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# Calculations of Line Shape for E.S.R. Absorption in Polycrystalline Substances

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The absorption for a polycrystalline substance is given by  $\mathcal{J} = \int_0^\pi \mathbf{I} \sin \vartheta \, d\vartheta$ , where  $\mathbf{I}$  is the line shape for a single crystal of uniaxial symmetry. We have performed calculations assuming the single crystal line shape to be (a) the Lorentzian  $\mathbf{I} = \frac{2\pi Ak}{1 + \pi^2 k^2 (x - c)^2}$  where  $A$  is proportional to the number of spins,  $k = 2/\pi\Delta x$  and  $\Delta x$  is the line width, and (b) the Gaussian  $\mathbf{I} = 2\pi^{3/2} Ak \exp. [-(x - c)^2 \pi^2 k^2]$  where  $A$  is proportional to the number of spins,  $k = \frac{2 (\ln 2)^{1/2}}{\pi \Delta x}$ , and  $\Delta x$  is the line width. (The factor  $\pi^{1/2}$  is introduced to ensure that the total absorption is the same for (a) and (b).)

If the absorption curve is obtained experimentally by sweeping the frequency  $\nu$ ,  $x = \frac{h\nu}{\beta H}$ , and  $c = g$ . If the absorption is obtained by sweeping the magnetic field  $H$ ,  $x = \frac{\beta H}{h\nu}$ , and  $c = \frac{1}{g}$ . Taking a variation of  $g$  with  $\theta$  of  $g^2 = g_\perp^2 + (g_\parallel^2 - g_\perp^2) \cos^2 \theta$ , and providing that  $|g_\parallel - g_\perp|$  is small, we may take  $c = c_\perp + (c_\parallel - c_\perp) \cos^2 \theta$ .

If the line width and  $A$  is assumed constant,  $\mathcal{J}$  can be found exactly for the Lorentzian, using the expression for  $c$  above [1]; for the Gaussian, approximate numerical methods have to be employed. We have evaluated  $\mathcal{J}$  for the Gaussian using a 16 point Gaussian quadrature. The results thus obtained were checked with a 100 point Simpson rule. Figure 1 shows a comparison of typical curves calculated for both line shapes. If  $|g_\parallel - g_\perp|$  is not small, both cases must be evaluated numerically. Also when there is considerable anisotropy allowance must be made for the change in transition probability with  $\theta$ , i.e. in  $A$  [2].

We have been able to fit one of these theoretical curves to a spectrum recorded experimentally from U. V. irradiated deuterium peroxide. This fit is shown in figures 2 and 3.

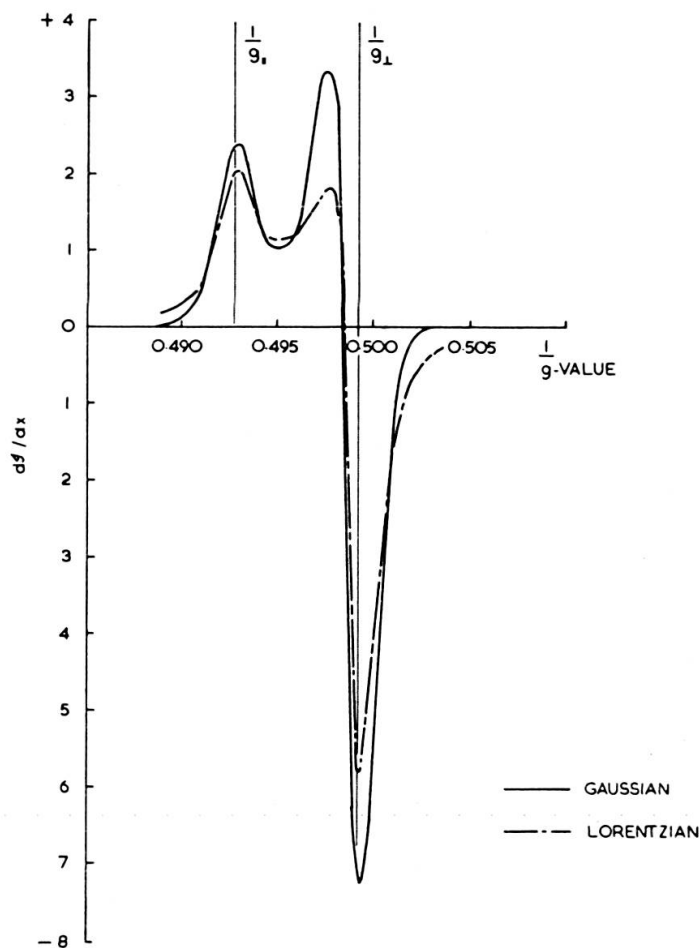


Fig. 1.

