Influence of hydrostatic pressure on the splitting of the Landau levels in tellurium

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The Shubnikov–de Haas effect in magnetic fields up to 120 kOe was used to study the influence of hydrostatic pressures up to 15 kbar on the splitting of the Landau levels in tellurium for $\mathbf{H} \parallel C_3$ resulting from the inversion asymmetry. A considerable increase in the amplitude of the 0^+ oscillation maximum and splitting of the first maximum were observed when the pressure was increased. The results were compared with a current model of the influence of pressure on the structure of the upper valence band of tellurium.

INTRODUCTION

A characteristic feature of the energy band structure of tellurium is a shift of the maxima of the upper valence band from the high-symmetry point M to points located at $\pm k_{zm}$ along the Brillouin zone edge parallel to the trigonal axis C_3.[1] The spin degeneracy of the states in the upper valence band at the point M is lifted completely by the strong spin-orbit interaction. Consequently, the application of a magnetic field does not cause an additional splitting of these states and the energy spectrum at the point M does not contain terms linear in H. However, when the extrema of this band are shifted from the high-symmetry point, the Hamiltonian in the effective mass method may contain terms proportional to the product of the wave vector and the magnetic field: $\mathbf{k}\cdot\mathbf{H}$. A dispersion relationship was obtained in[2] for the upper valence band of tellurium in a magnetic field $\mathbf{H} \parallel C_3$ and it contained the following term:

$$\varepsilon = Ak_z^2 - (\Delta^2 + C^2k_z^2)^{1/2} + \hbar\Omega(N + 1/2) \pm 1/2\, G\mu_B H_z, \quad (1)$$

where

$$G = 2Cg_1|k_z|/\mu_B(\Delta^2 + C^2k_z^2)^{1/2}, \quad \Omega = eH/m_\perp c,$$

g_1/μ_B is the spectroscopic splitting factor in the absence of the spin-orbit interaction.

It follows from Eq. (1) that in a magnetic field $\mathbf{H} \parallel C_3$ the valleys corresponding to $\pm k_{zm}$ shift in the opposite directions along the energy scale. The appearance of the G factor, which is a linear function of the component k_z, is a direct consequence of the absence of an inversion center in the crystal lattice of tellurium. We shall follow the terminology adopted in[2] and attribute the Landau level splitting to the inversion asymmetry.

Such splitting should be manifested in the Shubnikov-de Haas oscillations by the appearance of the zeroth oscillation maximum and by the splitting of the other maxima. The value of the G factor measured in the Shubnikov-de Haas experiments is governed by the separation of the noncentral extremal sections from the high-symmetry point. In a field $\mathbf{H} \parallel C_3$ the factor $G = G_m$ is governed by the value of k_{zm}. The first observations of the zeroth maximum of the Shubnikov-de Haas oscillations in the tellurium subjected to a magnetic field $\mathbf{H} \parallel C_3$ were reported in [2].

We found that the deviation of the magnetic field H from the C_3 axis reduced the amplitude of the zeroth maximum and shifted it in the direction of stronger magnetic fields until it disappeared at an angle $\varphi(\mathbf{H}, C_3) \lesssim 60°$. Thus, the range of angles in which the zeroth maximum was observed corresponded to the range of existence of the noncentral extremal sections of the Fermi surface of tellurium.[1] We concluded from these observations that the Landau levels of tellurium were split by the inversion asymmetry and the G factor was $G_m = 5 \pm 1$.

It was demonstrated in[3] that the dispersion relationship (1) could be obtained also by analyzing the valence band of tellurium with the aid of the $\mathbf{k}\cdot\mathbf{p}$ method.[4] A study of the cyclotron resonance in tellurium in the far infrared region (see[5]) revealed very weak absorption lines (P_4 in the notation used in[5]) in $\mathbf{H} \parallel C_3$. Linear extrapolation of the magnetic-field dependence of the transition energies corresponding to these lines passed through the origin of the coordinates. These lines could not be attributed to cyclotron transitions between the Landau levels usual for this orientation. We could assume that the lines were due to transitions between the Landau sublevels resulting from the inversion-asymmetry splitting. According to this interpretation the value of the G factor should be $G_m \approx 9$.

