Magnetic Susceptibility of Holes in Tellurium

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A calculation is carried out of the Landau contributions to inter-band interactions and magnetic susceptibility anisotropy of holes in tellurium. The experimental results obtained for hole concentrations $4 \cdot 10^{14} \leq n \leq 4 \cdot 10^{18}$ cm^{-3} qualitatively agree with the calculation and confirm the conclusions of the general theory of orbital magnetism. The most probable cause of quantitative discrepancy between the theory and experiments is the paramagnetic contribution related to inversion asymmetry of tellurium.

IT has been established by now[1] that the valence band of tellurium has a vertex on the side edge of the Brillouin zone, near the ALM plane, and is split on it by an energy gap 2Δ. The dispersion law for the holes is given in first approximation by

$$E(\mathbf{k}) = Ak_{\parallel}^2 + Bk_{\perp}^2 \pm \sqrt{\Delta^2 + C^2k_{\parallel}^2}, \qquad (1)$$

where

$$A = 3.63 \cdot 10^{-15}\ \text{eV-cm}^2,\ B = 3.26 \cdot 10^{-15}\ \text{eV-cm}^2,$$
$$\Delta^2 = 3.99 \cdot 10^{-3}\ \text{eV}^2,\ C^2 = 6.00 \cdot 10^{-16}\ \text{eV-cm}^2. \qquad (2)$$

Energies are considered positive if they lie below the center of the gap at the point M, from which the components of the wave vector are reckoned (the subscript $\parallel$ corresponds to the direction of the threefold axis).

It has turned out that the use of a model Hamiltonian for the spectrum (1) makes it possible to simplify the cumbersome general orbital-magnetism formula[2,3] to a relatively simple expression for the diamagnetism in terms of arbitrary values of the parameters (2).[4] The result obtained by Ruvalds[4] predicts a considerable role of interband contributions and unique singularities of the susceptibility near the critical points of the spectrum. In the valence band of tellurium, the spin degeneracy is completely lifted, so that tellurium might seem to afford a unique possibility of quantitatively verifying the theory of orbital magnetism. Unfortunately, owing to the absence of an inversion center, there is nevertheless a spin contribution to the hole susceptibility,[5] but no formulas describing this contribution have been derived as yet. The purpose of the present paper is to ascertain the degree of agreement between theory and experiment, so as to permit assessment of the roles of the individual contributions to the magnetism and of the possibility of refining the parameters of the band structure with the aid of the susceptibility. To this end, we investigated experimentally and theoretically the magnetic susceptibility of the anisotropy of the holes as a function of their density.

EXPERIMENTAL RESULTS

The use of the susceptibility anisotropy $\Delta\chi = \chi_{\parallel} - \chi_{\perp}$ has made it possible to separate and investigate the small increment due to the susceptibility of the holes against the background of the overwhelming isotropy part of the lattice contribution. The anisotropy was measured in the temperature interval 4.2–300°K by an automatic torsion balance with relative error ±1%. The hole density in the single-crystal tellurium samples was varied in the range $4 \times 10^{14} < n < 4 \times 10^{18}$ cm^{-3} by doping with antimony. Information on the magnetic susceptibility of pure tellurium at T = 293°K is given in the table, together with data obtained by others. The absolute value of $\chi_{\parallel}$ was measured by the Faraday method. We note that the earlier data[6-8] do not yield any information, suitable for quantitative comparison with the theory, concerning the susceptibility of the holes.

$\chi_{\parallel}^{sp} \cdot 10^7$	$\Delta\chi^{sp} \cdot 10^9$	Source
3.00	—	[8]
3.01	7.17	[9]
3.1±0.1	7.00±0.1	Present study

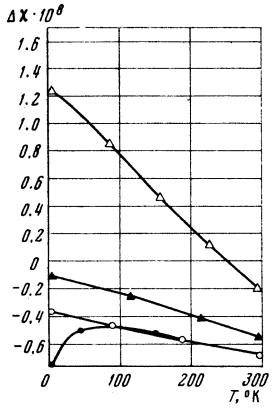

FIG. 1. Temperature dependences of the anisotropy of the specific magnetic susceptibility for samples of pure and doped tellurium. The points label curves with different values of n: ●–n = 4 × 10^4 cm^{-3}, ○–n = 9.3 × 16 cm^3, Δ–n = 7.3 × 10^{17} cm^{-3}, Δ–n = 2 × 10^{18}cm^{-3}.

As seen from Fig. 1, which shows the temperature dependences of $\Delta\chi$ for several samples, the anisotropy of the susceptibility of pure tellurium, for which the contribution of the free carriers is negligibly small, varies with the temperature. The anisotropy of the susceptibility of doped samples tends asymptotically to the anisotropy of pure tellurium with increasing temperature, when the susceptibility of the free carriers should vanish[9] (in the absence of generation processes). This means that the susceptibility of tellurium contains an anisotropic lattice contribution that is affected little by doping. Its detailed nature is of no importance to us now, and to obtain the hole contribution $\Delta\chi^h$ the lattice contribution should be eliminated from the susceptibil-

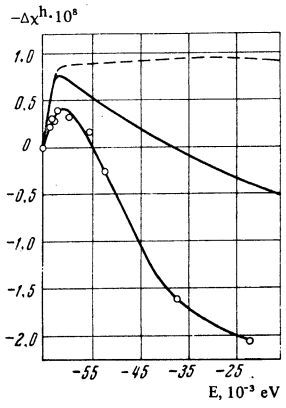

FIG. 2. Dependence of the anisotropy of the specific magnetic susceptibility on the level of the chemical potential at T = 4.2°K. The dashed curve is the anisotropy of the Landau-Peierls contribution, and the solid curve is the total diamagnetism anisotropy, while the curve with the points is a plot of the experimental data.

ity anisotropy of the doped sample and regarded as an additive increment: $\Delta\chi^h = \Delta\chi^{dop} - \Delta\chi^{Te}$. This is precisely how the points on the experimental curve of Fig. 2 were obtained at T = 4.2°K.

