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Trigonal Warping of the Energy Surfaces in Tellurium

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The period of the Shubinkov–de Haas oscillations, when the magnetic field is applied in the plane perpendicular to the c axis of single-crystal heavily doped Te($p=4.8\times10^{18}$ cm^{-3}), is observed to depend on the azimuthal angle. This angular dependence gives clear experimental evidence of trigonal warping of the constant-energy surfaces about the k_z axis in the Brillouin zone.

We present clear experimental evidence that the constant-energy surfaces in crystalline Te exhibit trigonal warping about the k_z axis of the Brillouin zone. This type of warping is expected on the basis of recent theoretical calculations[1,2] of the band structure, but has not been observed unambiguously, heretofore, experimentally. Our evidence is deduced from the angular dependence of the Shubnikov–de Haas (SdH) period as the applied magnetic field is rotated in the plane perpendicular to the crystallographic c axis.

Theoretical and experimental results[3–8] to date indicate that the constant-energy surfaces of crystalline p-Te consist of pairs of neighboring ellipsoids which are prolate in the k_z direction. In highly doped samples, these ellipsoids merge, as shown in Fig. 3(a), and the Fermi surface becomes dumbbell shaped. The center of this dumbbell is located at the H point of the Brillouin zone as in Fig. 3(c). Recent calculations[1,2] of the valence-band structure near the H point predict the existence of trigonal warping about the k_z axis. In particular, the $E(k)$ relation of the uppermost valence band was found to be of the form

$$E(k)=Ak_\perp^2-Bk_\perp^4-Ck_x(k_x^2-3k_y^2)+Dk_z^2+(S_1^2k_z^2+4\Delta_1^2)^{1/2}-\Delta_2\,,\qquad k_\perp^2=k_x^2+k_y^2\,. \tag{1}$$

The third term in Eq. (1) describes the trigonal warping as may be seen when it is written in polar coordinates as $Ck_\perp^3\cos3\varphi$, where φ is the aximuthal angle. As is well known, the plane of the orbit of a charge carrier in a strong magnetic field is perpendicular to the direction of the applied field. Our method of studying the trigonal warping is to cause a hole to traverse an orbit in the plane par-

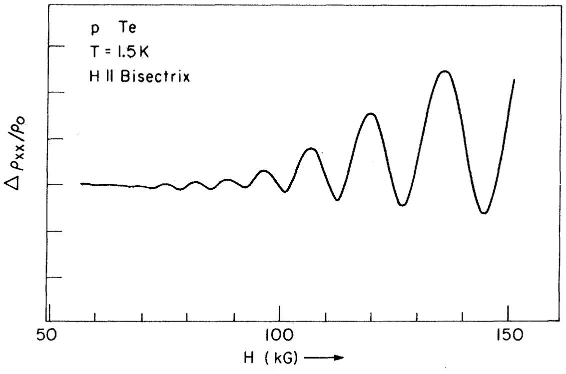

FIG. 1. Recorder tracing of the transverse magnetoresistance $\Delta\rho_{xx}$ of single-crystal p-type Te doped to a concentration of $p = 4.8 \times 10^{18}$ cm^{-3}.

allel to the k_z axis by fixing the applied magnetic field in the plane perpendicular to the crystallographic c axis. Rotating the field in this plane causes the hole orbit to rotate about this axis. In the absence of trigonal warping, i.e., if the Fermi surface is a solid of revolution, the SdH period which is observed for this configuration should be independent of the angle φ as the magnetic field is rotated. This is not observed to be the case.

We studied the transverse magnetoresistance ρ_{xx} of single-crystal Te doped to a hole concentration of $p = 4.8 \times 10^{18}$ cm^{-3}. The SdH periods were observed at $T = 1.5$ K in static magnetic fields up to 150 kG. A voltage proportional to ρ_{xx} was recorded on the Y axis of an X-Y recorder. A voltage proportional to the magnet supply current provided the X sweep and a fraction of this voltage was used to cancel the linear component of ρ_{xx}. This cancellation enhanced the amplitude of the oscillations and produced a trace of ρ_{xx} versus H which was free of any background. A typical recorder tracing is shown in Fig. 1 for H parallel to a bisectrix axis. These oscillations arise from the Landau levels with quantum numbers $7 \leq n \leq 13$. Similar traces were recorded at about 7° intervals over a total angle $\varphi = 170°$ in the (0001) plane. It is crucial to the analysis of the data that the trace in Fig. 1 shows no beat pattern, and this, in fact, is the case for all the angles studied.

The period at a fixed angle φ was determined to an accuracy of 2–3%. However, the relative accuracy between periods measured at successive angles was greater and amounted to 0.5%. As shown in Fig. 2, the period $P = \Delta(1/H)$, with H perpendicular to the c axis, depends on the angle φ and has maximum values for H parallel to the bisectrix and minimum values for H parallel to the binary. A least-squares fit to this angular dependence of P gives

$$P = (0.975 - 0.014 \cos 6\varphi) \times 10^{-6}\ \mathrm{G}^{-1}. \qquad (2)$$

According to the Onsager relation the extremal area A_0 of the Fermi surface in k space is

$$A_0 = (2\pi e/\hbar c)\ 1/P.$$

From this equation and Fig. 2 we find that the extremal cross sections perpendicular to the binary axis A_{BIN} are about 2.9% greater than those perpendicular to the bisectrix A_{BIS}. We attribute the φ dependence of P solely to the trigonal warping of the cross-sectional area perpendicular to the k_z axis, as shown in Fig. 3(b).