The assumption of the splitting of the Landau levels by the inversion asymmetry was used in[6] in discussing the results of an investigation of the magnetophonon resonance in tellurium. The value $G_m \approx 4$ obtained in[6] was in good agreement with our results.[2]

A strong influence of hydrostatic pressure on the amplitude and position of the zeroth maximum was also mentioned in[2]. The form of the upper valence band of tellurium described by the dispersion relationship (1) is governed by $\xi = 2A\Delta/C^2$ and we can distinguish two cases: 1) if $\xi < 1$, this band has a saddle point at $k_z = 0$ and two maxima at

$$k_z = k_{zm} = \pm\left[\frac{\Delta}{2A}\frac{1-\xi^2}{\xi}\right]^{1/2}, \quad (2)$$

where the saddle point is separated from the band edge by

$$\Delta\varepsilon = \Delta(\xi - 1)^2/2\xi; \quad (3)$$

2) if $\xi > 1$, the band is nearly parabolic with a single maximum at $k_z = 0$.

The first case corresponds to tellurium under normal pressure and then $\xi = 0.764$. A detailed study of the influence of a hydrostatic pressure on the Shubnikov-de Haas oscillations was used in[7] as the basis of a linear-approximation model of changes in the energy band structure of tellurium under pressure and the pressure

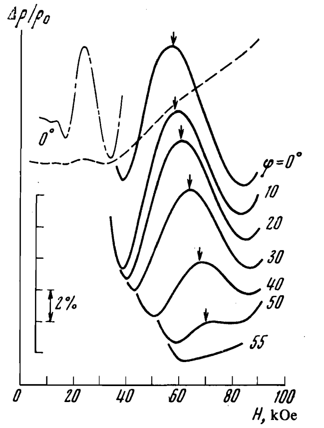

FIG. 1. Zeroth maximum of the Shubnikov-de Haas oscillations in a sample with $p = 1.4 \times 10^{17}$ cm^{-3} obtained for different angles $\varphi(H, C_3)$. The upper part of the figure shows the complete uncompensated magnetoresistance curve (dashed) and its amplified initial region (chain) for $\varphi = 0°$ ($H \parallel C_3$). The position of the zeroth maximum is identified by arrows.

coefficients of the parameters of the band structure were determined. According to this model, the value of ξ at $P_0 = 14$ kbar becomes equal to unity and it then follows from Eqs. (2) and (3) that k_{zm} and $\Delta\epsilon$ vanish so that the saddle point disappears in the energy spectrum, i.e., we now have the second case and the band is nearly parabolic.

An estimate of G_m obtained by the k · p approach[2] gives:

$$G_m \approx (m_0/m_\perp)\sqrt{1-\xi^2}. \tag{4}$$

Consequently, at 14 kbar, when $\xi = 1$, the G factor should vanish and all the manifestations of the splitting in the Shubnikov-de Haas effect should disappear.

In view of this, it would be interesting to investigate in greater detail than in[2] the influence of pressure on the behavior of the zeroth maximum of the Shubnikov-de Haas oscillations in tellurium.

EXPERIMENTAL RESULTS

We studied five tellurium single crystals with hole densities $p = 2 \times 10^{16} - 3 \times 10^{17}$ cm^{-3} by applying pressures up to 15 kbar at 1.5°K in magnetic fields up to 120 kOe. The hole densities in samples 1–5 were 2.0, 2.4, 4.2, 6.5, and 30×10^{16} cm^{-3}, respectively. All the measurements were carried out in a magnetic field $H \parallel C_3$. The method used in the investigation of the Shubnikov-de Haas oscillations under pressure was described earlier (see[7]).

Figures 2 and 3 show the influence of pressure on Shubnikov-de Haas oscillations in two samples: No 1 with $p = 2 \times 10^{16}$ cm^{-3} and No. 5 with $p = 3 \times 10^{17}$ cm^{-3}. Parts of the oscillation curves shown in Figs. 2 and 3 were obtained, as usual, by compensating the monotonic component of the magnetoresistance and amplifying the oscillatory component. Only one maximum with the quantum number N = 1 could be distinguished for sample No. 1 at P = 0 kbar (Fig. 2a); the zeroth maximum was not observed. At the highest pressure P = 15 kbar (Fig. 2b) the oscillation maxima with N = 0, 1, and 2 were observed clearly and the zeroth maximum was considerably stronger than the first maximum.

