PHONON SCATTERING AT ACCEPTORS WITH Γ_8 GROUND STATES IN SEMICONDUCTORS

Ernst Sigmund and Kurt Lassmann

Institut für Theoretische Physik and Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, D - 7000 Stuttgart 80, W-Germany

The ground state of acceptors in cubic semiconductors is fourfold degenerate and the interaction with the lattice vibrations leads to the possibility of a Jahn-Teller effect[1], causing a dynamical splitting of the electronic levels. However, due to the extended nature of the wavefunction of the defect, random internal fields may have dominant influence to destroy the J.T. effect. Such an influence should be smaller for deeper acceptors, where the wavefunctions are more concentrated.

In fact different types of experiments indicate a resonance energy in the meV range for the deeper acceptors GaAs(Mn), GaP(In), Si(In) and Si(B), which have been studied by the following methods:

α) Ultrasonic experiments and analysis of the relaxation attenuation[2,3]
β) Thermal conductivity measurements[4]
γ) Quasimonochromatic phonon scattering experiments[5]
δ) Luminescence measurements[6]
ε) Raman spectroscopy[7].

All these detected resonance energies are much larger than the splittings due to random internal fields, which may be of the order of 10 to 100 μeV.

The acceptor-hole-lattice interaction Hamiltonian can be written as

$$(1) \quad H_I = \sum_{q\lambda} \Lambda^{q\lambda}(b_{q\lambda}+b^+_{q\lambda})$$

where the electronic part $\Lambda^{q\lambda}$ contains Dirac's 4x4 matrices $\hat{\rho}_i$ and $\hat{\sigma}_j$ $(i,j=1,2,3)$:

$$(2) \quad \Lambda^{q\lambda} = D^{\varepsilon}(\hat{\rho}_1 r_1{}^{q\lambda} + \hat{\rho}_2 r_2{}^{q\lambda}) + D^{\tau}\hat{\rho}_3(\hat{\sigma}_1 s_1{}^{q\lambda} + \hat{\sigma}_2 s_2{}^{q\lambda} + \hat{\sigma}_3 s_3{}^{q\lambda})$$

This form is equivalent to the usual one[8] expressed in angular momentum operators. It is useful for our treatment. The following abbreviations are used

$$(3a) \quad r_1{}^{q\lambda} = \left(\frac{\omega_{q\lambda}}{2Mc_\lambda^2}\right)^{1/2} f(q)\ \frac{1}{3}\left[2\hat{q}_z e_{\lambda z} - \hat{q}_x e_{\lambda x} - \hat{q}_y e_{\lambda y}\right]$$

$$(3b) \quad r_2{}^{q\lambda} = \left(\frac{\omega_{q\lambda}}{2Mc_\lambda^2}\right)^{1/2} f(q)\ \frac{1}{\sqrt{3}}\left[\hat{q}_x e_{\lambda x} - \hat{q}_y e_{\lambda y}\right]$$

$$(3c) \quad s_1{}^{q\lambda} = \left(\frac{\omega_{q\lambda}}{2Mc_\lambda^2}\right)^{1/2} f(q)\ \frac{1}{\sqrt{3}}\left[\hat{q}_z e_{\lambda y} + \hat{q}_y e_{\lambda z}\right]$$

$$(3d) \quad s_2{}^{q\lambda} = \left(\frac{\omega_{q\lambda}}{2Mc_\lambda^2}\right)^{1/2} f(q)\ \frac{1}{\sqrt{3}}\left[\hat{q}_z e_{\lambda x} + \hat{q}_x e_{\lambda z}\right]$$

$$(3e) \quad s_3{}^{q\lambda} = \left(\frac{\omega_{q\lambda}}{2Mc_\lambda^2}\right)^{1/2} f(q)\ \frac{1}{\sqrt{3}}\left[\hat{q}_x e_{\lambda y} + \hat{q}_y e_{\lambda x}\right]$$

Here the long wavelength approximation is used, i.e. only acoustic phonons are coupled. $b_{q\lambda}$ and $b^{+}_{q\lambda}$ are the annihilation and creation operators for the phonon with wavevector $\vec{q}$ in the branch λ . $\omega_{q\lambda}$ is the angular frequency and c_λ the velocity of sound. $\hat{q}$ is the unit vector along $\vec{q}$ and $\vec{e}_\lambda$ is the polarization vector of the phonon. M is the mass of the crystal. $D^{\varepsilon}(=D^{a}_{\mathrm{u}})$ and $D^{\tau}(=D^{a}_{\mathrm{u}'})$ are the deformation potential constants for a $[1,0,0]$ and $[1,1,1]$ strain respectively. The extended nature of the defectstate is reflected in the cut-off function

$$(4) \quad f(q) \cong \left[1 + \frac{1}{4}\, a^{*2} q^2\right]^{-2}$$

where a^* is the effective Bohr radius.

