. In this case the determination of the values of the gaps from the temperature dependences of the longitudinal magnetoresistance becomes a complicated task and calls for computer calculation of the parameters ε_g and ε_{LT}, as well as a comparison of data obtained at various p and H in alloys with various compo-

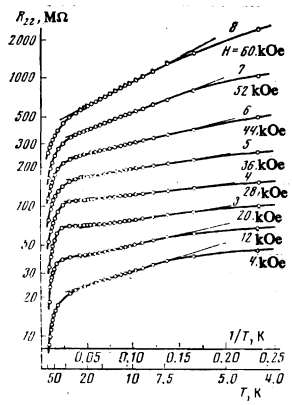

FIG. 4. Dependence of the longitudinal magnetoresistance R_{22} of the alloy $Bi_{0.911}Sb_{0.089}$ on $1/T$ at a pressure $p = 5.45$ kbar $> p_i = 5.1$ kbar and at different magnetic fields ($H \parallel C_1$). The ordinate scale corresponds to curve 1. The scale of curves 2—8 has been magnified for the sake of clarity by 2.5, 5.0, 8.9, 14.2, and 40 times.

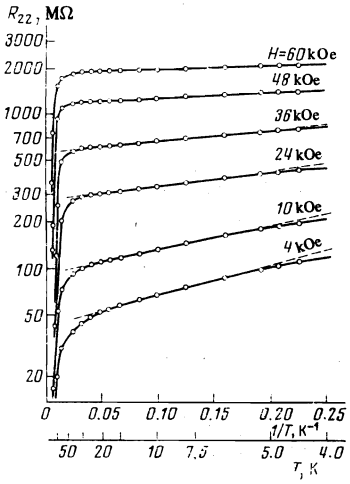

FIG. 5. Dependence of the longitudinal magnetoresistance R_{22} of the alloy $Bi_{0.871}Sb_{0.129}$ on $1/T$ at a pressure $p = 9.2$ kbar $> p_i = 8.25$ kbar and at different values of the magnetic field ($H \parallel C_2$).

sitions. This applies in particular to alloys with low Sb concentration, $6.6 \leq x \leq 7.5$ at.%, in which a semiconductor–metal transition accompanied by an overlap of the bands in L and T at $H = 0$ and a pressure close to the band inversion point $p = p_i$ is observed if $p < p_i$, and a reverse metal–semiconductor transition at which this overlap vanishes[19] is observed at $p > p_i$. The onset of a band overlap at the points L and T when $p \approx p_i$ in alloys with $6.6 \leq x \leq 7.5$ at.% of Sb causes the $R(T)$ dependence to acquire a metallic character at low temperatures. In this case it is impossible to determine the gap ε_g from temperature measurements.

Transitions to a zero-gap state in purest form can be observed in alloys of the first group with Sb concentration $x > 8.5$ at.%, which behave at low temperatures and at $p < p_i$ like semiconductors with a direct gap ε_g in the energy spectrum. The data on the motion of the L bands under pressure and in the magnetic field were consequently obtained in investigations of the alloys of the first group. On the other hand, a study of the alloys of the second group has made it possible to determine the direction and the velocity of the relative motion of the T extremum under the influence of a magnetic field and pressure.

We wish to stress once more that according to the theory developed in[16,7] for alloys with inverted spectra, the concept of the direct gap ε_g becomes meaningless, since the bands L_a and L_s overlap in this case and instead of a forbidden band with zero density of states between the terms L_a and L_s there appears a region of decreased (but not zero everywhere) density of states (see Fig. 3 of[7]). In experiments this region can imitate a certain thermal gap, the effective width ε_0 of which turns out to be less than the energy interval: $\varepsilon(L_s) - \varepsilon(L_a) = -\varepsilon_g$.

Thus, in the analysis of the experimental data it is more convenient to consider the activation energy ε_0, which is determined directly as a result of the measurements. It is obvious that in noninverted alloys with $\varepsilon_g \ll \varepsilon_{LT}$ the value of ε_0 coincides with the value of the direct gap ε_g in the spectrum.

2. Band inversion under the influence of pressure in the presence of a magnetic field

A characteristic feature of the low-temperature sections of the $\ln R(1/T)$ curves of alloys with $x > 8.5$ at.% is that *at all values of the magnetic field* their slope decreases with increasing pressure, goes through a minimum at a certain value $p = p_i$ that depends on H and on the alloy composition, and then increases again (Fig. 2). This variation of the $\ln R(1/T)$ curves means that the bands in L first come closer together (in this region $\varepsilon_0 \equiv \varepsilon_g$) and a ZGS is produced at $p = p_i$, while at $p > p_i$ the spectrum becomes inverted.

A typical plot of ε_0 against p, constructed by using the slope of the low-temperature section of the $\ln R_{11}(1/T)$ and formulas (1) for the alloy $Bi_{0.88}Sb_{0.12}$ at $H =$ kOe is shown in Fig. 6 (curve 1). The minimum value of ε_0 determines the pressure p_i of the band inversion for the given alloy and for the indicated value of the magnetic field. With increasing magnetic field, the value of p_i increases at a rate $\partial p_i/\partial H = (2.4 \pm 0.1) \times 10^{-2}$ kbar/kOe, which is practically independent of the alloy composition. Curves 2 and 3 in Fig. 6 show the dependence of ε_0 on p for the same alloy at two other values of the magnetic field: $H = 36$ and 60 kOe, respectively. In first-order approximation, the activation energy ε_0 in all values of H decreases linearly under pressure, at a rate

$$\partial\varepsilon_0/\partial p \equiv \partial\varepsilon_g/\partial p = -(2.5 \pm 0.2) \text{ meV/kbar at } p < p_i \qquad (2)$$

and increases linearly at a lower rate

$$\partial\varepsilon_0/\partial p = 1.5 \pm 0.15 \text{ meV/kbar at } p > p_i. \qquad (3)$$

It follows therefore that the inversion pressure $p_i(H)$ and the initial gap $\varepsilon_g(H)$ in the spectrum of the alloy at $p = 1$ bar are proportional to each other in first-order approximation:

$$\varepsilon_g(H)\,[\text{meV}]\big|_{p=1\text{ bar}} = (2.5 \pm 0.2)\, p_i\ [\text{kbar}]\ . \qquad (4)$$

We presented dependences of ε_0 and p typical of all the investigated alloys with $x > 8.5$ at.%.