The oscillation pattern obtained for sample No. 5 at P = 0 kbar (Fig. 3a) represented the well-known[1,7] beats of two components corresponding to the maximum

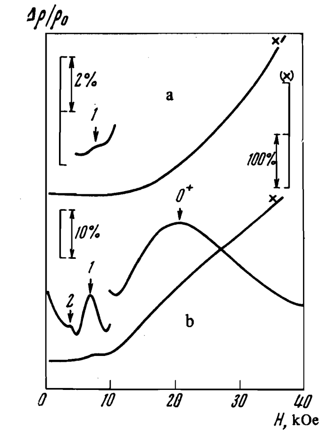

FIG. 2

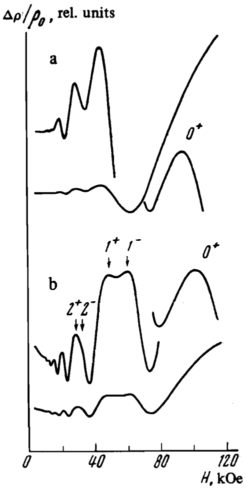

FIG. 3

FIG. 2. Shubnikov-de Haas oscillations in sample No. 1 ($p = 2 \times 10^{16}$ cm^{-3}): a—P = 0 kbar; b—P = 15 kbar. The scale on the right applies to the uncompensated curves identified by crosses.

FIG. 3. Shubnikov-de Haas oscillations in sample No. 5 ($p = 3 \times 10^{17}$ cm^{-3}): a—P = 0 kbar; b—P = 11.1 kbar.

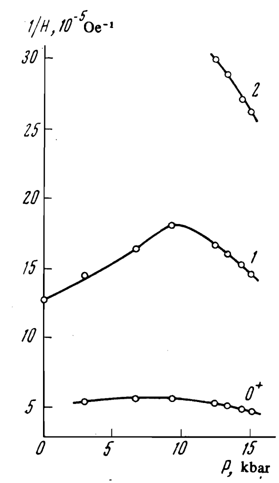

FIG. 4. Pressure dependences of the Shubnikov-de Haas oscillation maxima of sample No. 1 ($p = 2 \times 10^{16}$ cm^{-3}). Here, 0⁺, 1, and 2 are the numbers of the oscillation maxima.

and minimum (central) sections of the dumbbell-shaped Fermi surface. Moreover, in fields of about 100 kOe we observed a fairly strong zeroth maximum (the quantum numbers were identified by expanding the beats into components, as described in[1]).

At P = 11 kbar (Fig. 3b) the oscillations became nearly single-periodic and we observed not only the zeroth maximum but also the splitting of the first maximum. The second maximum was not split but became considerably flattened near the peak. Unfortunately, we were unable to determine accurately the position and amplitude of the zeroth maximum for this sample because fields up to 20 kOe, used in the present study, were insufficient to observe the last minimum.

The positions of the oscillation maxima on the reciprocal magnetic field scale are plotted for different pressures in Fig. 4 (sample No. 1). When the pressure was increased, all the maxima shifted toward weaker fields and then they began to shift back to stronger magnetic fields.

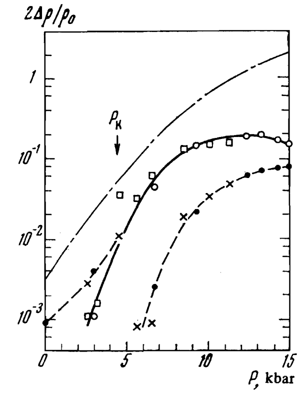

FIG. 5. Pressure dependences of doubled amplitude of the Shubnikov-de Haas oscillations in samples Nos. 1 and 2: O), □) zeroth maximum for samples Nos. 1 and 2; ●), X) first maximum for samples 1 and 2. The chain curve represents the calculated amplitude of the zeroth maximum and P_k is the point of merging of ellipsoidal Fermi surfaces.

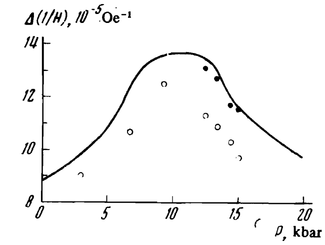

FIG. 6. Influence of pressure on the oscillation period governed by the noncentral extremal section of the Fermi surface of sample No. 1 ($p = 2 \times 10^{16}$ cm^{-3}) subjected to $\mathbf{H} \parallel \mathbf{C}_3$: O) periods deduced from the zeroth and first maxima; ●) periods deduced from the first and second maxima. The continuous curve represents calculations.