The scattering rate (or inverse life time) of a phonon q,λ is given by

$$(5) \quad \tau^{-1}_{q\lambda} = -\omega^{-1}_{q\lambda} \lim_{\varepsilon \to 0} \ \mathrm{Im}\ T(\omega_{q\lambda} + i\varepsilon)_{q\lambda,q\lambda}.$$

$T(\omega_{q\lambda}+i\varepsilon)$ is the T-matrix defined by the phonon Green's functions ($G=G_O-G_OTG_O$) of the unperturbed (G_O) and perturbed (G) crystal. Following refs. 9 and 10 the phonon Green's function can be replaced by Green's functions between the electronic operators $\hat{\rho}_i$ and $\hat{\sigma}_j$:

$$(6) \quad \tau_{q\lambda}^{-1} = 4\pi \lim_{\varepsilon\to 0} \; \mathrm{Im} \; \langle\langle \Lambda^{q\lambda};\Lambda^{q\lambda}\rangle\rangle .$$

We consider a longitudinally polarized phonon travelling in a [1,0,0] direction. This simplifies our further treatments considerably, because in this case we are only concerned with the "spin-spin" Green's function $\langle\langle\hat{\rho}_1;\hat{\rho}_1\rangle\rangle$.

Using the equation of motion method the Green's function hierarchy can be expanded up to the fourth order. In second order we factorize the quadratic forms of the phonon operators. In fourth order we close the hierarchy taking only the inhomogeneous part of the Green's functions into account.
The thermal expectation values are calculated by use of the exponential transformation

$$(7) \quad U = \exp\{\sum_{q\lambda} \omega_{q\lambda}^{-1} \Lambda^{q\lambda}(b_{q\lambda}-b_{q\lambda}^{+})\}$$

which guarantees that they are exact at least up to the second order in the coupling parameters.
Introducing an isotropic model for the crystal the mean scattering rate can be calculated analytically for zero temperature. As a final result we get the Lorentzian-like form

$$(8) \quad \langle\tau^{-1}\rangle(\omega) = \frac{P(\omega)}{(\omega-\Delta(\omega))^2+\Gamma(\omega)^2}$$

P,Δ and Γ are rather lengthy expressions, therefore we have omitted

TABLE I: Experimental and theoretical values of resonance energies. The small greek letters indicate the method of measurement (see text)

	GaAs(Mn)	GaP(In)	Si(In)	Si(B)
experimental values (meV)	3.1 ± 0.3 α, β	2.7 ± 0.3 ε	4.2 ± 0.2 $\alpha,\beta,\gamma,\delta,$	~2. α,β,γ
theoretical values (meV)	2.6	2.3	4.0	1.9

them. $\Gamma(\omega)$ represents the "width" of the resonance. The formal resonance frequency is given by the relation $\omega-\Delta(\omega)\equiv 0$. The results for several systems are given in table I. They are in good agreement with the experimental values.

REFERENCES

1. T.N. Morgan, Phys. Rev. Lett. 24:887 (1970)
2. K. Lassmann, Hp. Schad, Solid State Commun. 18:449 (1976)
3. Hp. Schad, K. Lassmann, Phys. Rev. Lett. 56A:409 (1976)
4. A. de Combarieu, K. Lassmann, "Phonon Scattering in Solids" Plenum Publishing Corp. p.340 (1976)
5. H. Schenk, W. Forkel, W. Eisenmenger, Frühjahrstagung DPG Freudenstadt 1978
6. R. Sauer, W. Schmid, J. Weber, Sold. State Commun. 27:705 (1978)
7. L.L. Chase, W. Hayes, J. Ryan, J. Phys. C 10:2957 (1977)
8. see e.g. G.L. Bir, E.J. Butikov, G.E. Pikus, J. Phys. Chem. Solids 24:1467 (1963)
9. M.V. Klein, Phys. Rev. B 186:839 (1969)
10. M. Rueff, E. Sigmund, M. Wagner, Phys. Stat. Sol. (b)81:511 (1977)