Inasmuch as the interval $|\varepsilon(L_a) - \varepsilon(L_s)|$ is small in

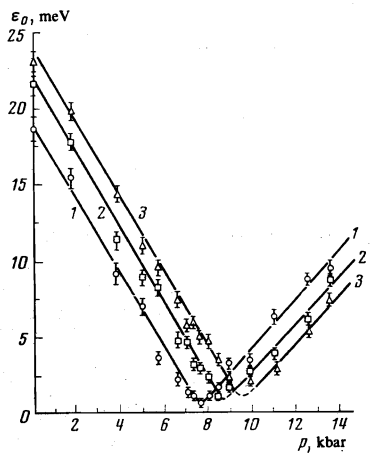

FIG. 6. Dependence of the activation energy ε_0 on the pressure for the alloy $Bi_{0.88}Sb_{0.12}$ at $H \parallel C_1$ in fields $H = 8$ kOe (1), 36 kOe (2), and 60 kOe (3).

comparison with atomic energies in $B_{1-x}Sb_x$ alloys at all values of the pressure, one can expect the rate and direction of the shift of the terms L_a and L_s themselves under pressure to remain the same on going from the direct arrangement of the L bands to the inverted one, as a result of which the energy interval $\varepsilon(L_a) - \varepsilon(L_s)$, which is equal to the width of the direct forbidden band ε_g at $\varepsilon(L_a) > \varepsilon(L_s)$ and whose modulus is equal to the overlap of the bands L_a and L_s at $\varepsilon(L_a) < \varepsilon(L_s)$, always changes under pressure at a rate determined by (2).

In accordance with the theory of Beneslavskiĭ and Fal'kovskiĭ,[7] the decrease of $|\partial\varepsilon_0/\partial p|$ on going from the region $p < p_i$ into the region $p > p_i$ means that when the inverted spectrum appears the direct gap ε_g disappears and there is produced an overlap of the bands L_a and L_s with a region of low density of states characterized by a certain activation energy $\varepsilon_0 < \varepsilon(L_s) - \varepsilon(L_a)$. One must also bear in mind another possibility, namely the production of a real gap $\varepsilon_g' < \varepsilon(L_s) - \varepsilon(L_a)$ in the inverted spectrum as a result of the lifting of the degeneracy at the term intersection points. Unfortunately, it is impossible to distinguish between these two possibilities on the basis of the obtained data.

Thus, on the basis of the presented data we can conclude that the semiconducting $Bi_{1-x}Sb_x$ goes into the ZGS under the influence of pressure *at all values of the magnetic field H*.

At pressures $p = p_i(x, H)$ corresponding to the onset of the ZGS the longitudinal magnetoresistances $R_{11}(H, p)$ and $R_{22}(H, p)$, measured at fixed values of the magnetic field, go through a minimum for all alloys. From the pressures at which R_{11} and R_{22} have minima we can determine uniquely and with sufficient accuracy the L-band inversion point $p = p_i(x, H)$ in the entire range of the investigated Sb concentrations in the alloys. The value of p_i at $H = 0$ can be determined also by an independent method from the characteristic change of the shape of the longitudinal magnetoresistance curve $R_{11}(H)$ ($\mathbf{H} \parallel C_1$) under pressure, as shown in[19]. This method of determining p_i at $H = 0$ was used in the present study to monitor the data obtained from the positions of the minima in the plots of R_{11} and R_{12} against p.

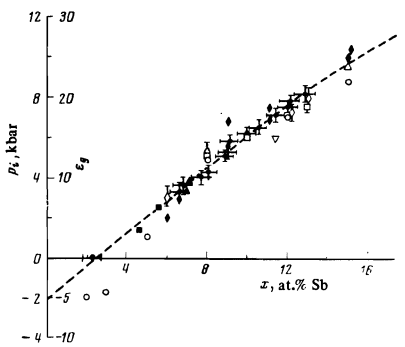

FIG. 7. Dependence of the inversion pressure (p_i) and of the direct energy gap (ε_g) of $Bi_{1-x}Sb_x$ alloys on the Sb concentration. Data for p_i: ●—present work, ■—[24], ▲—[19], ◆—[4]; data for ε_g (in meV): ○—[23], ▽—[25], △—[26], □—[27]. The point ● on the x axis corresponds to the maximum anisotropy of the electron Fermi surfaces of the semiconducting $Bi_{1-x}Sb_x$ alloys.[15]

The dependences of the inversion pressure p_i at $H = 0$ and of the gap ε_g at $p = 0$ and $H = 0$ in $Bi_{1-x}Sb_x$ alloys on the Sb concentration, as obtained from our data as well as from the data of[4,9,15,23-27], are shown in Fig. 7. The plot of p_i against x at $H = 0$ is essentially the phase diagram of the zero-gap state for the $Bi_{1-x}Sb_x$, plotted in the coordinates p and x. It constitutes the separation boundary between the regions of the direct ($p < p_i$) and inverted ($p > p_i$) spectrum on the (p, x) plane at $H = 0$. Extrapolation of this curve to $x = 0$ yields negative values of the critical pressure $p_i \approx -2$ kbar for pure Bi. It follows therefore that Bi should have an inverted spectrum structure in L and cannot be converted into ZGS by compression. The overlap of the terms L_a and L_s in the inverted spectrum of Bi amounts to ~ 5 meV. Upon compression, this overlap increases at a rate 2.5 ± 0.2 meV/kbar.

The value of $-\varepsilon_g$ obtained for Bi by extrapolating the curve in Fig. 7 agrees sufficiently well with the data of[28]. Of course, the extrapolation of the curve of Fig. 7 to $x = 0$ is not a sufficiently reliable operation for the determination of $-\varepsilon_g$ and p_i of pure Bi, since the values of ε_g and p_i have been determined reliably only for alloys with Sb concentration $x > 6.5$ at.%. The difficulty in the determination of $-\varepsilon_g$ of pure Bi is due to the fact that this parameter is small in comparison with the Fermi energy ε_F of the electrons in L. Consequently, no measurements of the Fermi level in L make it possible to calculate $-\varepsilon_g$ reliably, and this is apparently the main reason for the discrepancy between the calculated value $|\varepsilon_g|$ in different reports of the investigation of pure Bi (see, e.g., [17,18,28]).