The amplitude of the zeroth maximum of the lightly doped samples increased by more than two orders of magnitude in the pressure range up to 15 kbar (Fig. 5). The amplitude of the first maximum also increased. A singularity in the 4–6 kbar range (Fig. 5) arose because at these pressures and hole densities the topology of the Fermi surface changed[7] as a result of merging of two ellipsoidal surfaces into one dumbbell-shaped surface. This gave rise to beats in the Shubnikov-de Haas oscillations (the calculated pressure at which this merging of the Fermi surfaces occurred is identified by an arrow and P_k in Fig. 5).

DISCUSSION OF RESULTS

In the analysis of the results obtained we shall concentrate our attention on sample No. 1 investigated over a wider range of pressures (up to 15 kbar) than other samples, including those investigated earlier.[7]

Figure 6 shows the data on the period of the oscillations observed in this sample in the pressure range $P > 12$ kbar. The oscillation period is defined as $\Delta(1/H)_{12} = 1/H_2 - 1/H_1$, where H_1 and H_2 are the positions of the magnetoresistance oscillations with quantum numbers 1 and 2. It is known that this estimate of the period for ellipsoidal Fermi surfaces may be in error by about 2% because of the dependence of the position of the Fermi level on the magnetic field. The same figure includes the pressure dependence of the quantity $\Delta(1/H)_{01} = 1/H_1 - 1/H_0$ (H_0 is the position of the maximum which should be attributed to $N = 0$). The value of $\Delta(1/H)_{01}$ is less than $\Delta(1/H)_{12}$. This means that the zeroth maximum is located in weaker fields than the fields corresponding to the point of intersection of the Fermi level with the zeroth Landau level although the influence of the magnetic field on the Fermi level should shift the maxima with small quantum numbers in the direction of stronger fields. All these observations demonstrate that we are indeed dealing with the split-off 0^+ Landau sublevel.

The continuous curve in Fig. 6 represent the pressure dependence of the period of the oscillations which result from the quantization of the maximum section of the Fermi surface in $\mathbf{H} \to \mathbf{C}_3$ (this curve is calculated for the hole density in sample No. 1 using a linear model which describes well our earlier experimental data obtained up to 12 kbar[7]). We can see that in the present case the calculated curve fits quite well the experimental dependence up to 15 kbar. This is very remarkable if we bear in mind that in the model suggested in[7] the pressure coefficient of the effective mass $m_\perp$ has been estimated from the data given in[8] on the influence of pressure on the forbidden band width ϵ_g, which demonstrates that

$$\frac{1}{\varepsilon_{g0}}\frac{\partial \varepsilon_g}{\partial P} = -6 \cdot 10^{-2}\ \text{kbar}^{-1}$$

i.e., the value of ϵ_g extrapolated linearly vanishes at a pressure $P = 16.6$ kbar.

For the other samples used in the present study, the agreement with the theoretical model is just as good as in[7]. In particular, the results for sample No. 5 are compared with the calculations in Fig. 9 in[7].

The considerable rise of the zeroth maximum under pressure (Fig. 5) can be explained by a significant reduction in the broadening of the Landau levels as a result of the scattering of holes. This broadening is characterized by the Dingle temperature $T_b \sim \Gamma/\pi k$, where the width of the level is $\Gamma \sim \hbar/\tau$ and τ is the lifetime of carriers in the oscillatory states, which is of the order of the relaxation time in the expression for the electrical conductivity. Although in some cases the characteristic time τ which determines the Dingle temperature may differ considerably from the conductivity relaxation time, it has been demonstrated experimentally that for a large number of semiconductors, including tellurium,[9] these two quantities differ by not more than a factor of 1.5–2. Therefore, in order to estimate the pressure dependence of the oscillation amplitude we shall use the relaxation time $\tau_0 = m_\perp/e^2 p\rho_0$, where ρ_0 is the electrical resistivity in the absence of a magnetic field. We shall estimate the resistivity from the formula

$$\rho_\perp = \rho_0 \left\{ 1 + \frac{5}{2} \sum_{r=1}^{\infty} \frac{(-1)^r}{r^{1/2}} \left(\frac{\hbar\Omega}{2\varepsilon_F}\right)^{1/2} \frac{2\pi^2 rkT/\hbar\Omega}{\operatorname{sh}(2\pi^2 rkT/\hbar\Omega)} \times \cos(\pi\nu r) \exp\left(-\frac{2\pi\Gamma r}{\hbar\Omega}\right) \cos\left(\frac{2\pi\varepsilon_F r}{\hbar\Omega} - \frac{\pi}{4}\right) \right\}, \tag{5}$$

given in the review[10], where $\rho_\perp$ is the resistivity in a transverse magnetic field, ϵ_F is the Fermi energy, $\nu = (\frac{1}{2}) G_m m_0/m_\perp$ is the phase factor associated with the splitting of the Landau level. In the case of oscillations with a rapidly damped amplitude we need consider only the harmonic with $r = 1$.

