CYCLOTRON AND PARAMAGNETIC RESONANCE IN STRAINED CRYSTALS

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Recent studies on cyclotron and paramagnetic resonance in strained p-Si[1,2] have confirmed the earlier developed theory,[3,4] and have shown that investigations of this kind give important information concerning band structures and the nature of impurity centers. In connection with this, some new possibilities offered by measurements of the resonance effect in strained crystals are pointed out.

I. Measurements of the cyclotron resonance in strained Ge and Si make it possible to find not only the values of the constants A, B, and D determining the spectrum $E(\vec{k})$ in these crystals[5] but also the ratio of the deformation potential constants, b/d, which is very important for the theory of scattering.[6] Thus, according to reference 3, when the crystal is strained along [110], the inverse effective masses on the main axes, [110], $[1\bar{1}0]$, and [001], are equal to

$$A\pm\frac{D}{2}\,\frac{1+\gamma B/D}{(1+\gamma^2)^{1/2}},\quad A\mp\frac{D}{2}\,\frac{1-\gamma B/D}{(1+\gamma^2)^{1/2}},\quad A\mp\frac{B\gamma}{(1+\gamma^2)^{1/2}},\tag{1}$$

where

$$\gamma=\frac{2(b/d)c_{44}}{c_{11}-c_{12}}.$$

Here we assume that the upper choice of signs corresponds to $d\epsilon<0$ while the lower one corresponds to $d\epsilon>0$. The signs of the constants B and D cannot be determined by cyclotron resonance. Such experiments as well as measurements of the piezoresistance at high temperatures[7] allow us to determine only the signs of the products Bb and Dd. From the data[1] as well as from Smith's experiments[8] it is evident that for Si, $Bb>0$ and $Dd>0$.

II. The use of strained crystals with an InSb-type lattice makes it possible to obtain semiconductors with some special kind of spectrum when the surfaces of constant energy have toroidal shape and the extremum is in the ring. Taking into consideration terms linear[9] in $\vec{k}$ at low $\vec{k}$ for the lower band corresponding to the minimal energy of the holes, we obtain from the calculations

$$E(\vec{k})=E^0(\vec{k})\pm\frac{K}{(\mathcal{E}_\epsilon)^{1/2}}\Big(\sum_{i,j}\alpha_{ij}k_ik_j\Big)^{1/2}.\tag{2}$$

Here $E^0(\vec{k})$ has significance for the strained p-Ge corresponding to that determined by Eq. (18) of reference 3, K is Kane's constant,[9] $\mathcal{E}_\epsilon$ is determined by Eq. (16) of reference 3, and

$$\alpha_{xx}=3b^2(\epsilon_{yy}-\epsilon_{zz})^2+4d^2(\epsilon_{xy}{}^2+\epsilon_{xz}{}^2),$$

$$\alpha_{xy}=-2\sqrt{3}(\mathcal{E}_\epsilon)^{1/2}d\epsilon_{xy}+2d^2\epsilon_{xz}\epsilon_{yz},\ \text{etc.}$$

This formula is just for the strains when the band splitting, which is equal to $2(\mathcal{E}_\epsilon)^{1/2}$, exceeds kT and the difference $E(0)-E(k)_{\min}$, i.e., under conditions similar to those attained during the above-mentioned experiments.[1]

Toroidal surfaces occur, in particular, in the strains on the axes [001] and [111]: When $b\epsilon>0$,

$$E(\vec{k})=(A+\tfrac{1}{2}B)(k_\perp\pm k_{\perp 0})^2+(A-B)k_z{}^2;\tag{3}$$

when $b\epsilon<0$,

$$E(\vec{k})=(A-\tfrac{1}{2}B)(k_\perp\pm k_{\perp 0})^2+(A+B)k_z{}^2;\tag{4}$$

where

$$k_\perp{}^2=k_x{}^2+k_y{}^2,\quad k_{\perp 0}=\frac{\sqrt{3}}{2}\,\frac{|K|}{A\pm\frac{1}{2}B}.$$

