# *CHANGE OF THE PARAMETERS OF THE ELECTRON ENERGY SPECTRUM IN BISMUTH UNDER PRESSURE*

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The effective masses of carriers of both signs in bismuth under hydrostatic compression were determined from the temperature dependence of the amplitudes of the quantum oscillations of the electric resistance. At 8 kbar pressure, the effective masses of the electrons decrease by approximately 40%. The hole masses also have a tendency to decrease. The pressure-induced change of the main parameters of the energy spectrum of the bismuth are determined from the results of the present measurements and also from the published data[1-6]. The results are discussed.

THE reason for the great interest in the electron spectrum of bismuth has been the recent publication of numerous papers devoted to an elucidation of the features of the carrier dispersion in this metal. noteworthy among these papers are the theoretical work of Abrikosov and Fal'kovskiĭ[1], who considered, on the basis of general principles, the energy spectrum of bismuth at its genesis, and also the theories of Lax[2] and Cohen[3], who used model representations. It would be of interest to investigate the influence of the pressure on the main characteristics of the electron spectrum of bismuth.

In earlier investigations we measured the angular dependences of the periods of the electric-resistance oscillations (the Shubnikov-de Haas effect) in bismuth for both electrons and holes, up to pressures of 15 kbar[4,5]. It followed from these data that at 15 kbar only 20% of the initial volume of the Fermi surface of bismuth remains, and the hole surface (ellipsoid) has a tendency to become spherical.

In the present investigation we measured the effective masses of the carriers of both signs under pressure by determining the temperature dependence of the amplitudes of the quantum oscillations of the electric resistance. At the same time, Fal'kovskiĭ[6] considered the pressure-induced deformation of the electron spectrum of bismuth, which was calculated in[7]. On the basis of his paper, and also that of Lax et al.[2] and our experimental data we calculated the pressure-induced change of the main parameters of the energy spectrum.

## MEASUREMENT RESULTS

The cyclotron effective masses $m^* = (2\pi)^{-1}\,\partial S/\partial E$ of the electrons and holes in bismuth, and also the Dingle temperature $T_D$, were determined under a hydrostatic pressure up to 8 kbar from the measurements of the temperature dependence and the magnetic-field dependence of the amplitudes A of the quantum oscillations of the electric resistance:

$$A \sim \frac{1}{H^{1/2}}\frac{2\pi^2 kTm^*c}{e\hbar}\,\mathrm{sh}^{-1}\Big(\frac{2\pi^2 kTm^*c}{e\hbar H}\Big)\exp\Big(-\frac{2\pi^2 kT_D m^*c}{e\hbar H}\Big). \qquad (1)$$

The experiments consisted of measuring the quantum oscillations of the electric resistance of bismuth

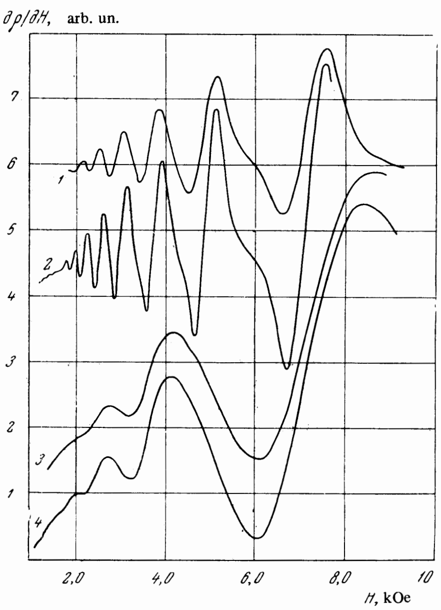


FIG. 1. Typical plots of quantum oscillations of the electric resistance $\partial\rho/\partial H$ against the field at different temperatures and pressures in the case $H \| C_2$: 1 – T = 4.2°K, P = 1 bar; 2 – T = 2.2°K, P = 1 bar; 3 – T = 4.2°K, P = 8 kbar; 4 – T = 1.95°K, P = 8 kbar.

by a modulation method[4] in the cases $H \parallel C_2$ (on the minor section of the electron ellipsoid) and $H \perp C_2$, $\sphericalangle(H, C_3) = 30°$ (on the minor section of the hole ellipsoid) at different temperatures $(1.5 \le T \le 4.2°K)$ and pressures (1 bar ≤ P ≤ 8 kbar) (Figs. 1, 2). The measurement procedure and the method of producing the pressure were described in detail in[4].

The results of the measurements of the effective masses for the electrons are as follows ($H \parallel C_2$):

| | | | |
|---|---|---|---|
| P, kbar: | 4,3 | 6,5 | 8 |
| $-\Delta m_e^*(P)/m_e^*(P=1\ \text{bar})$, %: | 22±20 | 29±20 | 41±25 |

The effective masses were obtained by averaging 15 – 20 values calculated at different temperatures and in different magnetic fields. The error was determined from the mean-square measurement error.