THEORY AND COMPARISON WITH EXPERIMENT

To calculate the anisotropy it is necessary to know both susceptibility components. One of them ($\chi_\perp$ in our notation) was obtained earlier by Ruvalds.[4] We have recalculated $\chi_\perp$ by an analogous method in a more compact form and obtained an expression for $\chi_\parallel$. In the limit T = 0, these expressions are given by

$$\chi_\perp^{L\text{-}P}(\pm) = -\frac{\Gamma}{8} y\left[1 \pm (y^2+\lambda^2)^{-1/2}\right] \Big|_{\eta_1(\pm)}^{\eta_2(\pm)},$$

$$\chi_\parallel^{L\text{-}P}(\pm) = -\frac{\Gamma B}{8A} y \Big|_{\eta_1(\pm)}^{\eta_2(\pm)},$$

$$\chi_\perp^{ind}(\pm) = \mp\frac{3\Gamma\lambda^2}{64}\left\{\ln\left[y+\sqrt{y^2+\lambda^2}\right] - \frac{(\varepsilon+\lambda^2)^2 y^3}{3\lambda^4(\lambda^2+y^2)^{3/2}} + \frac{(\varepsilon^2-\lambda^4-4\lambda^2)}{\lambda^4(y^2+\lambda^2)^{1/2}} y\right\}\Big|_{\eta_1(\pm)}^{\eta_2(\pm)} \quad (3)$$

$$\chi_\parallel^{ind}(\pm) = 0$$

Here $\chi^{L\text{-}P}(\pm)$ is the Landau-Peierls contribution; $\chi^{ind}(\pm)$ is the interband contribution,[10] called induced diamagnetism in [3]. The signs (±) pertains to bands whose tops are located at positive and negative energies, respectively;

$$\varepsilon = \frac{4A}{C^2}E, \quad \gamma = \frac{4A}{C^2}\Delta, \quad \lambda = \frac{\gamma}{2}, \quad \Gamma = \frac{2e^2C}{3\pi^2\hbar^2c^2};$$

y is the integration variable and the integration limits are indicated on the right, viz.,

$$\eta_2(+) = [\varepsilon+2-2(\varepsilon+1+\lambda^2)^{1/2}]^{1/2} \quad \text{for } \varepsilon > \gamma,$$
$$\eta_1(+) = 0;$$
$$\eta_2(-) = [\varepsilon+2+2(\varepsilon+1+\lambda^2)^{1/2}]^{1/2} \quad \text{for all } \varepsilon,$$
$$\eta_1(-) = 0 \quad \text{for } \varepsilon > -\gamma,$$
$$\eta_1(-) \simeq [\varepsilon+2-2(\varepsilon+1+\lambda^2)^{1/2}]^{1/2} \quad \text{for } \varepsilon < -\gamma.$$

The result is independent of the sign chosen for the energy scale, i.e., it is the same for hole and electron bands.

At arbitrary temperatures, it is impossible to obtain an analytic expression for the susceptibility, and its anisotropy for the parameters (2) and for the temperature T = 4.2°K was calculated with a computer. The results of the calculation are shown in Fig. 2 as functions of the chemical-potential level E at T = 0°K. They differ from (3) only in that the anisotropy peak is smoothed out at the critical point E = − Δ. The dashed curve demonstrates the anisotropy of the Landau-Peierls contribution, and the solid curve the total diamagnetism anisotropy.

A comparison of the theoretical and experimental curves (Fig. 2) leads to the following conclusions:

1. The theory of orbital magnetism is in qualitative agreement with experiment; an important role is played in this case by an allowance for the interband contribution.

2. The anisotropy peak on the experimental curve is connected with the critical point in the spectrum of tellurium, and its position corresponds fully to the assumed parameters (2).

3. A considerable discrepancy between theory and experiment is observed in the entire energy interval and, as discussed above, cannot be attributed to the influence of impurities.

4. Variation of the parameters of the tellurium spectrum (2) within the limits of the errors with which the effective masses have been determined in [11-12] does not eliminate the discrepancy with experiment, although it does point to a high sensitivity of the susceptibility to the values of these parameters. The deviation of the true spectrum from (1) under the influence of other levels is also small at the energies under consideration,[1] and can likewise not cause the discrepancies.

The most probable source of the discrepancies is the paramagnetic contribution due to the inversion asymmetry of tellurium.[5] This contribution turns out to be quite large and if formulas for its description become available, it will probably make it possible to calculate with sufficient accuracy the spin-splitting parameters. So long as no such formulas exist, the question of exact quantitative correspondence between theory and experiment for the orbital magnetism of tellurium remains open. There is no doubt, however, that the magnetic susceptibility will become a source of reliable quantitative information on complicated electronic spectra, and can even now be used successfully to observe and identify critical points in the spectra of metals,[13] semimetals,[14] and semiconductors.

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