Correspondingly, when $d\epsilon>0$,

$$E(\vec{k})=\left(A+\frac{D}{2\sqrt{3}}\right)(k_\perp\pm k_{\perp 0})^2+\left(A-\frac{D}{\sqrt{3}}\right)k_z{}^2,\tag{5}$$

where

$$k_{\perp 0}=\frac{|K|}{A+D/2\sqrt{3}}.$$

On the contrary, when $d\epsilon<0$,

$$E(\vec{k})=\left(A-\frac{D}{2\sqrt{3}}\right)k_\perp{}^2+\left(A+\frac{D}{\sqrt{3}}\right)(k_z\pm k_{z0})^2,$$

where

$$k_{z0}=\frac{\sqrt{2}\,|K|}{A+D/\sqrt{3}}.$$

The properties of semiconductors with toroidal energy surfaces have been studied in detail by Rashba et al.[10] Of great interest is the investigation of the cyclotron resonance and the combined resonance predicted by Rashba in these semiconductors.

III. In strained crystals p-Ge and p-Si it seems possible to observe a spin resonance of free carriers. In these nonstrained crystals such a resonance cannot be seen, because as a result of the large spin-orbit interaction an effective magnetic moment of the hole depends on its impulse direction. Therefore, instead of a resonance line, a broad resonance spectrum would result.

In strained crystals all the holes with low $\vec{k}$ possess the same effective magnetic moment depending on the strain direction, and their resonance frequency is determined by

$$(\hbar\omega_p)^2 = (\mu_0{}^2\mathcal{K}^2/\mathcal{E}_\epsilon)\langle\vec{H},\vec{H}\rangle, \tag{6}$$

where

$$\langle\vec{A},\vec{B}\rangle = \sum\beta_{ij}A_iB_j, \tag{7}$$

$$\beta_{xx} = [(\mathcal{E}_\epsilon)^{1/2} + b(\Delta - 3\epsilon_{xx})]^2 + 3d^2(\epsilon_{xy}{}^2 + \epsilon_{xz}{}^2),$$

$$\beta_{xy} = \sqrt{3}\,d\{\sqrt{3}\,d\epsilon_{xz}\epsilon_{yz} - \epsilon_{xy}[2(\mathcal{E}_\epsilon)^{1/2} - b(\Delta - 3\epsilon_{zz})]\}, \text{ etc.,}$$

where $\Delta = \epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}$ and $\mathcal{K}$ is Luttinger's constant.[11] In the case of strain along [001] and [111],

$$(\hbar\omega_p)^2 = \mu_0{}^2\mathcal{K}^2(g_\parallel{}^2H_z{}^2 + g_\perp{}^2H_\perp{}^2), \tag{8}$$

where $g_\parallel{}^2 = (1 \mp 2)^2$, $g_\perp{}^2 = (1 \pm 1)^2$, $H_\perp{}^2 = H_x{}^2 + H_y{}^2$, and μ_0 is the Bohr magneton. Here the upper sign corresponds to $b\epsilon > 0$ and $d\epsilon > 0$ while the lower one corresponds to $b\epsilon < 0$ and $d\epsilon < 0$.

The matrix element determining the probability of the transition under the influence of an alternating magnetic field h is equal to

$$|W_{12}|^2 = \frac{\mathcal{K}^2\mu_0{}^2}{\mathcal{E}_\epsilon}\,\frac{\langle\vec{H},\vec{H}\rangle\langle\vec{h},\vec{h}\rangle - \langle\vec{H},\vec{h}\rangle^2}{\langle\vec{H},\vec{H}\rangle}, \tag{9}$$

where $\langle\vec{A},\vec{B}\rangle$ may be determined according to (7). For the indicated directions [001] and [111], when $b\epsilon > 0$ or $d\epsilon > 0$,

$$|W_{12}|^2 = \mathcal{K}^2\mu_0{}^2\,\frac{[\vec{h}\vec{H}]^2 + 3[\vec{h}\vec{H}]_z{}^2}{H^2 + 3H_\perp{}^2}; \tag{10}$$

when $b\epsilon < 0$ or $d\epsilon < 0$, $W_{12} = 0$.

