

Calculations of line shape for E.S.R. absorption in polycrystalline substances

Autor(en): **Searl, J.W. / Smith, R.C. / Wyard, S.J.**

Objekttyp: **Article**

Zeitschrift: **Archives des sciences [1948-1980]**

Band (Jahr): **13 (1960)**

Heft 9: **Colloque Ampère**

PDF erstellt am: **24.05.2024**

Persistenter Link: <https://doi.org/10.5169/seals-738577>

Nutzungsbedingungen

Die ETH-Bibliothek ist Anbieterin der digitalisierten Zeitschriften. Sie besitzt keine Urheberrechte an den Inhalten der Zeitschriften. Die Rechte liegen in der Regel bei den Herausgebern.

Die auf der Plattform e-periodica veröffentlichten Dokumente stehen für nicht-kommerzielle Zwecke in Lehre und Forschung sowie für die private Nutzung frei zur Verfügung. Einzelne Dateien oder Ausdrucke aus diesem Angebot können zusammen mit diesen Nutzungsbedingungen und den korrekten Herkunftsbezeichnungen weitergegeben werden.

Das Veröffentlichen von Bildern in Print- und Online-Publikationen ist nur mit vorheriger Genehmigung der Rechteinhaber erlaubt. Die systematische Speicherung von Teilen des elektronischen Angebots auf anderen Servern bedarf ebenfalls des schriftlichen Einverständnisses der Rechteinhaber.

Haftungsausschluss

Alle Angaben erfolgen ohne Gewähr für Vollständigkeit oder Richtigkeit. Es wird keine Haftung übernommen für Schäden durch die Verwendung von Informationen aus diesem Online-Angebot oder durch das Fehlen von Informationen. Dies gilt auch für Inhalte Dritter, die über dieses Angebot zugänglich sind.

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

by J. W. SEARL
and R. C. SMITH and S. J. WYARD

Mathematics Department, Northampton College, London
Physics Department, Guy's Hospital Medical School, London

The absorption for a polycrystalline substance is given by $\mathcal{J} = \int_0^{\pi} I \sin \theta d\theta$, where 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 $I = \frac{2 \pi A k}{1 + \pi^2 k^2 (x - c)^2}$ where A is proportional to the number of spins, $k = 2/\pi\Delta x$ and Δx is the line width, and (b) the Gaussian $I = 2\pi^{3/2} Ak \exp[-(x - c)^2 \pi^2 k^2]$ where A is proportional to the number of spins, $k = \frac{2 (\ln 2)^{1/2}}{\pi \Delta x}$, and Δx 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 ν , $x = \frac{h\nu}{\beta H}$, 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 θ 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 θ , 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.

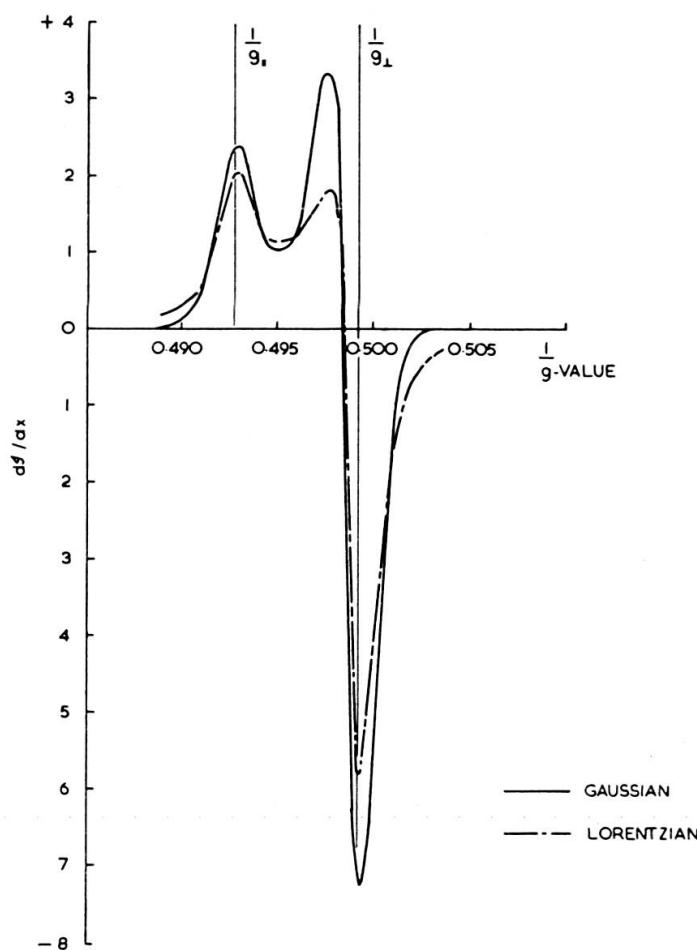


Fig. 1.