For our samples the value of ρ_0 decreases approximately by a factor of 8 when the pressure is raised to

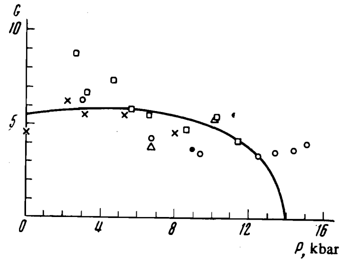

FIG. 7. The pressure dependence of the G factor: O) sample No. 1; □) No. 2; X) No. 3; Δ) No. 4; ●) No. 5; the continuous curve represents calculations based on Eq. (4).

15 kbar but the hole density p remains practically constant (compare Figs. 1 and 2 in[7]). This reduction is primarily due to an increase in the relaxation time. This pressure dependence of the relaxation time and, consequently of the Landau level broadening, ensures because of the exponential dependence of the amplitude of Γ, an increase in the amplitude of the zeroth maximum by more than two orders of magnitude, which is in agreement with the experimental resutls. The other factors in Eq. (5) are of the order of unity and vary weakly with pressure. In calculations of these factors we shall use the pressure coefficients given in[7]. The results of our calculation of the amplitude of the zeroth maximum of sample No. 1 is represented by the chain curve in Fig. 5

Thus, a considerable proportion of the experimental results obtained in the present study is explained satisfactorily by the linear model of the influence of pressure on the valence band of tellurium, suggested by us in[7]. However, contrary to this model, the zeroth maximum does not disappear on approach to $P_0 = 14$ kbar. The results presented in Fig. 5 demonstrate that the amplitude of the zeroth maximum reaches saturation close to 14 kbar and although it may begin to decrease, it certainly does not vanish.

Figure 7 gives the values of the G factor at different pressures deduced from the position of the zeroth maximum of samples Nos. 1–4 and from the splitting of the first maximum of sample No. 5 at pressures of 8, 9, and 11 kbar. The continuous curve in Fig. 7 represents the dependence $G_m(P)$ calculated using Eq. (4) and the pressure coefficients given in[7]. Thus, contrary to the model given in[7], the zeroth maximum does not disappear and the G factor does not vanish at $P_0 = 14$ kbar.

Apart from the terms included in the derivation of Eq. (1), the matrix Hamiltonian[1] does not include terms which could give rise to the splitting of the Landau levels for $k \neq 0$. Consequently, the existence of the zeroth maximum at $P \geq 14$ kbar can be explained only if we assume that throughout the investigated range of pressures the saddle point in the spectrum and the central minimal section of the Fermi surface are retained in spite of the fact that the oscillations are no longer observed.

The pressure $P_0 = 14$ kbar is suggested in[7] because at this pressure the experimental results agree best with the calculations throughout the investigated range of hole densities $3 \times 10^{16} - 1.3 \times 10^{18}$ cm^{-3} (see also Fig. 6 in the present paper) and, moreover, at pressures up to 12 kbar used in[7] the zeroth maximum is retained for $H \parallel C_3$. It is possible that the saddle point disappears at higher pressures (17–18 kbar), which are within the limits of the error (~30%) in the calculation of P_0 mentioned in[7]. An increase in P_0 by 2–3 kbar has no significant influence on the agreement between the experimental results given in[7] and the corresponding calculations. However, it is most likely that pressures $P \geq 14$ kbar are outside the range of validity of the linear model,[7] particularly in view of what we have said about the pressure dependence of ϵ_g.

The results reported in[2] and in the present paper demonstrate that the interpretation of the observed effects on the basis of the splitting of the Landau levels as a result of the absence of the inversion center is most appropriate in the case of tellurium. This is supported by the angular dependences of the position and amplitude of the zeroth maximum[2] (see also Fig. 1) and the observed splitting of the first and second maxima of the Shubnikov-de Haas oscillations. The existence of the zeroth maximum cannot be explained by the transfer of carriers from the zeroth Landau level to an impurity level because, in this case, the zeroth maximum would have existed for all angles between H and C_3, which is in conflict with the results reported in[2].

There is no doubt that the extension of the pressure range to $P > 20$ kbar will enable us to determine more reliably the nature of the observed effect.

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157