The determination of the effective mass under pressure was made difficult by the inevitable increase of the temperature $T_D$ as a result of a certain deteri-

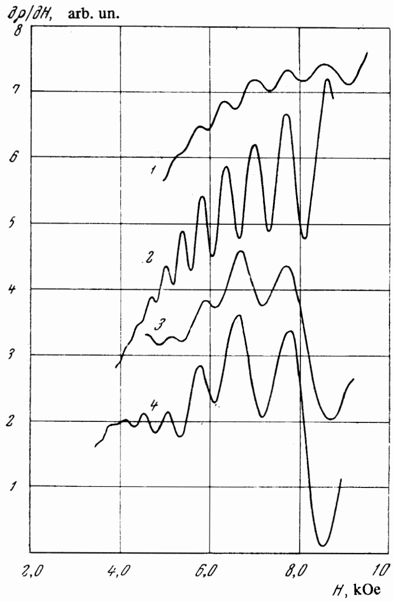


FIG. 2. Quantum oscillations of the electric resistance in the case $H \perp C_2$, $\measuredangle (H, C_3) = 30°$: 1 – T = 3.71°K, P = 1 bar; 2 – T = 1.95°K, P = 1 bar; 3 – T = 2.66°K, P = 8 kbar; 4 – T = 1.43°K, P = 8 kbar.

oration in the quality of the crystal, which led to a weak dependence of the oscillation amplitude on the temperature. It must also be taken into account that in bismuth under pressure the period of the quantum oscillations increases [4,5], and that for small cross sections of the electron ellipsoid they are observed in magnetic fields close to the quantum limit, where formula (1) is not exact.

From the foregoing results we see that $m_e^*$ decreases under pressure.

The decrease of the cyclotron effective mass for the electronic part of the surface under a pressure of 1.6 kbar was observed also earlier [8].

The hole cyclotron mass measured by us under pressure also had a tendency to decrease

$$|m_h^*| = (6.4 \pm 1.5) \cdot 10^{-2} \quad \text{for } P = 1 \text{ bar},$$
$$|m_h^*| = (5.2 \pm 1.5) \cdot 10^{-2} \quad \text{for } P = 8 \text{ kbar}.$$

The measurements of the Dingle temperature $T_D$ have shown that this temperature increases with increasing pressure and thus the quality of the crystal deteriorates under hydrostatic compression, owing to a certain inhomogeneity of the pressure.

## DISCUSSION OF RESULTS

1. Hole spectrum. Fal'kovskiĭ [6] investigated the influence of hydrostatic pressure on the electronic spectrum of bismuth, which he obtained earlier together with Razina [7]. In the first approximation, the hole ellipsoid changes in similarity to itself, and the relative decrease of its two principal extremal cross sections is the same:

$$\frac{dS_{max,\,min}}{S_{max,\,min}} = \frac{dE_F}{E_F} + \frac{d\gamma}{\gamma}. \tag{2}$$

In second approximation, the anisotropy of the Fermi surface and the effective mass of the holes change:

$$\frac{dS_{max}}{S_{max}} - \frac{dS_{min}}{S_{min}} = -\frac{dE_F}{4\Delta} - \frac{\Delta}{2\gamma^2}\,d\gamma, \tag{3}$$

$$\frac{dm_h^*}{m_h^*} = -\frac{dE_F - d\gamma}{\gamma - \Delta}. \tag{4}$$

Here $E_F$ is the Fermi energy reckoned from the top of the hole band, Δ the spin-orbit interaction energy, and $\gamma$ a quantity determined by the displacement u of the sublattices forming the crystal lattice of bismuth.

From the results of [5] and from formula (3) it might seem possible to calculate the change of $\gamma$ under pressure. This calculation, however, cannot be performed, owing to the large error in the determination of $dS_{max}/S_{max} - dS_{min}/S_{min}$ under pressure [5].

We can estimate the change of $\gamma$ under compression by means of formula (4). From the results obtained by us it follows that the mass of the holes on the minimal cross section apparently decreases. According to (4) this can be observed under the condition $d\gamma < dE_F \le E_F = 0.013$ eV. Thus, $d\gamma(P)/\gamma(1 \text{ bar}) \lesssim 2.5\%$, and the entire deformation of the spectrum can be explained as due to a decrease of the Fermi energy, neglecting the change in $\gamma$ and consequently in the parameter u of the bismuth lattice within the interval of our pressures. In this case we have in first approximation

$$\frac{\Delta E_F(P)}{E_F(P = 1\text{bar})} = \frac{\Delta S(P)}{S(P = 1\text{bar})}$$

and the change of the anisotropy of the hole ellipsoid at the point where the band overlap is lifted is approximately 2%. The effective mass of the holes decreases by ≈3%. The experimental results agree qualitatively with the conclusions of the theory.

