

12. ELECTRON PARAMAGNETIC RESONANCE OF BORON IN DIAMOND

C A J Ammerlaan

Natuurkundig Laboratorium, Universiteit van Amsterdam,Valckenierstraat 65, 1018 XE Amsterdam, The Netherlands

In type IIb natural diamond a new electron paramagnetic resonance spectrum, which we label C-NL1, was observed. The characteristics of the spectrum, as presented and briefly discussed below, allow the spectrum to be associated with holes bound to the shallow acceptor boron.

a. General appearance. The resonance consists of a single line without any resolved structure. In most cases the shape of the line is rather Gaussian. Depending on the conditions of the measurement, the full width at half maximum varies between 5 and 50 mT.

b. Stress dependence. The resonance is only observable when the sample is uniaxially stressed. This behaviour is similar to that of acceptor impurities in silicon<sup>(1)</sup>. The phenomenon is understood, on the basis of the effective mass theory, as the suppression of the line broadening due to random internal strains by the uniform external stress.

c. Temperature dependence. The resonance is only observable at low temperatures, typically below liquid helium temperature. This characteristic, which is exceptional for paramagnetic resonance in diamond, indicates a strong spin-lattice coupling. This may be associated with the orbital angular momentum in the acceptor ground state, which, according to the effective mass theory, is derived from p-states near the top of the valence band. The shallow acceptor impurities in silicon again show a similar behaviour<sup>(1)</sup>.

d. Angular dependence. Rotation patterns of the resonance field were measured with the magnetic field  $\vec{B}$  in the plane perpendicular to the external stress  $\vec{P}$ . For  $\vec{P} // [100]$ ,  $\vec{B} \perp \vec{P}$ , the resonance field is isotropic with an effective g-value  $g_{\text{eff}} = 2.16$ . Similarly, for  $\vec{P} // [111]$ ,  $\vec{B} \perp \vec{P}$ , the isotropic g-value is  $g_{\text{eff}} = 2.17$ . For  $\vec{P} // [0\bar{1}1]$ ,  $\vec{B} \perp \vec{P}$ , a real angular variation is observed with a maximal  $g_{\text{eff}} = 2.40$ , for  $\vec{B} // [100]$ , and a minimal

$g_{\text{eff}} = 1.92$  for  $\vec{B} // [011]$ . The appropriate spin-Hamiltonian  $H$  for analysis of these results is given by

$$\begin{aligned}
 H &= H_B + H_\epsilon \\
 H_B &= g_1 \mu_B (B_x I_x + B_y I_y + B_z I_z) \\
 &\quad + g_2 \mu_B (B_x I_x^3 + B_y I_y^3 + B_z I_z^3) \\
 H_\epsilon &= b' (\epsilon_{xx} I_x^2 + \epsilon_{yy} I_y^2 + \epsilon_{zz} I_z^2) \\
 &\quad + d' (2/\sqrt{3}) \{ \epsilon_{xy} (I_x I_y + I_y I_x) + \epsilon_{yz} (I_y I_z + I_z I_y) + \epsilon_{zx} (I_z I_x + I_x I_z) \}
 \end{aligned}$$

The constants  $g_1'$  and  $g_2'$  in the magnetic field dependent term  $H_B$  are the Zeeman  $g$ -factors for bound holes. In the strain dependent term  $H_\epsilon$  the strains are given by  $\epsilon_{xx}$ , etc, while  $b'$  and  $d'$  represent the deformation potential constants associated with normal and shear strains, respectively. The values of the parameters  $g_1'$ ,  $g_2'$  and  $d'/b'$  were determined by matching the theoretical expressions to the experimental data. Present results for boron in diamond are given in table I. For comparison, the table also includes values for the parameters for Si:B, both from the analysis by Bir, et al.<sup>(2)</sup> of the experiments of Feher, et al.<sup>(1)</sup> and from the recent experiments by Neubrand on virtually strain-free crystals<sup>(3)</sup>. The close similarity between the results for diamond and silicon supports the identification of the resonance C-NL1 with the neutral boron impurity.

Table I. Spin-Hamiltonian parameters of EPR spectrum C-NL1, and those of boron in silicon

System	$g_1'$	$g_2'$	$d'/b'$	Reference
C:B	$-1.10 \pm 0.05$	$+0.01 \pm 0.02$	1.65	This work
C:Si	-1.21	+0.002		Bir, et al.
	$-1.071 \pm 0.004$	$-0.031 \pm 0.001$	2.61	Neubrand

#### REFERENCES

- 1) Feher G, Hensel J C, and Gere E A, Phys.Rev.Letters 5 (1960) 309.
- 2) Bir G L, Butikov E I, and Pikus G E, J.Phys.Chem.Solids 24 (1963) 1467.
- 3) Neubrand H, Phys.Stat.Sol.(b) 86 (1978) 269.