Change of connectivity of the electron equal-energy surface of Bi under pressure

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A transition, induced by hydrostatic pressure, from ellipsoidal to dumbbell-shape, and then to a doubly connected form, has been observed in the electron equal-energy surface of Bi. In the pressure region where the cross section of the "neck" of the dumbbell becomes small enough, an intraband magnetic breakdown is observed. It is shown that the spectrum at the point L of the Brillouin zone of Bi is inverted and that the band overlap is $|\epsilon_g| = 4$–7 meV.

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The question of the inversion of the spectrum at the L point of the Brillouin zone remained until recently one of the least clear in the structure of the energy spectrum of Bi. There are many quantitatively and qualitatively differing results on this subject (see, e.g., [1–3]). The lack of exact data on the structure of the spectrum at the point L is attributed to the fact that the properties of the electrons on the Fermi surface of pure Bi depends little on the structure of the bottom of the band. Therefore information of the band structure obtained by investigating the properties of the electrons on the Fermi surface is quite inaccurate.

The most reliable information is obtained, from our point of view, by varying the ratio of the Fermi energy to the band overlap $|\epsilon_g|$ (or the gap ϵ_g in the case of an univerted spectrum) at the point L. One of the methods of changing the ratio $(\epsilon_F/|\epsilon_g|)$ is to smelt Bi with antimony. The character of the change of the spectrum of $Bi_{1-x}Sb_x$ alloys gives grounds for assuming that the spectrum of Bi at L is inverted and $\epsilon_g/\partial p = -(5 \pm 2)$ meV, [1] with the absolute value of ϵ_g increasing under hydrostatic compression at a rate $\partial\epsilon_g/\partial p = -2.5 \pm 0.2$ meV/kbar. On the basis of this result, it was of interest to increase the band overlap $|\epsilon_g|$ by hydrostatic compression to such an extent that it be-

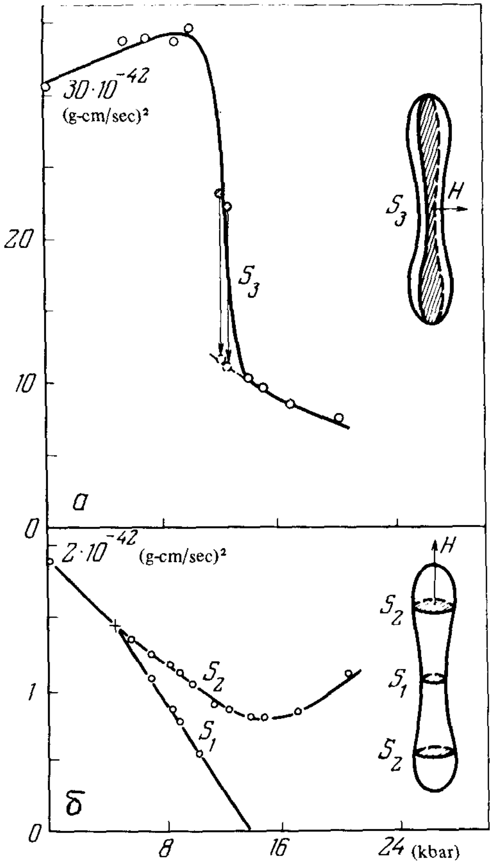

FIG. 1. Dependence of the extremal sections of the electron equal-energy surface on the pressure.

came comparable with or larger than the Fermi energy (Fig. 2b). Inversion of the spectrum should lead in this case to a qualitative change in the shape of the electron equal-energy surface (Fig. 2a).

With this in mind, we investigated the Shubnikov—de Haas (ShdH) effects of two single-crystal Bi samples of weakly doped Te (electron densities $n_e = 3.5\times 10^{17}$ cm^{-3} and 3.9×10^{17} cm^{-3}) in the pressure range up to 22 kbar. Since hydrostatic compression decreases rapidly the electron density,[4] doping with Te made it possible to observe distinctly a large number of oscillations in the entire range of employed pressures (the oscillations from small electron sections are difficult to observe in the case of pure Bi starting with a pressure ~ 12 kbar).

The pressure was produced by the procedure described in[5]. The ShdH oscillations were measured by a standard modulation method with the results delivered by an X–Y recorder. The sensitivity of the apparatus made it possible to observe oscillations from the three principal sections (S_1, S_2, S_3) of the electron equal-energy surface (Figs. 1a and 1b). The oscillation frequencies corresponding to these cross sections were determined accurate to ~ 5% by analyzing the experimental curves with a computer.

