VALENCE SPIN-ORBIT SPLITTING AND CONDUCTION g TENSOR IN Si†

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(Received May 15, 1961)

Roth et al. have calculated conduction g tensors in semiconductors, and have obtained excellent agreement with experiment for Ge[1,2] and InSb.[3] In the absence of crystal wave functions the calculations for these crystals and Bi[4] were based on a two-level approximation to the effective-mass sum rule. Then the g tensor could be estimated from observed spin-orbit splittings and effective masses. Roth also analyzed Si in the two-band approximation, but her original estimate of the isotropic g shift was too large by a factor of 3. Elliott pointed out[5] that because of the proximity of the conduction band edge along Δ to the point X, the crystal spin-orbit splitting should be small (at X it is zero by symmetry). Our calculations show that the valence spin-orbit splitting at Δ is actually too small by a factor of 3 to explain the experimental g shift. Yafet realized[6] that in Si the term considered by Roth might give the wrong sign for the isotropic g shift; our calculations have verified his conjecture. Finally, recent spin resonance experiments by Feher and Wilson[7] on strained Si samples have shown that $\delta g_{\perp}$, which is negligible in the two-band model, is actually greater than $\delta g_{\parallel}$. Therefore the two-band approximation is inadequate for Si, and a detailed calculation using crystal wave functions is required.

Several quantum-mechanical calculations of the g factor of electrons in crystals have been reported using cellular methods.[8,9] Here we use the orthogonalized plane wave (OPW) method, which is well suited to Si. We begin with the spin-orbit splitting of the valence band; the spin-orbit splitting was first calculated from OPW wave functions by Cohen and Falicov.[10]

OPW crystal wave functions are divided into a "smooth" plane wave part and a core part:

$$\psi_{\vec{k}}^{\alpha}=\sum_{\vec{K}} a^{\alpha}(\vec{k}+\vec{K})\,|(\vec{k}+\vec{K})^{\alpha}\rangle+\sum_{t} b_{\vec{k}}^{\alpha}\,|\phi_{t,\vec{k}}^{\alpha}\rangle, \tag{1}$$

where α labels irreducible representations, $(\vec{k}+\vec{K})^{\alpha}$ is a symmetrized combination of plane waves, and $b_{\vec{k}}^{\alpha}$ is determined from the requirement that $\psi_{\vec{k}}^{\alpha}$ be orthogonal to the core orbital ϕ_t. In computing $\langle\psi_{\vec{k}}^{\alpha}|H_{\text{s.o.}}|\psi_{\vec{k}}^{\beta}\rangle$, where $H_{\text{s.o.}}$ is the spin-orbit operator, we find that 96% of the matrix element comes from core-core terms. The spin-orbit splitting of the p valence bands along $\vec{k}=(\Delta 00)$ is therefore conveniently expressed in terms of the $2p$ core orbitals. For instance, at $\vec{k}=0$,

$$\Delta_{\text{s.o.}}(\Gamma_{25'})=3\,|A_{\Gamma_{25'}}|^{2}\,|\langle 2p_y|H_{\text{s.o.}}^{x}|2p_z\rangle|, \tag{2}$$

where

$$A_{\Gamma_{25'}}=(2/\sqrt{3})a(111)b_{2p}(111)+\sqrt{2}\,a(002)b_{2p}(002)+\cdots \tag{3}$$

The parameters a and b are taken from the band calculation of Kleinman and Phillips.[11] Sixty-five plane waves were used in the expansion (3).

Consider first the $2p$ spin-orbit splitting $3\,|\langle 2p_y|H_{\text{s.o.}}^{x}|2p_z\rangle|$. Tomboulian and Cady[12] completed the identification of the x-ray emission lines $2p^{3/2}\rightarrow 2s$ and $2p^{1/2}\rightarrow 2s$ for the second row of the periodic table. Their values for the $2p$ spin-orbit splitting for Mg and Si are listed in the first line of Table I. By invoking Slater's rule that the missing electron gives an extra screening charge $0.3e$, we can use Tomboulian and Cady's values for the spin-orbit splittings to estimate the $2p$ splitting in neutral Mg and Si (second line of Table I). Calculated values for Mg[13] and Si are listed in the third line. It will be seen that the discrepancies are quite similar for Mg and Si. These discrepancies are not understood; in the calculations quoted below, the corrected experimental value for the $2p$ spin-orbit splitting is used.