3. Shift of band boundaries of $Bi_{1-x}Sb_x$ alloys with noninverted spectrum in a magnetic field

The logarithm of the longitudinal magnetoresistance R_{11} (or R_{22}) as functions of the reciprocal temperature, measured at different values of the magnetic field in alloys with a direct spectrum at the point L (at $p < p_i$), and in alloys with inverted spectrum at L (at $p > p_i$), typical plots of which are shown in Figs. 3–5, make it possible to determine the character of the variation of the direct gap ε_g or of the activation energy ε_0 in a magnetic field. It is seen that in the region of the direct spectrum (Fig. 3) the slope of the low-temperature section of the $\ln R(1/T)$ curve increases with increasing magnetic field. Accordingly, the direct forbidden band ε_g at $p < p_i$ is an increasing function of H (curve 3–5).

Figure 8 shows plots of $\varepsilon_0(H)$ for the alloys $Bi_{0.911}Sb_{0.089}$ and $Bi_{0.88}Sb_{0.12}$ at several pressures $p < p_i$ (in this case $\varepsilon_0 \equiv \varepsilon_g$). The value of ε_0 at each value of H was determined from the slope of the low-temperature section of the $\ln R(1/T)$ curve by least squares. Analogous plots were obtained for all the investigated alloys with $x > 8.5$ at.% Sb. All indicate that, in the region of the direct spectrum, the gap ε_g of the semiconducting alloys $Bi_{1-x}Sb_x$ at $\mathbf{H} \parallel C_1$ and $\mathbf{H} \parallel C_2$, in first-order approximation, increases linearly in a magnetic field at a rate

$$\partial\varepsilon_g/\partial H = (6 \pm 1) \cdot 10^{-2} \text{ meV/kOe}, \qquad (5)$$

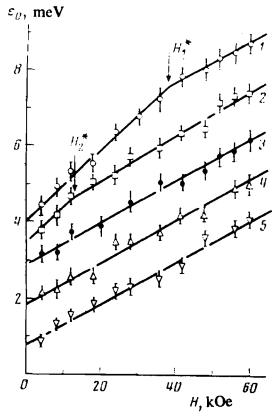

FIG. 8. Dependence of the activation energy ε_0 on the magnetic field $H \perp C_3$ at $p < p_i$ for alloys $Bi_{0.923}Sb_{0.077}$ ($p_i = 4.0$ kbar): 1) $p = 2$ kbar, 2) $p = 2.4$ kbar; $Bi_{0.911}Sb_{0.089}$ ($p_i = 5.4$ kbar): 3) $p = 4.05$ kbar; $Bi_{0.88}Sb_{0.12}$ ($p_i = 7.5$ kbar): 4) $p = 6.8$ kbar, 5) $p = 7.1$ kbar. The straight lines were drawn by least squares. H_1^* and H_2^* are the fields at which the kinks are observed on the plots against H.

that is practically independent of the composition of the alloy and of the pressure at $p < p_i$. It follows therefore that *no transitions to the* ZGS *can be induced by a magnetic field* $H \perp C_3$ *in the semiconducting* $Bi_{1-x}Sb_x$ *alloys at* $p < p_i$ (including the case of normal pressure $p = 1$ bar).

The increase of the gap ε_g in the magnetic field at $p < p_i$ means also that at the normal arrangement of the L bands the distance $\hbar\omega_c$ between the Landau levels exceeds their spin splitting, as a result of which the 0^- and 0^+ levels for the electrons and holes move away from each other in a magnetic field. The Landau level scheme corresponding to this situation is shown in Fig. 9a.

These data agree with the results of the theoretical calculations of Beneslavskiĭ and Fal'kovskiĭ,[7] according to which, in alloys with a direct spectrum, the direct gap ε_g at an orientation of H close to the elongation direction of the electron equal-energy surface in L should increase in the field at a rate $\partial\varepsilon_g/\partial H \approx e\hbar/m_y c$, where m_y is the electron effective mass in the elongation direction ($m_y \approx (0.6-1.0)m_0$ in Bi and in $Bi_{1-x}Sb_x$ alloys[16,17,29]). The obtained experimental value (5) agrees in order of magnitude with $e\hbar/m_y c \approx 2\times10^{-2}$ meV/kOe.[1)] Unfortunately, a more accurate quantitative comparison with the calculation data is impossible for lack of numerical values of the parameters of the geometrical model.[7]

4. $Bi_{1-x}Sb_x$ alloys with $x < 8.5$ at.%

For alloys with Sb concentration $x < 8.5$ at.%, a characteristic kink appears in a certain magnetic field H^* on the activation energy (ε_0) vs H plot determined from the slope of the low-temperature section of the $\ln R(1/T)$ curve at $p < p_i$. Two such typical plots of ε_0 against H, obtained for the alloy $Bi_{0.923}Sb_{0.077}$ at $p = 2.0$ and 2.4 kbar ($p_i = 4.0$ kbar at $H = 0$), are shown in Fig. 8 (curves 1 and 2).

The plot of ε_0 against H is in first approximation a straight line with slope $\partial\varepsilon_0/\partial H = (8.7 \pm 0.3)\times10^{-2}$ MeV/kOe, which goes over in a certain magnetic field $H^*(p)$ (H_1^* and H_2^* in Fig. 8) into another straight line with a smaller slope, $\partial\varepsilon_0/\partial H = (6 \pm 1)\times10^{-2}$ meV/kOe. The second slope coincides in value with $\partial\varepsilon_g/\partial H$ obtained for the alloys with $x > 8.5$ at.%. The magnetic field H^* at

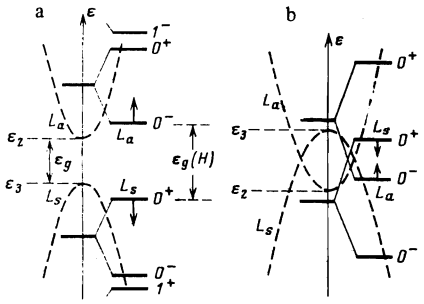

FIG. 9. Arrangement of the L bands for a momentum direction along the elongation of the equal-energy surface (dashed) and Landau-level scheme when H is oriented along the elongation for the direct (a) and inverse (b) spectra. In the case of the inverse spectrum, one of the possible arrangements of the lower levels relative to the edges of the corresponding bands is shown. This arrangement does not correlate with the degree of band intersection and can vary in a magnetic field.