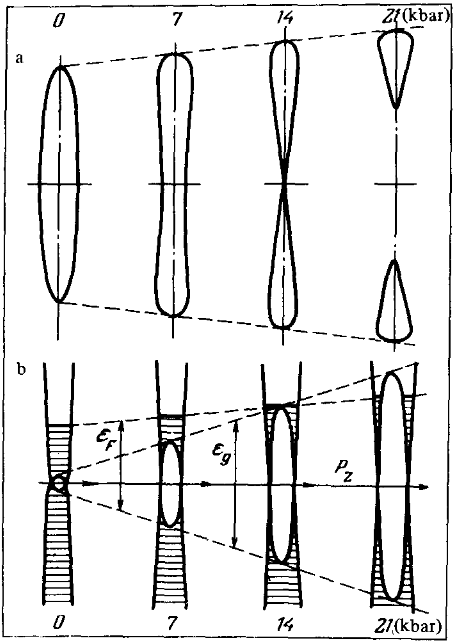

FIG. 2. Change in the shape of the electron equal-energy surface (a) when the pressure increases the band overlap ($-\epsilon_g$) in L (b).

The results obtained with the two investigated samples agree well with each other. We quote henceforth the data only for the sample with $n_e = 3.9 \times 10^{17}$ cm^{-3}.

The maximum principal section S_3 of the electron equal energy surface (corresponding to orientation of the field H along the binary axis) was observed to increase in the pressure region up to 10 kbar (Figs. 1a and 2a). With further increase of p, the oscillation frequency decreased abruptly. At $p = 13.8$ kbar, the rate of change of the frequency slows down greatly and at high pressures the oscillation frequency continues to decrease weakly with increasing pressure.

When the field is oriented along the elongation of the electron equal-energy surface, the frequencies of the oscillations vary in the following manner: the principal section S_1 on the electron equal-energy surface has at $p = 0$ a minimum that decreases monotonically with increasing pressure and vanishes at $p = 13.8$ kbar. Starting with $p \sim 5.5$ kbar, beats appear on the oscillation curves and are connected with the appearance of a new and higher frequency, which decreases much less with pressure. At $p = 14$ kbar, this frequency goes through a minimum and then increases (S_2, Fig. 1b).

The obtained pressure dependences of the oscillation frequencies at different field orientations can be interpreted in the following manner. When the pressure is increased, the ratio $|\epsilon_g|/\epsilon_F$ also increases. The increase of the band overlap at L changes the shape of the electron equal-energy surface, which becomes dumbbell-like starting with $p \sim 5.5$ kbar (cross on Fig. 1b). At this instant, when the field is oriented along the elongation of the electron equal-

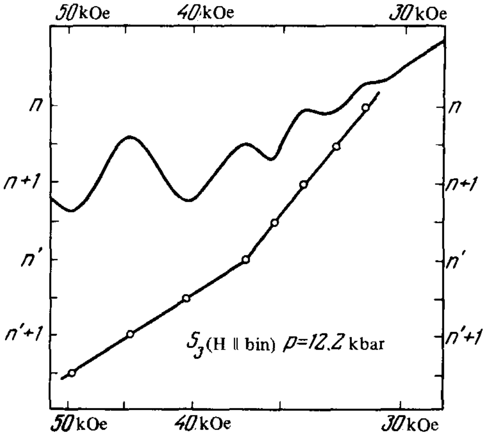

FIG. 3. Change of the character of the oscillations under intraband magnetic breakdown.

energy surface a second somewhat larger extremal section S_2 besides the minimum central section S_1 of the dumbbell "neck". At a pressure $p_k = 13.8$ kbar, S_1 degenerates into a point. With increasing pressure, the electron equal-energy surface breaks up into two drop-like equal-energy surfaces, the distances between which increases rapidly with pressure (Fig. 2a).

The obtained picture of the variation of the electron equal-energy surface agrees well with calculations by the Abrikosov-Fal'kovskiĭ model, in which the energy spectrum can be written in the form[3,6]

$$\left(\epsilon - \frac{p_z^2}{2M_1}\right)\left(\epsilon + \epsilon_g + \frac{p_z^2}{2M_2}\right) = v_x^2 p_x^2 + v_y^2 p_y^2 . \tag{1}$$

Here $\mathbf{p} = \mathbf{p}(p_x, p_y, p_z)$ is the quasimomentum; v_x, v_y, $(v_y < v_x)$, M_1, M_2, $(M_2 > M_1)$ are the parameters of the spectrum. The energy ϵ is reckoned from the bottom of the band. The quasimomentum components p_x and p_z are directed respectively along the binary axis and along the elongation of the electron equal-energy surface, while p_y is perpendicular to p_x and p_z.

