Structure of valence band of bismuth telluride

V. V. Sologub, R. V. Parfen'ev, and A. D. Goletskaya

A. F. Ioffe Physico-technical Institute, USSR Academy of Sciences
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A new model is proposed for the valence band of bismuth telluride to explain the singularities of the Shubnikov–de Haas oscillations observed at helium temperatures in single-crystal p–Bi_2Te_3 with hole density 2.9×10^{18}–2.4×10^{19} cm^{-3}.

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In bismuth telluride (Bi_2Te_3, $E_g = 0.13$ eV,[1] space group D_{3d}^5) we investigated with the aid of the Shubnikov—deHaas (SdH) effect the change in the shape of the Fermi surface of the holes as a function of the occupation of the valence bands. The extremal sections of the Fermi surface were determined from the periods of the SdH oscillations following changes in the orientation of the magnetic field **H** relative to the crystallographic axes. At helium temperatures, in magnetic fields up to 72 kOe, we investigated the dependences of the periods of the SdH oscillations on the orientation of the magnetic field in the mirror-reflection plane (c_1c_3) and in the plane (c_1c_2) perpendicular to the trigonal c_3 axis. The hole density was determined from the Hall coefficient $R_{321}(\mathbf{H}\perp c_3)$ in a strong magnetic field. We observed the fundamental and supplementary series of the SdH oscillations in the p-Bi_2Te_3 samples with density $p > p^* = 4\times 10^{18}$ cm^{-3} (No. 2 and No. 3). The fundamental series of the oscillations was ascribed earlier[2] to a band consisting of six inclined ellipsoids lying in mirror planes (the Drabble-Wolfe model[3]). The additional series of oscillations was measured only at $\mathbf{H}\parallel c_3$ and was connected with the second six-ellipsoid sub-band, located at a distance $\Delta E = 0.015$ eV from the fundamental band. In the proposed model of the Bi_2Te_3 valence band, the role of the second sub-band is played by tubes that connect the valleys of the fundamental band at a concentration $p > p^*$. The tubes are parallel to the mirror planes and are inclined 45° to the bisector axis (Fig. 1).

1. Figure 2 shows the rosettes of the fundamental series of the oscillations for the three investigated samples. The maximum value $\Delta_{max}(1/H)$ of the period at $\phi_0 = 75°$ was taken as unity. The dashed lines correspond to the rosette c_1c_3 for the six-ellipsoid model, the parameters of which were determined from the periods of the oscillations for sample No. 1, $\Delta_{max}(1/H) = 8.3\times 10^{-5}$ Oe^{-1} and $\Delta_2(1/H) = 7.4\times 10^{-5}$ Oe^{-1} at $\mathbf{H}\parallel c_2$, and $\Delta_3(1/H) = 5.9\times 10^{-5}$ Oe^{-1} at $\mathbf{H}\parallel c_3$.

The upper curve reflects the change in the principal section, i.e., the maximum section of the ellipsoid lying in the mirror plane and rotated 15° relative to the c_1 axis. The lower curve is connected with the change of the nonfundamental sections, i.e., the maximal sections of the equivalent ellipsoids located in two other mirror planes. The calculated angular dependence of the periods does not agree with the experimental data. Whereas for the six-ellipsoid model the smallest sections (the largest $\Delta(1/H)$ of the principal and the equivalent ellipsoids lie on opposite sides of the c_1 axis (in different quadrants), the experimental curves indicate that both sections reach the smallest values in the same quadrant. This is possible for valleys that are more complicated than ellipsoids and have no symmetry centers, thus indicating the need for taking into account the terms cubic in **k** in the energy spectrum of the holes.

2. Figure 3 shows the angular dependence of the periods of the fundamental (I) and supplementary (II) series of oscillations for sample No. 3. The additional series of oscillations has large periods corresponding to the appearance of small sections of the Fermi surface at a hole density $p > 4\times 10^{18}$ cm. The abrupt de-

FIG. 1. Overall view of the proposed model of the valence band of Bi_2Te_2 at $p > p^*$. $\theta_I = 15°$ is the angle of inclination of the valley to the mirror plane; $\theta_{II} = 45°$ is the angle of inclination of the tube centered on the binary axis c_2.