Significant changes in the resonance frequency of the hole of the acceptor center occur when the splitting of the ground fourfold-degenerate state[12] due to the strain exceeds the term splitting in the magnetic field. However, in the case of strains obtained in practice,[2] a main contribution to the ψ function of the impurity center comes from states with large k for which Eq. (6) does not apply. That is why the resonance frequency of the bound hole depends not only on the constants b and d but also on the ψ function.[2] Therefore it is not to be believed, as is accepted in Kleiner and Roth,[13] that the term splitting is equal to the splitting of the valence bands at $k = 0$, for the term splitting also depends on the change of the corresponding effective masses.

Only in cases when the strain is so large that the main contribution to the ψ function comes from states of low k, i.e., when the band splitting $2(\mathcal{E}_\epsilon)^{1/2}$ exceeds the activation energy of the impurity center E_i, will the resonance frequency be the same as for free holes. Therefore, in the case of lower strains this frequency must depend notably on the strain value according to

$$\Delta_p/\omega_p \simeq 2(\mathcal{E}_\epsilon)^{1/2}/E_i. \tag{11}$$

In the above-mentioned experiments[2] $\Delta g_\perp/\epsilon g_\perp = 30$ which, according to (11), gives for the constant b a value about 0.5 ev.

We have no grounds to believe that in this instance the ratio $g_\parallel/g_\perp$ undergoes considerable changes for the bound states when compared with the free ones. Therefore, comparing the results of the experiments[2] with Eq. (8), the conclusion may probably be drawn that in Si both constants b and d are negative; hence B and D are also negative, which corresponds to the theoretical estimate.[5]

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[1] J. C. Hensel and G. Feher, Phys. Rev. Letters 5, 307 (1960).

[2] G. Feher, J. C. Hensel, and E. A. Gere, Phys. Rev. Letters 5, 309 (1960).

[3] G. E. Pikus and G. L. Bir, Fiz. Tverd. Tela 1, 139, 1642 (1959)[translations: Soviet Phys.–Solid State 1, 136, 1502 (1959)].

[4] G. E. Pikus and G. L. Bir, report at the International Semiconductor Conference, Prague, August, 1960 (unpublished).

[5] G. Dresselhaus, A. F. Kip, and C. Kittel, Phys. Rev. 981, 368 (1955).

[6] G. L. Bir and G. E. Pikus, Fiz. Tverd. Tela 2, 2287 (1960).

[7] G. E. Pikus and G. L. Bir, Fiz. Tverd. Tela 1, 1828 (1959)[translation: Soviet Phys.–Solid State 1, 1675 (1960)].

[8] C. Smith, Phys. Rev. 94, 42 (1954).

[9] G. Dresselhaus, Phys. Rev. 100, 580 (1955); E. Kane, J. Phys. Chem. Solids 1, 249 (1957).

[10] E. I. Rashba and B. I. Sheka, Fiz. Tverd. Tela, Collected Articles 2, 162 (1959); E. I. Rashba, Fiz.

Tverd. Tela 2, 1224 (1960); I. I. Boiko and E. I. Rashba, Fiz. Tverd. Tela 2, 1874 (1960).

[11] J. M. Luttinger, Phys. Rev. 102, 1030 (1955).

[12] W. Kohn, in Solid-State Physics, edited by F. Seitz and D. Turnbull (Academic Press, New York, 1957), Vol. 5, p. 257.

[13] W. H. Kleiner and L. M. Roth, Phys. Rev. Letters 2, 334 (1959).