The transition to the dumbbell-like electron equal-energy surface occurs at a pressure p such that

$$\frac{\epsilon_F(p) + \epsilon_g(p)}{M_1} = \frac{\epsilon_F(p)}{M_2} . \tag{2}$$

The pressure p_k at which the dumbbell breaks into two droplike electron equal-energy surfaces is determined from the condition

$$\epsilon_F(p_k) + \epsilon_g(p_k) = 0. \tag{3}$$

The dependences of S_3 and S_1 on p, calculated on the basis of relation (1) at the parameter values[12]: $v_x = 1.0 \times 10^8$ cm/sec, $v_y = 0.735 \times 10^8$ cm/sec, $(M_2/M_1) \sim 1.3$, $(d\epsilon_g/dp) = -2.7$ meV/kbar, and $\epsilon_{g0} = -6$ meV agree well with the experimental data (the solid curves of Figs. 1a and 1b were obtained by calculation).

We note that calculations by the Abrikosov-Fal'kovskiĭ model under the assumption $\epsilon_g > 0$ (the spectrum of Bi is not inverted), and also in accordance with the models of Lax[7] and Cohen[8] disagree with the experiments not only quantitatively but also qualitatively.

In the calculation of the dependence of S_3 on p for different models, we took into account the shift of the Fermi levels in a magnetic field.[9]

At pressures $p \sim 12$ kbar, when the cross section of the "neck" of the dumbbell becomes small enough, and in fields $H > \sim 35$ kOe, intraband magnetic magnetic breakdown[13] is observed, wherein both prebreakdown values of the cross section (dashed points on Fig. 3) and cross sections decreased approximately by one-half (dashed circles) are observed simultaneously. The cross sections that appear in fields T kOe fit well the plots of S_3 against p at $p > 14$ kbar.

Thus, the breaking of the necks of the electron equal-energy surfaces, which is accompanied by the Lifshitz electronic phase transition,[10] and the transition from three electron equal-energy surfaces to six drop-like equal-energy surfaces occurs in a Bi sample with $n_e = 3.9 \times 10^{17}$ cm^{-3} at a pressure 13.8 kbar.

An analogous transition should occur in pure Bi at $p \sim 12$—13 kbar. It follows therefore that under hydrostatic compression the three electron equal-energy surfaces of pure bismuth first split into six, and then these six surfaces contract into points and an electronic metal-insulator transition takes place at $p \sim 26$ kbar.[11]

[1] N. B. Brandt, S. M. Chudinov, and V. G. Karavaev, Zh. Eksp. Teor. Fiz. **70**, 2296 (1976) [Sov. Phys. JETP **43**, 1198 (1976)].
[2] V. S. Edel'man, Adv. Phys. **25**, 555 (1976).
[3] A. A. Abrikosov, Low Temp. Phys. **8**, 315 (1972).
[4] N. B. Brandt, E. S. Itskevich, and N. Ya. Minina, Usp. Fiz. Nauk **104**, 459 (1971) [Sov. Phys. Usp. **14**, 438 (1971)].
[5] N. B. Brandt and Ya. G. Ponomarev, Zh. Eksp. Teor. Fiz. **55**, 1215 (1968) [Sov. Phys. JETP **28**, 635 (1969)].
[6] S. D. Beneslavskiĭ and L. A. Fal'kovskiĭ, Fiz. Tverd. Tela **16**, 1360 (1974) [Sov. Phys. Solid State **16**, 876 (1975)].
[7] B. Lax and J. G. Mavroides, Advances in Solid State Physics **11**, 1960 (ed. by F. Seitz and D. Turnbull).
[8] M. H. Cohen, Phys. Rev. **121**, 387 (1961).
[9] G. E. Smith, G. A. Baraff, and J. M. Rowell, Phys. Rev. **135**, A1118 (1964).
[10] I. M. Lifshitz, Zh. Eksp. Teor. Fiz. **38**, 1569 (1960) [Sov. Phys. JETP **11**, 1130 (1960)].
[11] D. Balli and N. B. Brandt, Zh. Eksp. Teor. Fiz. **47**, 1653 (1964) [Sov. Phys. JETP **20**, 1111 (1965)].
[12] B. A. Akimov, Cand. Dissertation, Moscow University, 1975.
[13] Yu. V. Kosichkin, Cand. Dissertation, Moscow, Phys. Inst. Acad. Sci. 1970.