which the kink occurs decreases rapidly with pressure:

$$\partial H^*/\partial p = -(58 \pm 5) \text{ kOe/kbar} \qquad (6)$$

Inasmuch as in alloys with $x < 8.5$ at.%, at $H = 0$ and low pressures, the minimal gap in the spectrum is ε_{LT}, it is natural to connect the observed kinks with the motion of the term $T_{\overline{45}}$ in a magnetic field, as a result of which the minimal gap in the spectrum is no longer ε_{LT} but ε_g in magnetic fields larger than $H^*(p)$. From this point of view, the slope of the low-temperature section in fields $H < H^*(p)$ determines the gap ε_{LT}, and in fields $H > H^*(p)$ it determines the gap ε_g. The transition from the dependence of ε_{LT} on H to the dependence of ε_g on H occurs in a field $H = H^*$ in which the gaps ε_{LT} and ε_g become equal to each other. A scheme corresponding to this model, of the motion of the terms L_a, L_s, and $T_{\overline{45}}$ in a magnetic field, is shown in Fig. 10a.

With increasing pressure, ε_g decreases much more rapidly (see (2)) than the downward motion of the term $T_{\overline{45}}$ (see Fig. 10b).[19] Therefore the difference $\varepsilon(T_{\overline{45}}) - \varepsilon(L_s) = \varepsilon_g - \varepsilon_{LT}$ decreases with increasing pressure ($\partial(\varepsilon_g - \varepsilon_{LT})/\partial p = -(1.5 \pm 0.2)$ meV/kbar), and the field $H^*(p)$ decreases accordingly.

The proposed model of the motion of the L and T bands in a magnetic field, as well as the values (5) and (6) obtained by us at $p < p_1$ and the value

$$\partial\varepsilon_{LT}/\partial H = (8.7 \pm 0.3)\cdot10^{-2} \text{ meV/kOe} \qquad (7)$$

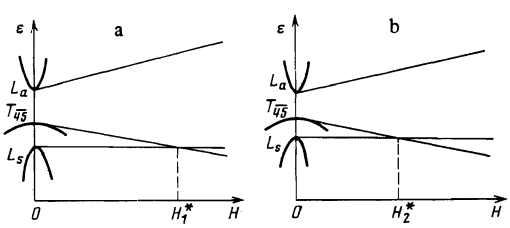

FIG. 10. Motion of the boundaries of the L and T bands in a magnetic field $H \perp C_3$ for $Bi_{1-x}Sb_x$ alloys at $x < 8.5$ at.%. The indirect gap ε_{LT} becomes equal to the direct gap ε_g in fields H_1^* and H_2^* corresponding to the pressures p_1 (Fig. 10a) and $p_2 > p_1$ (Fig. 10b).

allow us to draw definite conclusions concerning the degree of similarity of the electron and hole bands in L.

We assume for simplicity that all the equal-energy electron surfaces are equivalently oriented with respect to **H**. In this case the rates of change of the gaps ε_g and ε_{LT} in the field can be expressed in the form

$$\frac{\partial \varepsilon_g}{\partial H}=\frac{1}{2}\frac{e\hbar}{m_0 c}\left[\left(\frac{m_0}{m^c_{eL}}-\frac{m_0}{m^s_{eL}}\right)+\left(\frac{m_0}{m^c_{hL}}-\frac{m_0}{m^s_{hL}}\right)\right], \tag{8}$$

$$\frac{\partial \varepsilon_{LT}}{\partial H}=\frac{1}{2}\frac{e\hbar}{m_0 c}\left[\left(\frac{m_0}{m^c_{eL}}-\frac{m_0}{m^s_{eL}}\right)+\left(\frac{m_0}{m^c_{hT}}-\frac{m_0}{m^s_{hT}}\right)\right] \tag{9}$$

where m^c_{eL}, m^c_{hL}, m^c_{hT} are the cyclotron masses and m^s_{eL}, m^s_{hL}, m^s_{hT} are the spin masses of the L electrons, L holes, and T holes. Expressions (8) and (9) are perfectly rigorous in a strong magnetic field at $\mathbf{H}\parallel C_1$, when, as a result of the transfer of the carriers,[29] the principal role in the spectrum is played by only two equivalent L extrema.

With respect to the T holes in $Bi_{1-x}Sb_x$ alloys it is known that they are described by a quadratic dispersion law and that their cyclotron and spin masses are practically independent of the alloy composition.[14] According to the experimental data of [14,17], at $\mathbf{H}\perp C_3$ we have $m^c_{hT}\approx 0.2m_0$, and the spin splitting of the T holes is small in comparison with the orbital splitting ($m^s_{hT}\gg m^c_{hT}$). We assume that these data are valid also for the $Bi_{1-x}Sb_x$ alloys at $6.6\leq x\leq 13$ at.% Sb. Substituting in (8) and (9) the values of m^c_{hT}, m^s_{hT}, $\partial\varepsilon_g/\partial H$ and $\partial\varepsilon_{LT}/\partial H$, we obtain the differences of the reciprocal spin and cyclotron masses, which determine the absolute rates of motion in a magnetic field of the 0^- and 0^+ terms respectively for the electron and holes in L:

$$\begin{aligned} m_0/m_{eL}{}^c-m_0/m_{eL}{}^s&=10.3\pm1.5,\\ m_0/m_{hL}{}^c-m_0/m_{hL}{}^s&=0\pm1.5. \end{aligned} \tag{10}$$

The strong disparity of these differences means that the main change of ε_g in the field occurs as a result of the upper shift of the electronic 0^- level (the L_a term), whereas the hole 0^+ level (the L_s term) remains practically stationary (see Fig. 10):

$$\begin{aligned} \partial\varepsilon(L_a)/\partial H&=(6\pm1)\cdot10^{-2}\ \text{meV/kOe}\\ \partial\varepsilon(L_s)/\partial H&=(0\pm0.9)\cdot10^{-2}\ \text{meV/kOe} \end{aligned}$$

Thus, for electrons at the point L the spin splitting is somewhat smaller than the orbit splitting and this causes the growth of the gap ε_g in the magnetic field. For the holes of L, the spin and orbit splittings are equal to each other within the limits of experimental accuracy.

