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X-ray attenuation coefficient of carbon for Cu $K\alpha_1$ radiation.

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The X-ray attenuation coefficient of carbon at λ(Cu $K\alpha_1$) has been measured with a specimen of highly oriented pyrolytic graphite, tilted to average inhomogeneities and change the beam path length. The values determined are μ(Cu $K\alpha_1$) = 9·246 (5) cm^{-1} and μ/ϱ(Cu $K\alpha_1$) = 4·080 (2) cm^2 g^{-1}. For Cu $K\bar{\alpha}$, the derived value is 4·089 (2) cm^2 g^{-1} and this differs significantly from the latest value, 4·219 cm^2 g^{-1} given in Vol. IV of *International Tables for X-ray Crystallography*.

The attenuation coefficient of carbon for Cu $K\alpha_1$ (λ = 1·54056 Å) X-rays was measured in the course of studies of the polarization factors for highly-oriented pyrolytic graphite crystals (Calvert, Killean & Mathieson, 1974*a*). The crystal examined in this particular experiment was a commercially available Union Carbide product, grade ZYA, with a nominal mosaic spread of 1°. A uniform plane-polarized beam of X-rays having a divergence of 7′, a circular cross section of diameter approximately 1 mm and an intensity of 17 kcounts s^{-1} was produced by reflexion from a pyrolytic graphite crystal (Calvert, Killean & Mathieson, 1974*b*). This beam was passed through another pyrolytic graphite crystal in order to determine the attenuation coefficient of carbon. The measurements were carried out using a device previously described (Mathieson, 1968). With this device the tilt angle of the specimen can be varied in angular steps from about 10° to the direct beam to 100° to the direct beam. This reduces effects due to possible inhomogeneities in the specimen crystal although these are small (Moore, 1973). It also assists in detecting and hence avoiding the occurrence of any diffraction conditions.

The thickness of the specimen crystal was measured several times at the corners of the crystal with a micrometer having a sensitivity of $2{\cdot}5\times10^{-5}$ cm, and over the area traversed by the X-ray beam with a specially constructed Sheffield air gauge sensitive to $2{\cdot}5\times10^{-4}$ cm. The mean thickness was determined as 0·1092(3) cm. The density was taken to be 2·266 g cm^{-3} (Moore, 1973). The low impurity level in highly oriented pyrolytic graphite specimens – probably less than 20 p.p.m. by weight and mostly due to silicon (Moore, 1973) – was neglected.

At each setting of the crystal 10^6 counts were accumulated and the direct beam was measured to this same precision before and after the transmitted-beam measurements. This established the mechanical and electronic stability of the system and showed that no corrections for drift needed to be applied. The counts were corrected for the system dead-time, which was measured by the method due to Chipman (1969) as $2{\cdot}54\times10^{-6}$ s. A correction was also applied for the background counting rate of 0·15 counts s^{-1}. Tests showed that no $\lambda/2$ component was detectable.

The linear and mass attenuation coefficients were determined respectively by calculating the mean values of μ and μ/ϱ from the data in Table 1 from the relationship

$$\mu=\frac{\sin\omega}{t}\cdot\ln\left[\frac{I_0}{I(\omega)}\right] \qquad (1)$$

where

ω is the angle between the crystal face and the direct beam,
I_0 is the intensity of the direct beam incident on the crystal,
$I(\omega)$ is the intensity of the direct beam after passing through the crystal,
t is the thickness of the crystal,
ϱ is the density of the specimen crystal.

Table 1. *The linear attenuation coefficient, μ, calculated from* (1)

The dead-time corrected incident beam had an intensity of 17437·7 c s^{-1}. The mean value of μ is 9·246 (5) cm^{-1} and of μ/ϱ is 4·080 (2) cm^2 g^{-1}. The angle ω was reset for each measurement.

ω (°)	$I(\omega)$ (c s^{-1})	μ (cm^{-1})
89·997	6325·5	9·286
89·997	6350·8	9·250
89·997	6355·4	9·243
89·997	6371·2	9·220
88·95	6348·8	9·251
88·90	6337·5	9·267
88·90	6368·5	9·222
88·35	6360·3	9·232
87·79	6337·6	9·262
87·79	6367·2	9·219
87·79	6361·9	9·227
87·79	6358·4	9·232
87·79	6328·0	9·276
87·24	6342·7	9·251
86·69	6339·3	9·251

The statistical errors in both I_0 and $I(\omega)$ are negligible compared with those in t, the standard error in the mean value of μ being 0·007 cm^{-1}. This error is to be compared with the statistical standard error in the mean value computed from the spread of values in Table 1 of 0·005 cm^{-1}. The values of the coefficients obtained are μ(Cu $K\alpha_1$) = 9·246(5) cm^{-1} and μ/ϱ(Cu $K\alpha_1$) = 4·080(2) cm^2 g^{-1}.

The experimental values of the mass attenuation coefficient for Cu $K\bar{\alpha}$ listed in *International Tables for X-ray Crystallography* (1962) range from 3·84 to 5·56 cm^2 g^{-1} The nearest to our linearly interpolated value for μ/ϱ(Cu $K\bar{\alpha}$) of 4·089(2) is 4·15 cm^2 g^{-1} (Chipman, 1955) but unfortunately there is no standard error quoted for this value. It is of interest that *International Tables* (1962) quotes a private communication from Dr H. J. Milledge which gives a mean value for the mass attenuation co-

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efficient of carbon of 4·17 $cm^2\ g^{-1}$. This value was obtained from twenty-three measurements on thirteen different diamond crystals with a spread of results from 3·95 to 4·54 $cm^2\ g^{-1}$.

