38. LINEWIDTH STUDIES ON THE C:B ELECTRON PARAMAGNETIC RESONANCE

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In type IIb diamond an electron paramagnetic resonance is observed which presumably arises from holes bound to the acceptor boron. The state is described by spin J = 3/2 and a spin-Hamiltonian H, with

$$H = H_B + H_\varepsilon,$$

$$H_B = g_1'\mu_B(B_xJ_x + B_yJ_y + B_zJ_z) + g_2'\mu_B(B_xJ_x^3 + B_yJ_y^3 + B_zJ_z^3),$$

$$H_\varepsilon = b'(\varepsilon_{xx}J_x^2 + \varepsilon_{yy}J_y^2 + \varepsilon_{zz}J_z^2) + d'(2/\sqrt{3})\left[\varepsilon_{xy}(J_xJ_y + J_yJ_x) + \varepsilon_{yz}(J_yJ_z + J_zJ_y) + \varepsilon_{zx}(J_zJ_x + J_xJ_z)\right].$$

The Hamiltonian constants are $g_1' = -1.10 \pm 0.05$, $g_2' = +0.01 \pm 0.02$ and $d'/b' = 1.65$ [1].

The resonance is only observable when an external uniaxial stress $\vec{P}_{ext}$ is applied to the diamond. Results for $\vec{P}_{ext}//[100]$ and magnetic field $\vec{B}$ rotated in the plane perpendicular to $\vec{P}_{ext}$ are shown in figure 1. The magnetic field value at which resonance is observed, B_{res}, is isotropic with an effective g-value $g_{eff} = 2g_1' + 5g_2'$. Linewidth ΔB and line intensity χ, on the other hand, have a pronounced angular dependence. The linewidth variations are probably caused by internal stresses $\vec{P}_{int}$ in the diamond.

One may assume the presence of internal stresses with a random direction and with a strength distribution according to a Gaussian function. It is useful to decompose the internal stress into its components $\vec{P}_{int,//}$ parallel to the external stress direction [100] and $\vec{P}_{int,\perp}$ perpendicular to it. Then the total stress $\vec{P}_{tot}$ is given by $\vec{P}_{tot} = \vec{P}_{ext} + \vec{P}_{int,//} + \vec{P}_{int,\perp}$.

First the effect of $\vec{P}_{int,//}$ is considered. Using perturbation theory a more accurate formula for the effective g-value can be derived. It reads:

$$g_{eff} = 2g_1' + 5g_2' - \{\frac{3}{16}(2g_1' + 5g_2') - \frac{9}{32}g_2' \cos 4\phi\}.\left\{\frac{(g_1' + 7/4g_2')\mu_B B}{b'(S_{11} - S_{12})P_{tot}}\right\}^2.$$

As the formula indicates a dependence of g_{eff} with $\cos 4\phi$ (ϕ = azimuthal angle) on P_{tot}, as is observed experimentally, is obtained. However, the correction to $g_{eff} = 2g_1' + 5g_2'$ is too small to be of practical significance.

The perpendicular component of $\vec{P}_{int}$ has a larger influence. For the effect of tilting $\vec{P}_{tot}$ away from [100] one derives by series expansion in the polar angle θ:

$$g(\theta,\phi) = g(0,\phi) + \left(\frac{dg}{d\theta}\right)_{\theta=0} . \theta + \frac{1}{2}\left(\frac{d^2g}{d\theta^2}\right)_{\theta=0} . \theta^2.$$

Since the linear term vanishes

$$\frac{\Delta g}{g_{eff}} = \frac{g(\theta,\phi)-g(0,\phi)}{g_{eff}} = \frac{1}{2g_{eff}}\left(\frac{d^2g}{d\theta^2}\right)_{\theta=0} . \theta^2.$$

Small angles θ will give no broadening; large angles would do so but have a low probability of occurring. An effective θ_{eff} is therefore introduced. Some angles ϕ will cause a positive g-shift Δg; others will give a negative g-shift. The line broadening is due to the difference. A measure for the relative linewidth is thus given by:

$$\frac{\Delta B}{B_{res}} = \frac{1}{2g_{eff}}\left\{\left(\frac{d^2g}{d\theta^2}\right)_{max} - \left(\frac{d^2g}{d\theta^2}\right)_{min}\right\} . \theta^2_{eff}.$$

The quantity $\frac{1}{2g_{eff}}\left\{\left(\frac{d^2g}{d\theta^2}\right)_{max} - \left(\frac{d^2g}{d\theta^2}\right)_{min}\right\}$ can be calculated from the spin-Hamiltonian. A graphical representation of it in figure 2 shows a satisfactory agreement with the linewidth $\Delta B/B$ as measured. For measurements with $\vec{B}$ in the (100) plane a linewidth anisotropy can be introduced as the ratio of the linewidths ΔB for $\vec{B}//[010]$ and $\vec{B}//[011]$. It is given by

$$\frac{\Delta B_{[010]}}{\Delta B_{[011]}} = \frac{\left\{\left(\frac{d^2g}{d\theta^2}\right)_{max} - \left(\frac{d^2g}{d\theta^2}\right)_{min}\right\}_{[010]}}{\left\{\left(\frac{d^2g}{d\theta^2}\right)_{max} - \left(\frac{d^2g}{d\theta^2}\right)_{min}\right\}_{[011]}} .$$

For C:B the linewidth anisotropy is an experimental 2.2, in quite good agreement with the calculated value 1.8. The significance of the agreement is corroborated by a comparison to a different but similar system, i.e. to Si:Al. For this system both the calculated and measured anisotropy are smaller than one, which implies that the linewidth variation is out of phase with C:B.