In previous experiments[7] on Te, doped to the same carrier concentration as in the present study, the anisotropy of the SdH period in the trigonal-bisectrix plane was studied. Using these data, under the assumption of rotational symme-

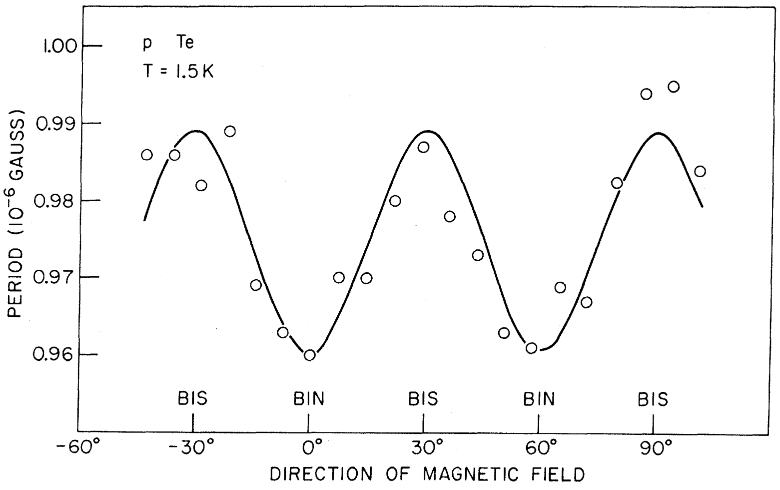

FIG. 2. Azimuthal variation of the SdH period when the applied magnetic field is rotated in the plane perpendicular to the crystallographic c axis. The open circles are the data points and the solid line is a least-squares fit to the data according to Eq. (2). The binary (BIN) and bisectrix (BIS) axes are labeled at the bottom of the figure.

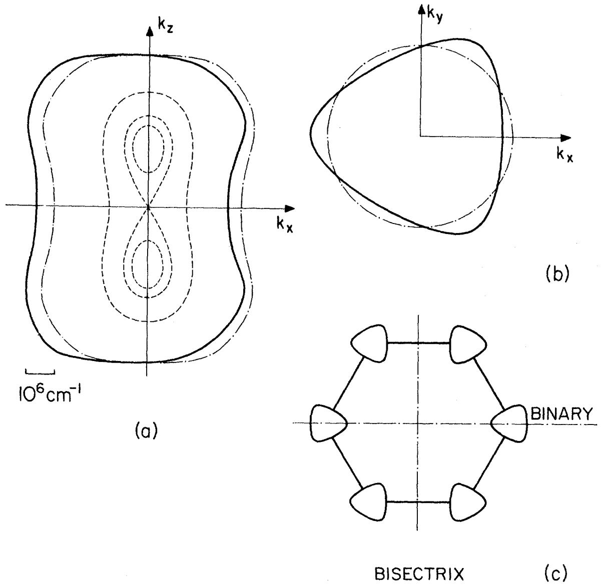

FIG. 3. (a) Constant-energy surfaces of p-Te at various carrier concentrations. At the lowest concentrations they consist of separated ellipsoids which merge into dumbbell shape as the concentration is increased. Dashed line: calculated from Eq. (1) neglecting trigonal warping; dash-dot line: calculated from experimental data, on a sample with $p = 4.8 \times 10^{18}$ cm^{-3}, using Mueller's inversion scheme but neglecting trigonal warping; solid line: present results with trigonal warping included. (b) Central cross section at $k_z = 0$. The solid line shows the trigonal warping as determined from Eq. (3) with $\alpha = 0.08 \times 10^{-6}$ cm. (c) Arrangement of the warped constant-energy surfaces in the Brillouin zone. The H point lies at the corners of the hexagon. The binary and bisectrix axes are indicated.

try, the constant-energy surfaces were constructed by employing a modification of Mueller's inversion scheme.[9] This inversion gave the important result that for large carrier concentrations ($p \gtrsim 10^{18}$ cm^{-3}) the constant-energy surface in the vicinity of $(k_z)_{\max}$ is flatter than predicted by Eq. (1). In order to account for the trigonal warping observed in the present study we made use of this empirically determined Fermi surface as follows. We describe the cross sections at $k_z =$ const by the equation

$$k_x^2 + k_y^2 - \alpha k_x \cdot (k_x^2 - 3k_y^2) = \beta(k_z), \qquad (3)$$

where β depends on k_z and is found from the condition that the area enclosed by the warped cross section at $k_z =$ const is equal to the area known from the previous experiments[7] performed with H parallel to the c axis. The parameter α, which characterizes the extent of the warping quantitatively, is then determined from the present experimentally observed ratio of the extremal areas, namely, $A_{\mathrm{BIN}}/A_{\mathrm{BIS}} = 1.029$. The value of α determined by this method is $\alpha = 0.08 \times 10^{-6}$ cm, and the central cross section at $k_z = 0$ described by Eq. (3) is shown in Fig. 3(b).

The arrangement of the warped constant-energy surfaces in the Brillouin zone is shown in Fig. 3(c). Since only a single period is observed for all φ, the angular disposition of all six constant-energy surfaces relative to the Brillouin-zone center must be identical. From our experiments it is not possible to decide whether some or each of the six surfaces are rotated by 180° about the k_z axis. It is evident from Fig. 3(c) that each valley gives the same φ dependence of P.

In summary, trigonal warping of the constant-energy surfaces about the k_z axis in crystalline Te has been observed unambiguously for the first time. This warping is small, but its presence is an important feature in the Fermi surface of Te and it may have importance for the interpretation of other experiments.

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