From (2) and (3) we now find $\Delta_{\text{s.o.}}(\Gamma_{25'})=0.042$ ev, in good agreement with the infrared value 0.0441 ± 0.0004 ev of Zwerdling et al.[14] A plot of $\Delta_{\text{s.o.}}(\Delta_5)$ is given in Fig. 1.

Starting from the effective-mass $(\vec{k}\cdot\vec{p})$ Hamiltonian and treating $H_{\text{s.o.}}$ as a perturbation, Roth[1] has derived the following formulas for the g tensor in Si:

$$\delta g_{\parallel}=\delta g_{x}=\mathrm{Re}\frac{4}{mi}\sum_{\mu,\nu}\frac{1}{E_{0\mu}E_{0\nu}}\langle\Delta_1|p_y|\Delta_5^{\mu y}\rangle\langle\Delta_5^{\mu y}|H_{\text{s.o.}}^{x}|\Delta_5^{\nu z}\rangle\langle\Delta_5^{\nu z}|p_z|\Delta_1\rangle$$

$$+\mathrm{Re}\frac{8}{mi}\sum_{\mu,\nu}\frac{1}{E_{0\mu}E_{0\nu}}\langle\Delta_1|H_{\text{s.o.}}^{x}|\Delta_{1'}^{\mu}\rangle\langle\Delta_{1'}^{\mu}|p_y|\Delta_5^{\nu z}\rangle\langle\Delta_5^{\nu z}|p_z|\Delta_1\rangle, \tag{4}$$

$$\delta g_{\perp} = \delta g_{y,z} = \mathrm{Re}\frac{4}{mi}\sum_{\mu,\nu}\frac{1}{E_{0\mu}E_{0\nu}}\langle\Delta_1|p_z|\Delta_5^{\mu z}\rangle\langle\Delta_5^{\mu z}|H_{\mathrm{s.o.}}^{y}|\Delta_1^{\nu}\rangle\langle\Delta_1^{\nu}|p_x|\Delta_1\rangle$$

$$+\mathrm{Re}\frac{4}{mi}\sum_{\mu,\nu}\frac{1}{E_{0\mu}E_{0\nu}}\langle\Delta_1|H_{\mathrm{s.o.}}^{y}|\Delta_5^{\mu z}\rangle\langle\Delta_5^{\mu z}|p_z|\Delta_1^{\nu}\rangle\langle\Delta_1^{\nu}|p_x|\Delta_1\rangle$$

$$+\mathrm{Re}\frac{4}{mi}\sum_{\mu,\nu}\frac{1}{E_{0\mu}E_{0\nu}}\langle\Delta_1|p_z|\Delta_5^{\mu z}\rangle\langle\Delta_5^{\mu z}|p_x|\Delta_5^{\nu z}\rangle\langle\Delta_5^{\nu z}|H_{\mathrm{s.o.}}^{y}|\Delta_1\rangle. \quad (5)$$

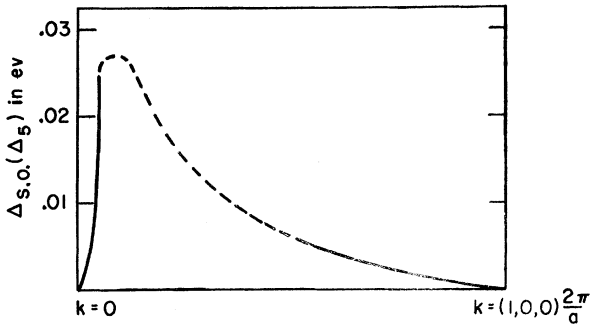

FIG. 1. Sketch of the spin-orbit splitting of the Δ_5 valence band of silicon. The dashed curve represents interpolation from the calculated results. Note that although there is a spin-orbit splitting for the valence state $\Gamma_{25'}$ at $\vec{k}=0$, the lower split level is associated with $\Delta_{2'}$. So as far as Δ_5 band is concerned, the splitting is equal to zero at the zone center.