An acceptable match between the two curves in figure 2 is obtained for $\theta_{eff} = 12^{\circ}$. Since $tg\theta_{eff} = |\vec{P}_{int}|/|\vec{P}_{ext}|$ and the experiments were performed with $|\vec{P}_{ext}| = 0.50$ GPa, this leads to an estimated internal stress of about 0.1 GPa. Multiplying with the compliance of diamond, $S_{11}-S_{12} = 1.05 \times 10^{-12}\ Pa^{-1}$, the corresponding internal strain ε_{int} is calculated to be 10^{-4}.

Reference

[1] C.A.J.Ammerlaan, Diamond Conference 1981, p.33.

Figure captions

Figure 1. Angular dependence, for $\vec{B}$ in the (100) plane, of the resonance field B_{res}, the resonance linewidth ΔB, and its intensity χ. Compressive stress of 0.50 GPa//[100].

Figure 2. The relative linewidth $\Delta B/B_{res}$ as a function of the direction of the magnetic field $\vec{B}$ in the (100) plane. Upper curve: experimental result for $|\vec{P}_{ext}|$ = 0.50 GPa; lower curve: calculated for $\theta_{eff} = 1^{\circ}$.

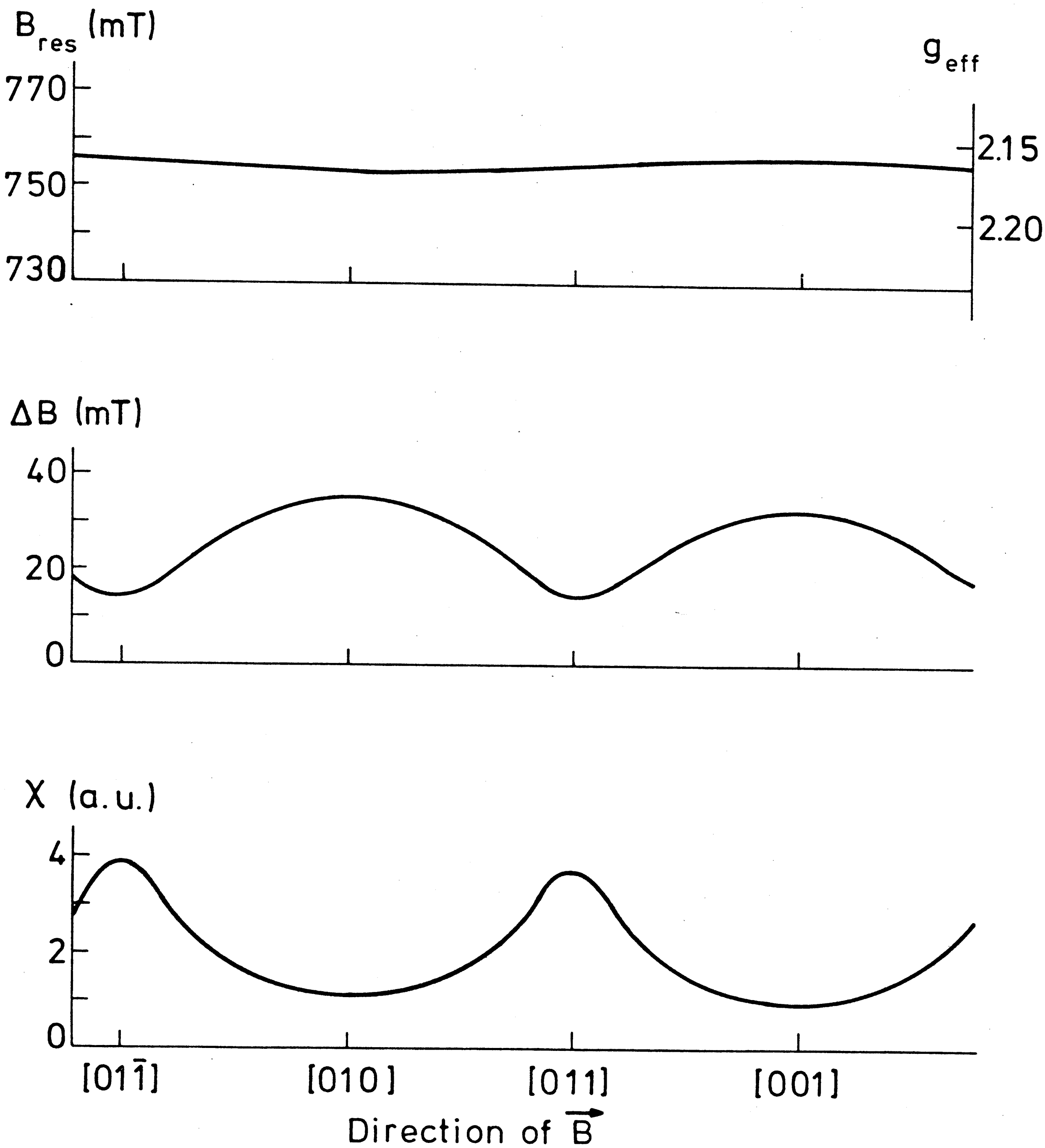

Figure 1. Angular dependence, for $\vec{B}$ in the (100) plane, of the resonance field B_{res}, the resonance line width ΔB, and its intensity χ. Compressive stress of 0.50 GPa // [100].

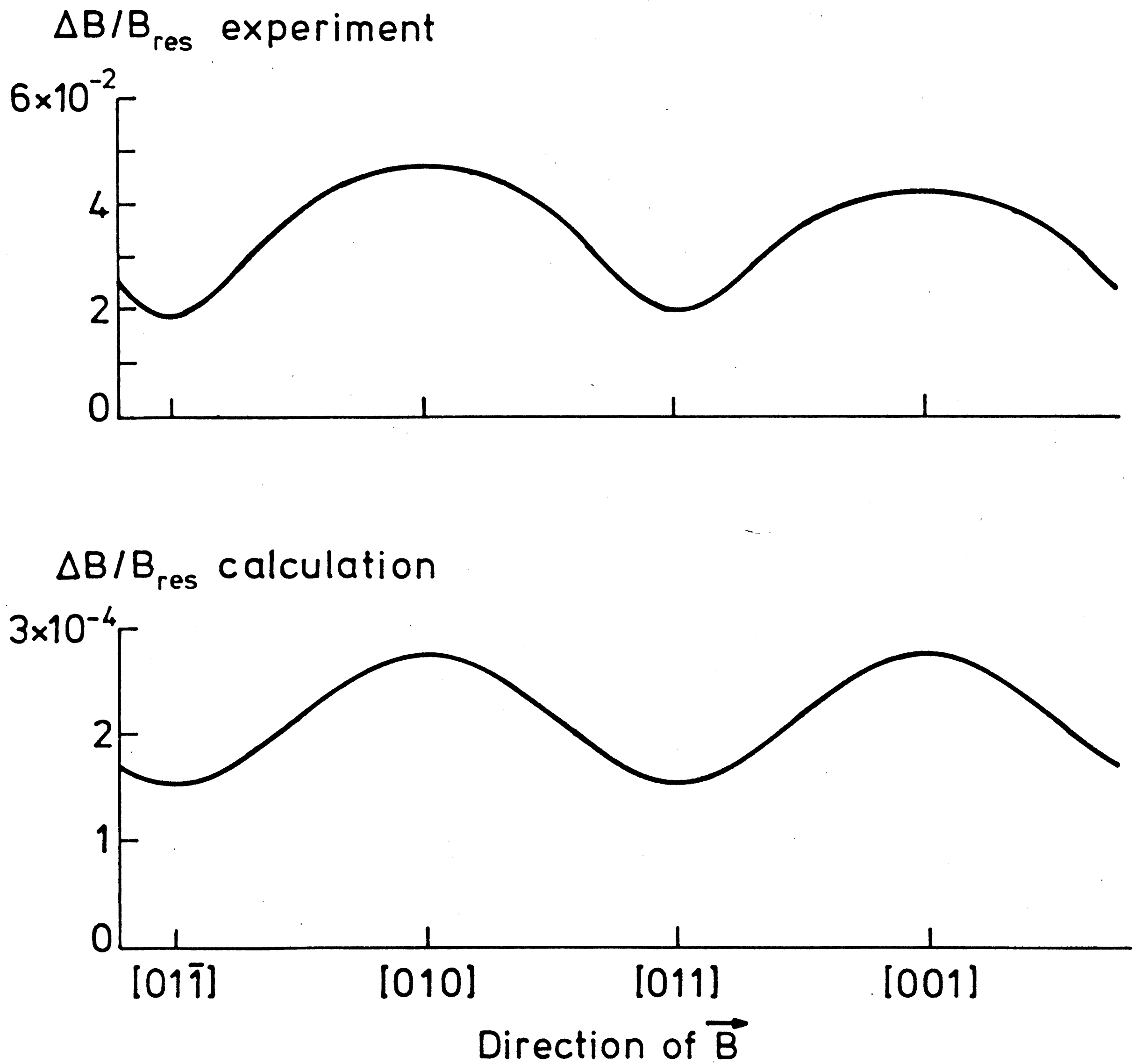

Figure 2. The relative linewidth $\Delta B/B_{res}$ as a function of the direction of the magnetic field $\vec{B}$ in the (100) plane. Upper curve: experimental result for $|\vec{P}_{ext}|$ = 0.50 GPa; lower curve: calculated for θ_{eff} = 1°.