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Spin-Orbit Interaction and the Effective Masses of Holes in Germanium*

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We reported[1] earlier the observation of cyclotron resonance of electrons and holes in germanium crystals; in particular, we reported the observation of two approximately isotropic effective masses for holes, $m^*/m=0.04$ and 0.3. The association of these masses with the motion of holes has been confirmed by experiments at K band with circularly polarized radiation, which also reveal a structure to the $m^*=0.3m$ resonance. These experiments, which will be published shortly, determine the sign of the charge carrier. The questions which arise are: (1) Why are there two masses? (2) Why can the masses be resolved, in view of the warped nature of energy surfaces[2] near degenerate points? (3) Why are the masses so light? We consider these questions below.

(1) Herman and Callaway[3] have carried out calculations suggesting that the top of the valence band in germanium occurs at the center of the Brillouin zone and is threefold degenerate, corresponding to p bonding orbitals on the Ge atoms. We suggest that spin-orbit interaction[4] is responsible for the observation of essentially two, rather than three, masses. The top of the valence band has point group symmetry properties related to atomic $p_{\frac{3}{2}}$ states and is quadruply degenerate, but in crystals with a center of symmetry the contact is that of two double-degenerate bands. There is therefore a possibility of two different masses. The band arising from atomic $p_{\frac{1}{2}}$ states is lower (for holes) by perhaps 500 to 2000 cm^{-1}, as estimated from atomic spectra and by a suggested interpretation of the infrared absorption[5] of $p-$Ge.

(2) We have carried out for this proposed level scheme a general second-order perturbation determination of the energy surfaces near $\mathbf{k}=0$, following the method of Shockley.[2] The calculation hinges largely on symmetry properties of the bands and is *not* based on a strong-binding model. The perturbation is

$$H'=\hbar\mathbf{k}\cdot[(\mathbf{p}/m)+\zeta(\mathbf{S}\times\mathbf{r}], \qquad (1)$$

where the spin-orbit term is not important; its inclusion however does not alter the general form of the result. Here $\mathbf{k}$ is the wave vector and $\mathbf{p}$ the momentum operator. We paid special attention to tracing the origin of spherical and nonspherical (warping) contributions to the energy surface. The symmetry properties and representations of the bands as given by Elliott are useful in this connection. The most general form of the energy to second order may be written as

$$E(k)=Ak^2\pm[B^2k^4+C^2(k_x^2k_y^2+k_y^2k_z^2+k_z^2k_x^2)]^{\frac{1}{2}}, \qquad (2)$$

where A, B, C, are constants derived from the matrix elements of H' connecting the valence band edge (representation Γ_{8g}) with other states. It turns out that the principal nonspherical perturbation (which enters through C) arises from the perturbation by a state with antibonding s character (Γ_{7u}) which is separated[3] from Γ_{8g} by some 6 ev. The spherical perturbations A, B arise principally from the antibonding $p_{\frac{1}{2}}$ and $p_{\frac{3}{2}}$ states (Γ_{6u},Γ_{8u}) which are separated from Γ_{8g} by 0.7–0.8 ev. The perturbations involve the usual energy denominator, so that the spherical terms could be larger than the nonspherical, but other arguments suggest that the differences may not be great.

Nonspherical energy surfaces give cyclotron resonance if the tube mass[6] on a plane in $\mathbf{k}$ space perpendicular to the magnetic field is independent of the energy. Otherwise, an accelerated electron will enter a tube of different period, and the phase will be destroyed. With the nonspherical term, it is possible to define for certain field directions two sets of tubes for which cyclotron resonance is possible. With the field parallel to the [100] axis, and $C^2\ll 4B^2$, the two resonances on a single energy surface are separated by

$$\Delta\omega\cong\omega_0\frac{C^2}{16B}\left(\frac{2m}{\hbar^2}\right)\frac{m^*}{m}, \qquad (3)$$

to first order. For strong warping only one of the lines will be strong.

Our preliminary measurements with H in the [100] direction indicate that there are actually two peaks near $m^*/m=0.3$, with a separation $\Delta\omega/\omega_0\approx 0.2$, which leads to the rough estimate $B^2/C^2\approx 1$. For the $0.04m$ effective mass we would then estimate $\Delta\omega/\omega_0\approx 0.03$, which cannot be resolved at present. The $0.3m$ structure should be somewhat anisotropic.