First differential of absorption for a polycrystalline substance using  $g_{\parallel} = 2.0295$ ,  $g_{\perp} = 2.0034$  and  $K$  (for Lorentzian) = 289, calculated for both Lorentzian and Gaussian line shapes.

It is possible to accommodate within these calculations variable line width. If  $\Delta x = \Delta x_{\perp} + (\Delta x_{\parallel} - \Delta x_{\perp}) \cos^2 \theta$  for example, it is still possible to evaluate the Lorentzian exactly and the Gaussian numerically. There is, however, a dearth of information of the variation of line width with  $\theta$ .

<sup>1</sup> SEARL, J.W., R. C. SMITH, S. J. WYARD, 1959, *Proc. Phys. Soc.*, 74, 491.

<sup>2</sup> BLEANEY, B., 1960, *Proc. Phys. Soc.*, 75, 621.

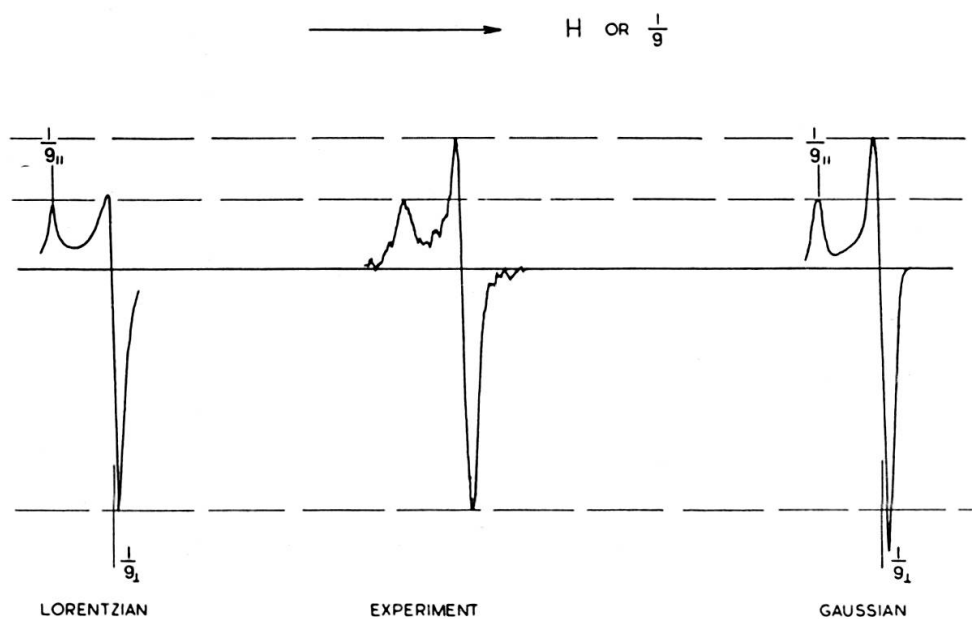


Fig. 2.

Comparison of an experimental E.S.R. first differential recording with curves calculated by  $g$ -value anisotropy theory. Experimental curve obtained from 80%  $D_2O_2$  3100Å U.V. irradiated at 90° K, subsequently warmed for 5 minutes at 133.5° K.

Calculated curves use  $g_{||} = 2.039$ ,  $g_{\perp} = 2.006$ , line width (in  $\frac{1}{g}$ ) = 0.00168.

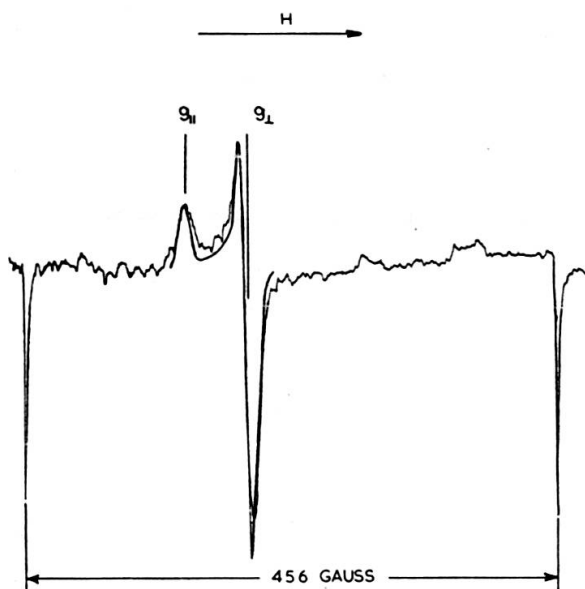


Fig. 3.

From figure 2, fit of Gaussian calculation to experimental curve.