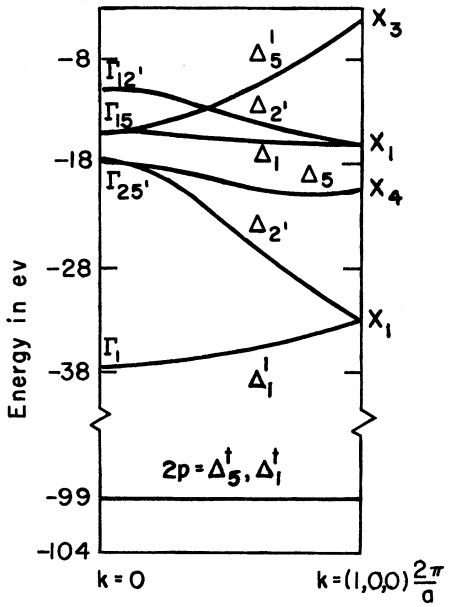

FIG. 2. Sketch of the energy bands of silicon along [100] axis of the Brillouin zone, after Kleinman and Phillips. Superscript t is used to denote the $2p$ core states.

Figure 2 shows the relevant energy levels. The conduction band edge is believed[15] to be at $\Delta = 0.85(2\pi a^{-1})$. Note the $2p$ core levels.

Because of the selection rule $\langle X_4^n|H_{\mathrm{s.o.}}|X_4^n\rangle = 0$, the most important matrix elements of $H_{\mathrm{s.o.}}$ are $\langle\Delta_5^n|H_{\mathrm{s.o.}}|\Delta_5^{n'}\rangle \simeq \langle X_4^n|H_{\mathrm{s.o.}}|X_4^{n'}\rangle \neq 0$. From Table II we see that terms of this form, in which one of the levels is a $2p$ core state, make the largest contribution to δg. Comparison with Feher and Wilson's values is made in Table III; the agreement is excellent.

According to Roth[16] the "one-valley" interband term H_2 is responsible for donor spin-lattice relaxation for $H \parallel (100)$. Roth's expression for H_2 is

$$H_2 = \tfrac{1}{2}A\beta\{\epsilon_{xy}(\sigma_x H_y + \sigma_y H_x) + \text{cyclic term}\}, \quad (6)$$

where A is given in terms of the deformation potential E_{yz} by

$$A = \frac{4i}{3m}\frac{\langle\Delta_{2'}|p_x|\Delta_{2'}\rangle\langle\Delta_{2'}|E_{yz}|\Delta_1\rangle}{E_{12'}{}^2E_{15}}$$

$$\times\{\langle\Delta_1|p_y|\Delta_5^{y}\rangle\langle\Delta_5^{y}|H_{\mathrm{s.o.}}^{y}|\Delta_{2'}\rangle$$

$$+\langle\Delta_1|H_{\mathrm{s.o.}}^{y}|\Delta_5^{z}\rangle\langle\Delta_5^{z}|p_y|\Delta_{2'}\rangle\}. \quad (7)$$

We have calculated all the matrix elements in A except that of the deformation potential. From Feher and Wilson's measured value[7] of A (0.44 $\pm$ 0.04), we find that $\langle\Delta_{2'}|E_{yz}|\Delta_1\rangle = 23$ ev. For comparison, the intraband shear deformation

Table I. Spin-orbit splitting of $2p$ core state.

	Mg	Si
Exp. (ev)	0.27	0.72
Corr. exp. (ev)	0.22	0.60
Calc. (ev)	0.17	0.49

Table II. Relative magnitude of contributions to g tensor. The first term in $\delta g_{\parallel}$ is the only one contributing in the two-band approximation.