SELECTION RULE FOR THE INTERACTION OF MICROWAVE ULTRASONICS WITH SPINS

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Theory and results for iron-group paramagnetism in crystals[1] show that the dominant contribution, of noncubic crystalline fields, to the ground-state spin Hamiltonian is quadratic in the spin. This indicates a quadrupolar form for the relevant spin operator in spin resonance transitions induced by lattice vibrations. Quadrupole selection rules for spin-phonon transitions have been explicitly derived by Mattuck and Strandberg[2] for non S-state ions of the iron group. However, their low-frequency acoustic experiments[3] were unable to verify the selection rule. Using microwave ultrasonics in conjunction with standard spin resonance techniques,[4] we have experimentally confirmed the quadrupole selection rule for a non S-state ion, Cr^{3+} in Al_2O_3, and also for two S-state ions, Mn^{2+} and Fe^{3+} in MgO.

9-kMc/sec longitudinal phonons were generated in quartz rods bonded to the paramagnetic host crystals.[5,6] The wave propagation direction was parallel to the c axis in the Al_2O_3, and parallel to a cubic axis in the MgO. CW resonance saturation techniques were used to observe the interaction of the ultrasonics with the spin resonances, and relative spin-phonon matrix elements were extracted by comparison of the saturation by ultrasonics with saturation by a microwave source, at the resonance frequency, which was not coherent with the electron spin resonance spectrometer power.[6] Measurements of the matrix elements were made as a function of the angle θ between the dc magnetic field direction and the wave axis.

The dominant quadrupole nature of the relevant spin operator is shown by comparison of the observed angular variations with those computed, using the quadrupole spin operator. Good agreement was obtained for all three ions. As an example, Fig. 1 shows the experimental and theoretical angular variations of the square of the matrix element for the (-3/2, -1/2) transition of Fe^{3+} in MgO. In the absence of crystal field terms in the spin Hamiltonian, m_S is a good quantum number along H_{dc}, independent of the angle θ, and the probability for $\Delta m_S = \pm 1$ transitions, caused by a longitudinal wave, varies as

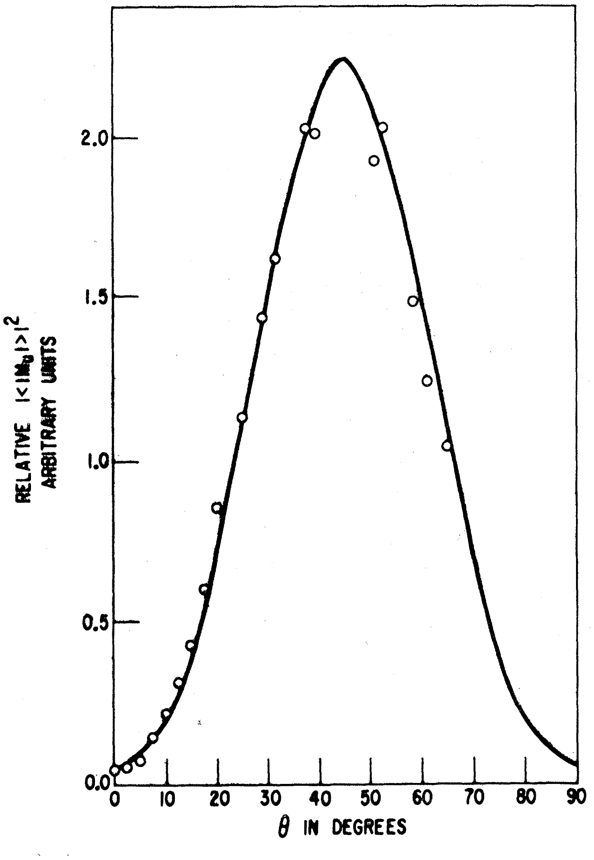

FIG. 1. Angular variation of the spin-phonon matrix element for the (-3/2, -1/2) transition of Fe^{3+} in MgO. The theoretical expression is normalized to the average of the experimental values. The small background level is believed due to generation of other acoustic modes, either in the quartz-MgO bond, or in the MgO crystal.