We note that the indicated character of the field-induced shift of the electron and hole L levels is in good agreement with the value (6) obtained from the shift of the kink of curves of 1 and 2 on Fig. 8. Indeed, if it is assumed that the level L_s is stationary, then it is easy to show that at the rates (5) and (7) the difference $\varepsilon_g-\varepsilon_{LT}$ decreases at a rate

$$\partial(\varepsilon_g-\varepsilon_{LT})/\partial H=-(2.5\pm0.5)\cdot10^{-2}\ \text{meV/kOe}$$

The value of $\partial H^*/\partial p$ can be obtained from the ratio of the derivatives $|\partial(\varepsilon_g-\varepsilon_{LT})/\partial p|$ and $|\partial(\varepsilon_g-\varepsilon_{LT})/\partial H|$, which amounts to

$$\frac{\partial H^*}{\partial p}=\frac{1.5\pm0.2}{2.5\pm0.5}\cdot10^2=(60\pm8)\frac{\text{kOe}}{\text{kbar}}.$$

Thus, the electron and hole bands in L are far from equivalent.

In order to estimate the extent to which the spin ($\Delta\varepsilon_s$) and orbit ($\Delta\varepsilon_0$) splitting of electrons differ, and also to determine the order of magnitude of the small parameter in the Baraff theory[6]

$$\delta=\frac{\varepsilon(n+1,\ s=-1)-\varepsilon(n,\ s=+1)}{\varepsilon(n+1,\ s=-1)-\varepsilon(n,\ s=-1)}=1-\frac{\Delta\varepsilon_s}{\Delta\varepsilon_0}=1-\frac{m_{eL}}{m^s_{eL}} \tag{11}$$

($s=\pm1$ is the spin variable), which characterizes the deviation of the electron spectrum of Bi in L, from the simple two-model of Cohen and Blount[31] ($m^c_{eL}\equiv m^s_{eL}$, $\Delta\varepsilon_s\equiv\Delta\varepsilon_0$), we rewrite (10) in the form

$$1-m_{eL}{}^c/m_{eL}{}^s\approx10m_{eL}{}^c/m_0. \tag{12}$$

For estimating purposes we assume, in accord with the work of Herrmann *et al.*,[29] a cyclotron mass $m^c_{eL}=10^{-3}m_0$ for the L electrons at the bottom of the band in superconducting $Bi_{1-x}Sb_x$ alloys at an orientation of **H** close to the direction of elongation of the equal-energy surface. From (12) we obtain $\delta\sim10^{-2}$. As expected, at this orientation of H the deviation from the two-band model, connected with the influence of the more remote bands, is quite small. This difference, however, is of principal significance, since the magnitude and sign of the parameter δ determine the direction and relative rate of displacement of the bands in L in a magnetic field. At $\delta>0$ the orbital splitting goes over into spin splitting and the term L_a shifts upward in a magnetic field.

5. Motion of band boundaries of alloys with inverted spectrum and formation of ZGS in a magnetic field

In the inverted-spectrum region at $p>p_i$, the slope of the low-temperature section on the $\ln R(1/T)$ curves decreases in a magnetic field (see Fig. 5). It follows therefore that with increasing H the effective gap ε_0 decreases, and consequently also the overlap of the bands L_a and L_s. The dependences of ε_0 on H for the alloys $B_{0.911}Sb_{0.89}$ and $Bi_{0.88}Sb_{0.12}$ at certain pressures $p>p_i$ are shown by way of example in Fig. 11 (curves 1–3). The data obtained for a large number of alloys at different pressures $p>p_i$ show that, in first-order approximation at $\mathbf{H}\parallel C_1$ and $\mathbf{H}\parallel C_2$ the effective gap ε_0 decreases in a magnetic field linearly at a rate

$$\partial\varepsilon_0/\partial H=-(4\pm0.6)\cdot10^{-2}\ \text{meV/kOe} \tag{13}$$

which is practically independent of the alloy composition and of the pressure.

The decrease of ε_0 in a magnetic field leads to a more complicated character of the $\ln R(1/T)$ curve in the pressure region $p_i\lesssim p<p_i+1$ kbar near the inversion pressure. A family of curves typical of this pressure region is shown in Fig. 4. The slope of the low-tem-

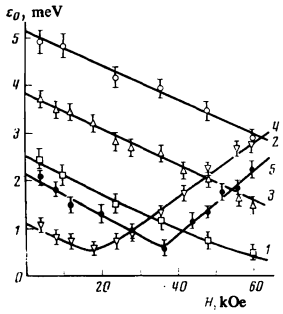

FIG. 11. Dependence of the activation energy ε_0 on the magnetic field $\mathbf{H} \perp C_3$ at $p > p_i$ of the following alloys: $Bi_{0.879}Sb_{0.121}$ ($p_i = 7.9$ kbar): 1—$p = 9.2$ kbar, 2—$p = 11.4$ kbar; $Bi_{0.88}Sb_{0.12}$ ($p_i = 7.5$ kbar): 3—$p = 10.0$ kbar; $Bi_{0.911}Sb_{0.089}$ ($p_i = 5.1$ kbar): 4—$p = 8.2$ kbar, 5—$p = 5.45$ kbar.

perature section first decreases in the magnetic field, goes through a minimum at a certain $H = H_i$ that depends on x and p, and then again increases. The corresponding dependences of the activation energy ε_0 on H are shown in Fig. 11 (curves 4 and 5). At $H < H_i$ the value of ε_0 decreases at the rate (13), and at $H > H_i$ it increases at the rate (5). It follows therefore that H_i is directly proportional to ε_0 at $H = 0$:

$$H_i\ [\text{kOe}] = (25 \pm 3.5)\,\varepsilon_0\ [\text{meV}]$$

The obtained form of the dependence of ε_0 on the magnetic field indicates that the semiconducting $Bi_{1-x}Sb_x$ alloys with inverted spectra ($p > p_i$) go over into the zero-gap state at definite values of H_i.