	Term in Eqs. (4) and (5) involving:			Relative magnitude with respect to first term in Eq. (4)
$\delta g_{\parallel}$	$\langle\Delta_1\|p_y\|\Delta_5^{y}\rangle$,	$\langle\Delta_5^{y}\|H_{s.o.}^{x}\|\Delta_5^{z}\rangle$,	$\langle\Delta_5^{z}\|p_z\|\Delta_1\rangle$	1
	$\langle\Delta_1\|p_y\|\Delta_5^{1y}\rangle$,	$\langle\Delta_5^{1y}\|H_{s.o.}^{x}\|\Delta_5^{z}\rangle$,	$\langle\Delta_5^{z}\|p_z\|\Delta_1\rangle$	0.7
	$\langle\Delta_1\|p_y\|\Delta_5^{y}\rangle$,	$\langle\Delta_5^{y}\|H_{s.o.}^{x}\|\Delta_5^{1z}\rangle$,	$\langle\Delta_5^{1z}\|p_z\|\Delta_1\rangle$	0.7
	$\langle\Delta_1\|p_y\|\Delta_5^{ty}\rangle$,	$\langle\Delta_5^{ty}\|H_{s.o.}^{x}\|\Delta_5^{z}\rangle$,	$\langle\Delta_5^{z}\|p_z\|\Delta_1\rangle$	-2.6
	$\langle\Delta_1\|p_y\|\Delta_5^{y}\rangle$,	$\langle\Delta_5^{y}\|H_{s.o.}^{x}\|\Delta_5^{tz}\rangle$,	$\langle\Delta_5^{tz}\|p_z\|\Delta_1\rangle$	-2.6
$\delta g_{\perp}$	$\langle\Delta_1\|p_z\|\Delta_5^{z}\rangle$,	$\langle\Delta_5^{z}\|p_x\|\Delta_5^{z}\rangle$,	$\langle\Delta_5^{z}\|H_{s.o.}^{y}\|\Delta_1\rangle$	-0.5
	$\langle\Delta_1\|p_z\|\Delta_5^{z}\rangle$,	$\langle\Delta_5^{z}\|H_{s.o.}^{y}\|\Delta_1^{1}\rangle$,	$\langle\Delta_1^{1}\|p_x\|\Delta_1\rangle$	0.3
	$\langle\Delta_1\|p_z\|\Delta_5^{tz}\rangle$,	$\langle\Delta_5^{tz}\|H_{s.o.}^{y}\|\Delta_1^{1}\rangle$,	$\langle\Delta_1^{1}\|p_x\|\Delta_1\rangle$	-0.2
	$\langle\Delta_1\|p_z\|\Delta_5^{z}\rangle$,	$\langle\Delta_5^{z}\|H_{s.o.}^{y}\|\Delta_1^{t}\rangle$,	$\langle\Delta_1^{t}\|p_x\|\Delta_1\rangle$	-3.1
	$\langle\Delta_1\|p_z\|\Delta_5^{tz}\rangle$,	$\langle\Delta_5^{tz}\|H_{s.o.}^{y}\|\Delta_1^{t}\rangle$,	$\langle\Delta_1^{t}\|p_x\|\Delta_1\rangle$	-0.3

Table III. g tensor for Si.

	$\delta g_{\parallel}$	$\delta g_{\perp}$
Calc.	-0.0027	-0.0036
Exp.	-0.0028	-0.0040

potential matrix element is $E_2 = \langle\Delta_1|E_{yy}|\Delta_1\rangle = 7$ ev.[17] Evaluation of this discrepancy requires a detailed theory of deformation potentials.

The author wishes to express his gratitude to Professor J. C. Phillips for suggesting the problem and for many helpful comments, to Professor M. H. Cohen and Dr. L. M. Falicov for interesting discussions, and to Dr. L. Kleinman for showing him the Si wave functions.

†Work supported in part by the Office of Naval Research.

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