First differential of absorption for a polycrystalline substance using $g_u = 2.0295$, $g_{\perp} = 2.0034$ 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 $\Delta x = \Delta x_{\perp} + (\Delta x_{\parallel} - \Delta x_{\perp}) \cos \theta^2$ 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 θ .

¹ SEARL, J.W., R. C. SMITH, S. J. WYARD, 1959, *Proc. Phys. Soc.*, **74**, 491.
² BLEANEY, B., 1960, *Proc. Phys. Soc.*, **75**, 621.

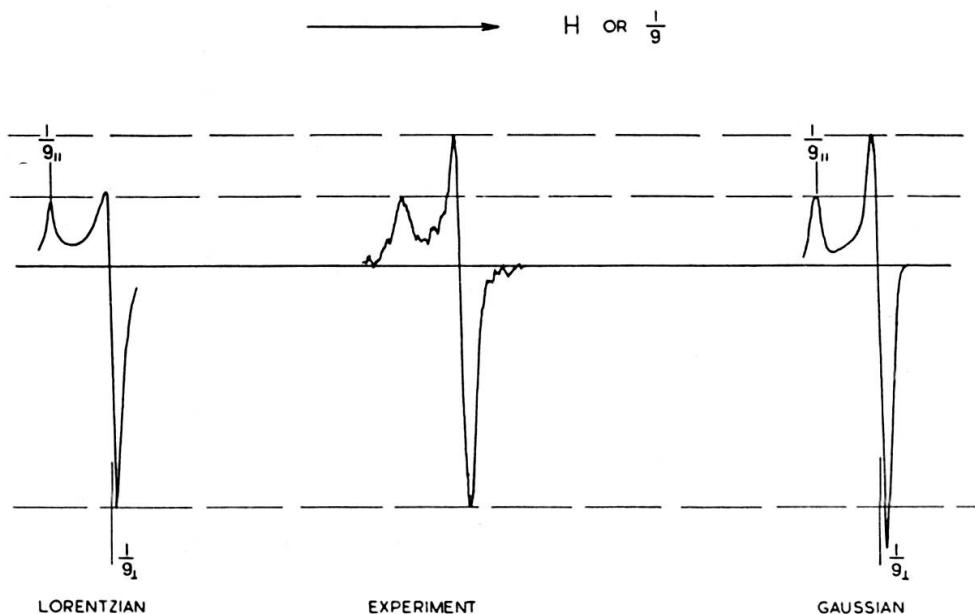


Fig. 2.

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 3100Å U.V. irradiated at $90^\circ K$, subsequently warmed for 5 minutes at $133.5^\circ K$.

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

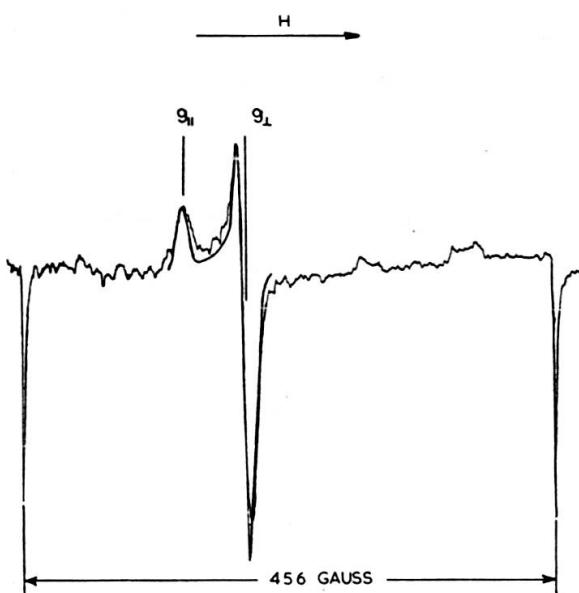


Fig. 3.

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