The transitions to the ZGS are the consequence of the fact that the overlap of the L_a and L_s terms, which is a result of their inversion under pressure at $p > p_i$ in the magnetic field, decreases and vanishes at $H = H_i$. At $H = H_i$, a second inversion of the L bands is produced, due in this case to the action of the magnetic field, as a result of which the spectrum in L returns to the non-inverted state with a true direct gap ε_g between the terms L_a and L_s. Such a character of the restructuring in the magnetic field is indicated also by the change in the rate $|\partial\varepsilon_0/\partial H|$ from the value (13) at $H < H_i$ due to the value (5) at $H > H_i$, which coincides in the region $H > H_i$ with the rate of the increase of ε_g in the magnetic field for alloys with non-inverted spectra at $p < p_i$.

For alloys with an inverted spectrum and with $\varepsilon_0 > 2.5$ meV at $H = 0$ it is possible to observe in fields H up to 65 kOe only the pre-inversion decrease of $\varepsilon_0(H)$ (curves 1–3 in Fig. 11).

The character of the motion of the energy levels in a magnetic field at $p > p_i$ is illustrated by the diagram in Fig. 9b. It was constructed under the assumption[7] that the rate and direction of the displacements of the terms L_a and L_s in a magnetic field (just as in hydrostatic compression) does not depend on their sequence: the term L_a in a field always moves upward in energy. This motion of the term leads to an increase in the gap ε_g in the non-inverted spectrum and to a decrease of the band overlap $|-\varepsilon_g|$ in the inverted spectrum.[2)]

The reversal of the sign and of the magnitude of the derivative $\partial\varepsilon_0/\partial H$ on going from the direct spectrum to the inverted spectrum was observed also in $Pb_{1-x}Sn_xSe$ alloys, which have band energy structures close to that of Bi at the points L of the Brillouin zone.[32] A comparison of the data of Calawa *et al.*[32] with our data shows that the reversal of the sign[32] and the change in the magnitude of $\partial\varepsilon_0/\partial H$ on going through the inversion point is a common phenomenon for substances with spectrum of the Bi type and does not depend on the cause of the inversion (pressure, magnetic field, or change of alloy composition).

6. Zero-gap surface for $Bi_{1-x}Sb_x$ in the coordinates x, p, and H

The aggregate of the available experimental data on the pressure-induced and magnetic-field-induced L-band inversion in $Bi_{1-x}Sb_x$ alloys with different compositions make it possible to construct the surface of the zero-gap state in the space of the parameters, namely the composition (x), the pressure (p), and the magnetic field (H) (Fig. 12). This surface is the geometric locus of the points whose coordinates x, p, and H determine the values of the parameters at which the gap ε_g in the spectrum of the $Bi_{1-x}Sb_x$ vanishes. The surface bounding the region of the existence of the ZGS on the right determines the pressures at which Bi and the alloys $Bi_{1-x}Sb_x$ experience polymorphic transformations and go over into the metallic state.[33]

When constructing the ZGS surface we used the fact that in $Bi_{1-x}Sb_x$ the inversion pressure p_i increases in proportion to the magnetic field H:

$$p_i(x, H)\ [\text{kbar}] = p_i(x, 0)\ [\text{kbar}] + (2.4 \pm 0.1)\cdot 10^{-2} H\ [\text{kOe}].$$

This means that in a magnetic field the plot of p_i against x shifts parallel to itself into the region of higher pressures.

Naturally, the ZGS shift shown in Fig. 12 is approximate, since it is constructed on the basis of a linear extrapolation of the obtained data into the region of higher pressures, magnetic fields, and antimony concentrations. However, this extrapolation is apparently reasonable, since there are no grounds for expecting deviations from the linear character of the motion of the band boundaries in a magnetic field, at least up to fields $H \sim 10^6$ Oe.

We can thus expect the region of the existence of the ZGS in $Bi_{1-x}Sb_x$ alloys in the three-dimensional (x, p, H) space to be bounded by the following values of the parameters: $x \lesssim 40$ at.%, $p \lesssim 35$ kbar, $H \lesssim 1500$ kOe.

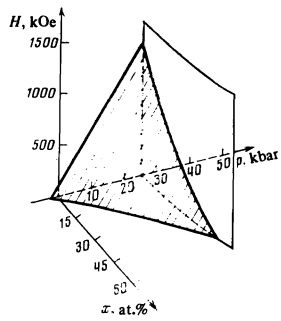

FIG. 12. Zero-gap-state surface (shaded) for $Bi_{1-x}Sb_x$ alloys, plotted in composition–pressure–magnetic field coordinates.

CHANGE IN THE ANISOTROPY OF THE TRANSVERSE MAGNETORESISTANCES ON FORMATION OF THE ZG STATE IN A MAGNETIC FIELD

It was indicated above that the zero-gap state is induced by a magnetic field only in $Bi_{1-x}Sb_x$ alloys with inverted spectrum in the ultraquantum region of magnetic fields, in which the boundaries of the bands are the Landau 0^- and 0^+ levels for the electrons and holes, respectively. This circumstance creates appreciable difficulties when it comes to determining the character of the change of the spectrum parameters (effective masses, relaxation times of the carriers, etc.) in the transition to the ZGS.

The point is that at the present time there is no sufficiently rigorous theory for the calculation of the longitudinal and transverse conductivities in the ultraquantum limit of magnetic fields, even for substances with a simple band spectrum. The main cause is that, owing to the quasi-one-dimensional character of the carrier motion in the ultraquantum region, the role of collisions with impurities is altered in principle. On the one hand, in the ultraquantum limit, the frequency of collisions with impurities decreases with increasing magnetic field owing to the decrease of the characteristic diameter $l_H = (c\hbar/eH)^{1/2}$ of the diameter of the electron orbits. On the other hand, in the ultraquantum limit, an even greater "one-dimensionalization" of the electron system takes place, causing an increase in the role of interference effects in scattering, which hinder the motion of the electron in the direction of the magnetic field.

Bychkov [34] has shown that in a strictly one-dimensional system the static conductivity should be entirely suppressed as a result of the interference of the scattering acts. The electron system in the ultraquantum limit is not strictly one-dimensional, for in this case there remains a possibility of changing the center of the electron orbit in collisions with impurities. Consequently, there is no complete blocking of the longitudinal motion of the electron, and a finite conductivity along the field remains. The need for taking into account the interference effects greatly complicates the calculation of the components of the magnetoconductivity tensor $\sigma_{ij}(H)$ and leads to great mathematical difficulties. The known theoretical papers [35,37] devoted to the calculation of $\sigma_{ij}(H)$ in the ultraquantum region do not take into account the interference effect and are based on rather crude assumptions.