2. Electron spectrum. The decrease of the effective masses of the electrons with pressure, when the carrier density decreases, is connected with the nonquadratic dispersion law for the electronic part of the Fermi surface of bismuth, which was observed in a number of investigations [2,9,10]. The magnetooptic measurements of Lax et al. [2] have shown that there is a small energy gap $E_g$, equal to 0.015 eV, in the energy spectrum of the bismuth electrons. Indeed, as shown theoretically, only two out of the four branches of the spectrum are quite close [7]. In this case, neglecting the influence of the remote energy bands, we can obtain from the total spectrum of Abrikosov and Fal'kovskiĭ, for small cross sections of the electron surface, the so-called two-band model [6] first introduced by Lax for the interpretation of data on optical absorption [2]. In this model, which takes into account the interaction between the conduction and valence bands, the cyclotron effective mass at the Fermi level $m_e^*(E_F) = (2\pi)^{-1}(\partial S/\partial E)_{extr}$ and the areas of the small extremal sections of the electronic ellipsoid $S(E_F)$ are functions of the electron Fermi energy $E_F$. These quantities are expressed as follows in terms of the constants describing the spectrum:

$$S(E_F) = 2\pi m_0^* E_F (1 + E_F / E_g), \tag{5}$$

$$m_e^*(S) = m_0^* [1 + 2S / \pi m_0^* E_g]^{1/2}, \tag{6}$$

where $m_0^*$ is the cyclotron mass at the bottom of the conduction band, which is proportional as usual [11] to

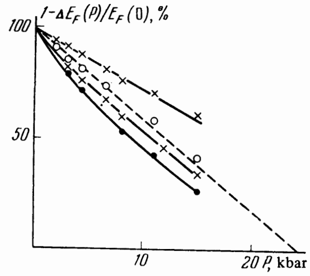


FIG. 3. Plot of f(P) [Eq. (7)] for electrons with different rates of change of $E_g$ with changing pressure: ×– $\frac{\partial E_g}{\partial P}\frac{1}{E_g(P=1\text{ bar})}=\pm 5\cdot 10^{-5}\text{ bar}^{-1}$, ●– $10^{-4}$ bar$^{-1}$; ○–$E_g$ = const. The dashed straight line shows the plot of f(P) = 1 – ΔS/S(P = 1 bar) for holes.

| $P$, bar | Experiment | | Calculation | | |
|---|---|---|---|---|---|
| | $S(P)\cdot 10^{42}$, CGS | $-\frac{\Delta S(P)}{S(1\text{ bar})}$, % | $E_F(P)\cdot 10^{14}$, erg | $-\frac{\Delta E_F(P)}{E_F(1\text{ bar})}$, % | $\frac{\Delta m_e^*(P)}{m_e^*(1\text{ bar})}$, % |
| 1 | 1.47 | | 4.4 | | |
| 1900 | 1.23 | 15±2 | 4 | 9±1 | 7±1 |
| 3000 | 1.15 | 21±3 | 3.7 | 16±2 | 11±2 |
| 4300 | 1,,05 | 29±4 | 3.5 | 20±2 | 16±2 |
| 6500 | 0.9 | 39±4 | 3.2 | 27±2 | 21±2 |
| 8000 | 0.85 | 48±6 | 2.9 | 32±4 | 27±4 |

the aforementioned small gap $E_g$.

It would be of interest to calculate by means of formula (6) the $E_g(P)$ dependence from the results of [4,5] and the present data for the effective masses of the electrons, and also of [6,12]. We could not do this, however, owing to the large error in the determination of the quantity $\pm m_e^*(P)/m_e^*(P = 1\text{ bar})$.

Information on the change of $E_g(P)$ can be obtained by comparing the relations

$$f(P) \equiv 1 - \Delta E_F(P)\,/\,E_F(P = 1\text{ bar}) \qquad (7)$$

for holes and electrons, extrapolating these relations to high pressures. Both curves should cross the pressure axis at one point. The values of $\Delta E_F(P)/E_F \times (P = 1\text{ bar})$ for the electrons can be calculated from formula (5) and from the data of [4,5] at different rates of change of $E_g$ with changing pressure. The results of the calculations are shown in Fig. 3. It can be concluded from the presented data that $E_g$, most likely, does not decrease under pressure.

Assuming that $E_g$, and consequently also $m_0^*$ do not depend on the pressure, we calculated by means of formula (6) the dependence of the effective mass on the pressure $\Delta m_e^*(P)/m_e^*(P = 1\text{ bar})$. The results of the calculations of $m_e^*$ and $E_F$ are shown in the table. In the calculation we used the following numerical values of the parameters of the electron spectrum at P = 1 bar: $E_F = 4.4 \times 10^{-14}$ erg, $E_g = 2.4 \times 10^{-14}$ erg, $m_0^*/m_0 = 2.09 \times 10^{-3}$ [2].

The calculated values of $\Delta m_e^*(P)/m_e^*(P = 1\text{ bar})$ agree satisfactorily with the measured values given in the preceding section.

In conclusion, the authors consider it their pleasant duty to thank Academician L. F. Vereshchagin for interest in the work, L. A. Fal'kovskiĭ for a discussion of the results, and I. P. Krechetova for taking part in the experiments.


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