(3) The spherical terms in the energy are quite large, as the perturbing levels are unusually close. It is quite reasonable that the masses should be light: the coefficients A, B will be $\gg\hbar^2/2m$.

It appears that it is possible to account for the features of the hole resonances, as observed up to the present. The effect of spin-orbit interaction on the electron cyclotron resonance is to lift the degeneracy of the antibonding p band so that the $p_{\frac{1}{2}}$ band is lowest. The ellipsoid model proposed for $n-$Ge by Meiboom and

Abeles[7] and Lax and co-workers[8] probably would not work unless the degeneracy, in this case along $\langle 111\rangle$ axes, where lifted by the spin-orbit interaction.

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Nuclear Spin and Hyperfine Structure Interaction of the 3.1-hr Cs^{134} Isomer*

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We have performed an atomic beam magnetic resonance[1] experiment on the 3.1-hr isomer of Cs^{134}. The results of this experiment indicate that $I=8$ in units of $\hbar$, and $\Delta\nu=3675.6\pm0.6$ Mc/sec.

The apparatus is of the "flop-in" type in which one observed those atoms which have undergone the transition in the homogeneous magnetic field for which $[I+\frac{1}{2}, -(I+\frac{1}{2})]\rightleftarrows[I+\frac{1}{2}, -(I-\frac{1}{2})]$. At very weak magnetic fields this transition frequency is linear in H and is independent of $\Delta\nu$, depending only upon I. At intermediate fields the dependence upon $\Delta\nu$ becomes significant and is given accurately by the modified Breit-Rabi[1] expression permitting one to calculate $\Delta\nu$.

The Cs^{134m} for each run was prepared by irradiating approximately 100 mg of CsCl in the Brookhaven reactor for about 9 hours. It was then placed in a Monel oven with freshly cut chips of metallic barium. At about 450°C a strong steady beam of Cs atoms emerged from the oven. The focused atoms, selected by a 0.004-in. slit, are allowed to impinge for an arbitrary time interval upon a thin, flat tungsten target upon which they are adsorbed. The target could then be removed via an airlock and its activity measured with a proportional counter, thus giving a measure of the focused beam intensity for one set of magnetic field and frequency conditions. For deposition times of the order of five minutes counting rates of approximately 70 counts/min at the peak with a background of about 15 counts/min were obtained. The magnetic field was calibrated by observing the rf spectrum of Cs^{133} and using $\Delta\nu^{133}=9192.76$ Mc/sec as given by Kusch and Taub.[2]

TABLE I. Observed resonances.

Cs^{133} (Mc/sec)	Cs^{134m} (Mc/sec)
1.990	0.940
4.504	2.125
9.995	4.750
15.252	7.325
29.865	14.612
48.850	24.540
99.500	53.582±0.010
213.500	136.280±0.010

The frequencies at which Cs^{134m} resonances were observed are given in Table I along with the calibrating frequencies of Cs^{133}. The lower-frequency results serve to establish the spin. The constant $\Delta\nu^{134m}$ was calculated for the two highest field runs as given in the table. These combine to give a value of 3675.6±0.6 Mc/sec. Using the value[3] 0.731 for g_I of Cs^{133} and neglecting any hfs anomaly, we calculate the magnetic moment of Cs^{134m} to be $\mu=1.10\pm0.01$, with the sign undetermined.

The available proton-neutron configurations, agreeing with the measured spin, on the basis of the shell model[4] are $d_{5/2}$, $h_{11/2}$ and $g_{7/2}$, $h_{11/2}$. In the limit of a strict $J-J$ coupling two-particle wave function, the magnetic moments calculated for these two pure states are $+2.72$ nm and -0.35 nm, respectively. Thus it would appear that a mixed configuration, such as suggested by de-Shalit and Goldhaber,[5] is necessary to account for the magnitude of the observed moment. The proper admixture would then be 53 percent ($g_{7/2}$, $h_{11/2}$) and 47 percent ($d_{5/2}$, $h_{11/2}$) with the theory predicting a positive sign. In this connection it is interesting to note that no combination of "stripped"[6] moments for the proton and neutron, calculated from pure states, yields a magnetic moment in agreement with the observed value. Furthermore, if one analyzes the data of Bellamy and Smith[7] concerning the ground state of Cs^{134}, one finds that the above conclusion also holds here. Thus it would appear that the magnetic moments of Cs^{134} and Cs^{134m} make rather a strong case for the use of mixed configurations if one restricts the discussion to single proton-single neutron wave functions.

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