In addition, in the analysis of the dependence of σ_{ij} on H in the ultraquantum limit, it is necessary to take into account the possibility of changing the character of the screening as a result of the change in the ratio of the screening radius r_D, the magnetic length l_H, and the values of the reciprocal Fermi or thermal momenta $1/k$ of the electrons, [36] the change in the carrier density, and also the possibility of the change from degenerate statistics to Boltzmann statistics as a result of the decrease of the Fermi energy in the magnetic field. [38] The impossibility of taking into account all these mechanisms does not enable us to draw unambiguous conclusions on the character of the restructuring of the band spectrum of the substance in the magnetic field only on the basis of the form of the $\sigma_{ij}(H)$ dependences.

The problem becomes much simpler if instead of studying the initial curves of the longitudinal and transverse magnetoresistance we analyze the magnetic-field dependence of the anisotropy of the transverse components. In a certain direction of the magnetic field H (for example, along one of the principal axes of the crystal) it is possible to measure experimentally, under identical conditions, four independent components of the magnetoresistivity tensor $\rho_{ij}(H)$. At $\mathbf{H} \parallel C_1$, these components are: the longitudinal magnetoresistivity $\rho_{11}(H)$ $(\mathbf{i} \parallel \mathbf{H} \parallel C_1)$, the transverse magnetoresistivities $\rho_{22}(H)$ $(\mathbf{i} \parallel C_2, \mathbf{H} \parallel C_1)$ and $\rho_{33}(H)$ $(\mathbf{i} \parallel C_3, \mathbf{H} \parallel C_1)$, and the Hall component $\rho_{23}(H)$ $(\mathbf{i} \parallel C_2, \mathbf{H} \parallel C_1)$, which coincides, according to the Onsager reciprocity principle, with the component $\rho_{32}(H)$ $(\mathbf{i} \parallel C_3, \mathbf{H} \parallel C_1)$. The anisotropy of the transverse components is determined by the relation

$$\eta(H) = \rho_{22}(H)/\rho_{33}(H).$$

The transition to anisotropy makes it possible to exclude the change of the carrier density in a magnetic field, and also to exclude the influence of various mechanisms that make identical contributions to the H dependence of the components ρ_{22} and ρ_{33} in both quasiclassical and ultraquantum fields. [30]

In the analysis of the experimental data we confine ourselves to consideration of the anisotropy curves

$$\eta(H_i) = \rho_{22}(H_i)/\rho_{33}(H_i)$$

$(\mathbf{H} \parallel C_1)$, obtained at helium temperatures only for $Bi_{1-x}Sb_x$ alloys with $x > 8.5$ at.%, in which the transition to the ZGS is observed in the purest form.

In the region of the direct spectrum at $p < p_i$, the general character of the $\eta(H)$ dependence changes little with changing composition and pressure of the alloy. The functions $\eta(H)$ are smooth with maxima at $H \sim 10$–12 kOe), and decrease monotonically in stronger fields (curves 1 on Figs. 13 and 14). The absolute value of $\eta(H)$ depends on the pressure; as $p = p_i$ is approached from below, the maximum of the $\eta(H)$ curves becomes

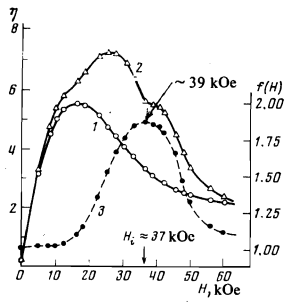

FIG. 13. Dependence of the anisotropy of the transverse magnetoresistivities $\eta = \rho_{22}/\rho_{33}$ on the magnetic field $\mathbf{H} \parallel C_1$ ($T = 4.2$ °K) for the alloy $Bi_{0.91}Sb_{0.09}$ ($p_i = 5.1$ kbar at $\mathbf{H} = 0$): 1) $p = p'' = 4.8$ kbar, 2) $p = p'' = 6.4$ kbar, 3) the function $f(H) = \eta(H, p > p_i)/\eta(H, p < p_i)$. At $p = p'$, the ZGS is observed at $H_i \approx 37$ kOe.

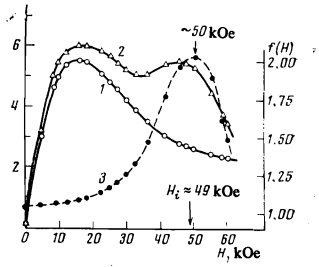

FIG. 14. Dependence of the anisotropy $\eta = \rho_{22}/\rho_{33}$ of the transverse magnetoresistences on the magnetic field $\mathbf{H} \parallel C_1$ ($T = 4.2$ °K) for the alloy $Bi_{0.91}Sb_{0.09}$ ($p_i = 5.1$ kbar at $H = 0$): 1) $p = p''$ = 4.6 kbar, 2) $p = p' = 6.75$ kbar, 3) the function $f(H)$ is equal to the ratio of the curves 2 and 1. At $p = p'$, the ZGS is observed at $H_i \approx 49$ kOe.

sharper and higher. The value of $\eta(0)$, which is close to unity at $p = 1$ bar for each alloy, decreases rapidly as $p \to p_i$ and reaches ~ 0.1–0.05, which is minimal in the purest alloys. At $p > p_i$, the value of $\eta(0)$ again increases under pressure and tends to unity.

It was shown in[30] that in $Bi_{1-x}Sb_x$ with a direct spectrum the anisotropy is $\eta(0) = 2\mu_3/\mu_1$, where μ_1 and μ_3 are the transverse components of the electron-mobility tensor in the directions of the C_1 and C_3 axes. A typical plot of $2/\eta(0) = \mu_1/\mu_3$ against pressure is shown in Fig. 15. The same figure shows for comparison the results of preceding work[4] (dashed curve). It is seen that on going over to the ZGS under pressure, a significant increase of the mobility anisotropy is observed, with the component μ_1 becoming dominant.