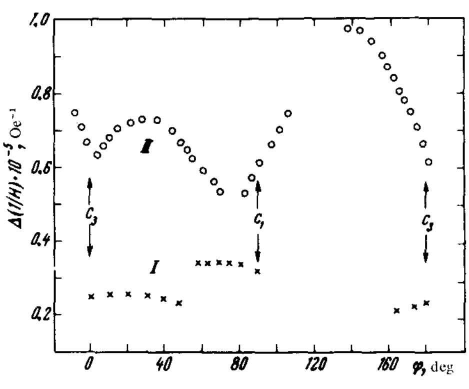

FIG. 2. Variation of $\Delta(1/H)$ of the fundamental (I) and supplementary (II) series of SdH oscillations when **H** is rotated in the mirror plane, for p-Bi_2Te_3 sample No. 3 at $T = 1.6$ °K ($\mathbf{J}\parallel c_2$).

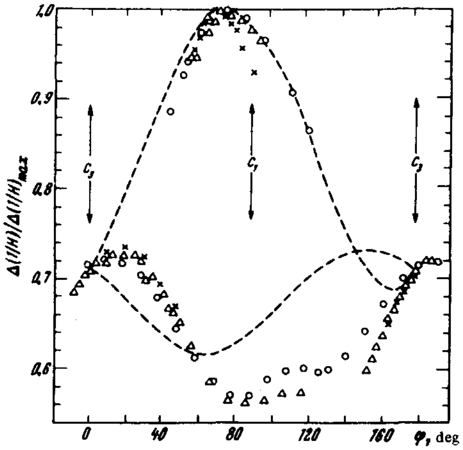

FIG. 3. Angular dependences of the periods of the SdH oscillations in p-Bi_2Te_3 following rotation of H in the mirror plane: J $\parallel c_2$, $T = 1.6$ °K; $\Delta_{max}(1/H) = 8.3\times10^{-5}$ Oe^{-1}, 6.0×10^{-5} Oe^{-1}, and 3.45×10^{-5} Oe^{-1} for samples No. 1, 2, and 3, respectively. The sample parameters p (cm^{-3}) and $R_{321}\sigma_{22}$ (cm^2/V-sec) at $T = 1.6$ °K are equal to: ○ (No. 1)—2.9×10^{18} and 3.7×10^4; Δ (No. 2) —7×10^{18} and 1.7×10^4; ×(No. 3) — 2.4×10^{19} and 5.6×10^3.

crease of the period of the second series from the maximum value at $\phi_{II} = 135°$ following an angular displacement cannot be attributed to the angular dependence of the maximum section of the ellipsoid or even of a cylinder, and corresponds to a change in the minimum section of a hyperboloid tube that is parallel to the mirror plane and is inclined 45° to the c_1 axis. The change of the additional period on the left of c_1 agrees with the change of the sections of the equivalent hyperboloid tubes (rotated 120° around c_3). That the orientation of the tubes is parallel to the mirror planes is confirmed by the rosette c_1c_2, from which it follows that the minimum section is observed at H $\parallel c_1$.

3. At a hole density $p < p^*$, the tubes break (the additional series of oscillations vanishes). The shape of the valleys can still differ in this case from ellipsoidal, owing to stubble that remains at the tube junction points. It appears that the stubble influences most strongly the angular dependence of the extremal sections of the equivalent valleys (Fig. 2, sample No. 1).

4. The hyperboloid tubes, while having a small minimal section, can have a noticeable volume, and this explains the disparity, observed in[2,4] between the hole densities determined from the period of the SdH oscillations of the fundamental series at H $\parallel c_3$ and those determined from the Hall coefficient R_{321}.

5. The appearance of tubes with small cross section at $p > p^*$ can lead to a change in the relations between the components of the magnetoresistance tensor in a weak magnetic field. In the investigated samples with concentrations $p = 1.6\times10^{18}$–2.4×10^{19} cm^{-3} at $T = 4.2$ °K there was observed an increase of the ratio of the Hall coefficients at H $\perp c_3$ and H $\parallel c_3$ (R_{321}/R_{123}), from 1.5 at $p < p^*$ to 2.6 at $p > p^*$, as well as a decrease of the ratio ρ_{1133}/ρ_{1122} for the transverse magnetoresistance, from 3.5 to 1.6, respectively.

The noted experimental facts indicate that the purely ellipsoidal model of the valence band of Bi_2Te_3 does not apply at a hole density $p \gtrsim 3\times10^{18}$ cm^{-3}. The observed additional sections belong to tubes that are centered on the binary axes, and appear as a result of the anisotropic nonparabolicity of the fundamental band.

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