Recently the tabulated value of the mass attenuation coefficient derived from smoothed functions of the mass attenuation coefficient against wavelength has been revised from 4·60 $cm^2\ gm^{-1}$ (*International Tables for X-ray Crystallography*, 1962) to 4·219 $cm^2\ gm^{-1}$ (*International Tables for X-ray Crystallography*, 1974): with this value is associated a $\pm \leq 2\%$ 'envelope of uncertainty' *i.e.* $\pm \leq 0{\cdot}084$ $cm^2\ g^{-1}$ and hence the outer limits of 4·219 $cm^2\ g^{-1}$ are $\leq 4{\cdot}303$ $cm^2\ g^{-1}$ and $\geq 4{\cdot}135$ $cm^2\ g^{-1}$. If these limits are taken to imply $\sigma \leq 0{\cdot}028$ $cm^2\ g^{-1}$ then the difference between the *International Tables* value of 4·219 $cm^2\ g^{-1}$ and our derived value of 4·089(2) $cm^2\ g^{-1}$ (for Cu $K\bar{\alpha}$) is significant. Clearly, in the most accurate experimental work, it is still essential to determine the mass attenuation coefficient experimentally.

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The information contained in neutron powder diagrams of magnetic materials.

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A reciprocal-space treatment is given of the effects of reflexion averaging on the information available from magnetic neutron powder diagrams. The results confirm those previously obtained by spin-density Patterson methods.

Introduction

Shirane (1959) has described the effects of reflexion overlap in powder patterns of magnetic materials which have a unique spin direction. The results have been extended to multi-spin axis structures by Wilkinson & Lisher (1973) using a spin density Patterson (real-space) treatment and subsequently verified by Litvin (1974) using group-theoretical methods. The present note reports the equivalent reciprocal-space treatment for multi-spin axis structures.

Theory

From the work of Halpern & Johnson (1939), the magnetic contribution to the *hkl* neutron diffraction line from a magnetically ordered material can be shown to be proportional to $I(\mathbf{k}) = |\mathbf{P}(\mathbf{k})|^2 - |\hat{\mathbf{k}} \,.\, \mathbf{P}(\mathbf{k})|^2$, where $\mathbf{P}(\mathbf{k})$ is a 'vector structure factor' defined by $\mathbf{P}(\mathbf{k}) = \sum_{i=1}^{n} \mathbf{S}_i f_i(\mathbf{k}) \times \exp 2\pi j \mathbf{k} \,.\, \mathbf{r}_i$ for a magnetic unit cell in which the atoms are in positions $\mathbf{r}_i$ and have spins $\mathbf{S}_i$ and form factors f_i. $\mathbf{k}$ is the scattering vector for the *hkl* reflexion and $\hat{\mathbf{k}}$ is a unit vector in the direction of $\mathbf{k}$.

Thus

$$\begin{aligned} I(\mathbf{k}) &= |\mathbf{P}(\mathbf{k})|^2 - |\hat{\mathbf{k}} \,.\, \mathbf{P}(\mathbf{k})|^2 \\ &= |\mathbf{P}(\mathbf{k})|^2 [1 - \hat{\mathbf{k}} \,.\, \hat{\mathbf{P}}(\mathbf{k})]^2 \\ &= |\mathbf{P}(\mathbf{k})|^2 \sin^2 \tau \end{aligned}$$

where τ is the angle between $\mathbf{k}$ and $\mathbf{P}(\mathbf{k})$.

Now

$$|\mathbf{P}(\mathbf{k})|^2 = \sum_{i=1}^{n} |\mathbf{S}_i|^2 f_i^2 + 2 \sum_{i \neq j}^{n} \mathbf{S}_i \,.\, \mathbf{S}_j f_i f_j \cos 2\pi \mathbf{k} \,.\, (\mathbf{r}_i - \mathbf{r}_j)$$

and the information contained in $|\mathbf{P}(\mathbf{k})|^2$ therefore concerns the magnitudes of the spins $\mathbf{S}_1 \ldots \mathbf{S}_n$ and the relative angles between them. There are no terms involving the orientation of the spins relative to the crystallographic axes of the material. This dependence is contained within the term $\sin^2 \tau$, and as shown by Shirane it is the averaging of this term over overlapped reflexions which results in a loss of information when the configurational symmetry is higher than orthorhombic.

In fact, it is easy to show that $\mathbf{P}(\mathbf{k})$ is identical for reflexions of the form $\{hkl\}$ related by the configurational symmetry axis. Consider, for example, a magnetic structure with tetragonal configurational symmetry. Atoms in positions x,y,z; $\bar{y},x,z$; $\bar{x},\bar{y},z$; $y,\bar{x},z$ related by the configurational tetrad have identical spins $\mathbf{S}$ and the expression for $\mathbf{P}(\mathbf{k})$ is

$$\begin{aligned} \mathbf{P}(hkl) = \sum_{i=1}^{n} \mathbf{S}_i f_i \{ & \exp [2\pi j(hx_i + ky_i + lz_i)] \\ & + \exp [2\pi j(h\bar{y}_i + kx_i + lz_i)] \\ & + \exp [2\pi j(h\bar{x}_i + k\bar{y}_i + lz_i)] \\ & + \exp [2\pi j(hy_i + k\bar{x}_i + lz_i)] \} \end{aligned}$$

where the symmation is taken over all groups related by the fourfold axis. The reflexion $\bar{k}hl$ has

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