As shown in[30], in the region of quasiclassical fields $\eta(H)$ increases from $\eta(0) = 2\mu_3/\mu_1$ at $H = 0$ to $\eta(H) \approx \mu_3/3\mu_2$ at $H > (\frac{3}{2}\mu_2\mu_3)^{-1/2}$, where μ_2 is the mobility component along the direction of elongation of the electron surface. On going to the ultraquantum region, the growth of $\eta(H)$ slows down and gives way to a smooth decrease. This change of the $\eta(H)$ dependence is the consequence of the outflow of the electrons from the ellipsoid that is elongated along a direction perpendicular to the field at $\mathbf{H} \parallel C_1$. After the complete outflow, which ends at $n \sim 10^{15}$ cm^{-3} in fields $H \sim 20$ kOe, the anisotropy $\eta(H)$ becomes equal to $4\mu_3/3\mu_1$[30] ($\mu_1 = e\tau_1/m_1$, $\mu_3 = e\tau_3/m_3$, τ_1, τ_3 and m_1 and m_2 are the components of the electron relaxation time and effective-mass tensors respectively along the axes C_1 and C_3).

The monotonic variation of $\eta(H)$ at $p < p_i$ in fields $H > 20$ kOe is a reflection of the further one-dimensionalization of the electron system in the ultraquantum region and of the monotonic increase of the gap ε_g in the spectrum.

For alloys with inverted spectrum ($p > p_i$), the plots of $\eta(H)$ assume a different form; near the inversion field H_i a second maximum appears on the $\eta(H)$ curves (Figs. 13 and 14, curves 2). With increasing pressure, I_i increases and accordingly the position of the second maximum shifts to the right.

It can be assumed that the second maximum on the $\eta(H)$ curves at $p > p_i$ is connected with the change of the anisotropy of the transverse mobilities on going to the ZGS under the influence of the magnetic field. To separate the influence of the inversion of the L bands in a magnetic field on the anisotropy of the mobilities μ_3/μ_1, it is necessary to exclude the contributions of all the other mechanisms (which are connected with the transfer of carriers between the L extrema, with the transition of the magnetic field to the ultraquantum region, with the one-dimensionalization of the electron system etc.) to the variation of $\eta(H)$. This can be done by considering the ratio of two functions $\eta(H)$ corresponding to pressures p' and p'' that are symmetrical about the inversion point p_i. The function

$$f(H) = \frac{\eta(H,\ p = p' > p_i)}{\eta(H,\ p = p'' < p_i)}, \quad p' - p_i = p_i - p''$$

is represented by a curve with a maximum at $H = H_i$ (curves 3 in Figs. 13 and 14). At $H < H_i$ and $H > H_i$ the value of $f(H)$ tends to unity. This form of the function $f(H)$ shows that the dependence of the anisotropy η on the field in alloys with inverted ($p > p_i$) and non-inverted ($p < p_i$) spectrum is identical at all fields, with the exception of a rather narrow region $H \sim H_i$. A comparison of the data obtained at different pressures p' and p'' allows us to conclude that $f(H)$ is a universal function of the argument H/H_i. Thus, the results indicate that $f(H)$ characterizes the time-dependent part of the anisotropy μ_3/μ_1, which is connected only with a transition to the ZGS under the influence of the magnetic field.

Comparing the $f(H)$ curves on Figs. 13 and 14 with the plot of μ_i/μ_3 against p in Fig. 15, we see easily that the change of the anisotropy of the mobilities μ_1/μ_3 on going over to the ZGS is the inverse of the change observed on going to the ZGS under the influence of pressure. In a magnetic field there is no predominant growth of μ_1 on going to the ZGS and, to the contrary, isotropization of the mobilities is observed. Since the transition to the ZGS in a magnetic field is the result of the approach and inversion of two non-interacting levels 0^- and 0^+ for the electrons and holes, it follows that according to Beneslavskiĭ and Fal'kovskiĭ[7] the effective masses m_1 and m_3 should not change. Thus, the change of the anisotropy of the mobilities $\mu_1/\mu_3 = \tau_1 m_3/\tau_3 m_1$ on

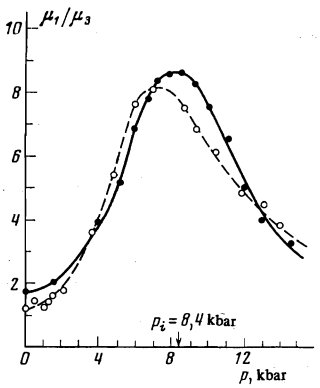

FIG. 15. Solid curve—anisotropy of the transverse electronic mobilities $1/3 = 2/(0)$ vs pressure for the n-type $Bi_{0.871}Sb_{0.129}$ alloy at $T = 4.2$ °K; dashed—analogous plot for $Bi_{0.91}Sb_{0.09}$ at $T = 4.2$ °K according to the data of [4].

going to the ZGS in a magnetic field seems to be entirely due to the change of the anisotropy of the relaxation times, which is such as to cause isotropization of the carrier scattering processes as $H \to H_i$.

[1)]At $\mathbf{H} \parallel C_2$ the elongation direction of one of the electron surfaces coincides with H, and the elongation directions of the two others make angles 60° with H. In this case the changes of the gaps ε_g in a magnetic field, in each of the L extrema, are close to one another and experiment seems to yield some average value of $\partial\varepsilon_0/\partial H$. At $\mathbf{H} \parallel C_1$ the elongation direction of one of the surfaces is perpendicular to H, while those of the two others make angles 30° with H. In this case the nonequivalence of the surface orientations relative to H is quite appreciable.[7] As shown in[30], however, in a strong magnetic field at $\mathbf{H} \parallel C_1$ all the carriers flow over into two equivalent extrema. Therefore the experimental value of $\partial\varepsilon_0/\partial H$ at $\mathbf{H} \parallel C_1$ determines the rate of change of the equal gaps ε_g of the two equivalent extrema.

[2)]We note that in our earlier paper,[9] owing to an error in the determination of the pressure, we have drawn the incorrect conclusion that a ZGS is produced in a magnetic field both at $p < p_i$ and at $p < p_i$. Repeated measurements on the same samples have shown that both curves of Fig. 3 of[9] pertain to pressures $p \gtrsim p_i$.

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Translated by J. G. Adashko