SPECTRUM CORRECTION FACTORS FOR SAMPLE HOLDER AND SELF-SHIELDING EFFECTS FOR PLANAR SAMPLES IN THERMAL NEUTRON SCATTERING STUDIES

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ABSTRACT

Spectrum correction factors, for application to neutron scattering data, due to sample holder and self-shielding effects in planar samples have been derived for three cases: (1) a bare sample, (2) a sample contained in a can, and (3) a two-component sample (eg a metal hydride) in a can where the scattering from one component has to be separated from the scattering from the second component.

1. INTRODUCTION

When a monochromatic neutron beam is incident upon a flat sample contained in a sample holder then it is usually necessary when analysing the scattered polychromatic neutron spectrum to correct for the effect of the scattering and absorption properties of the sample holder on the spectrum as well as the self-shielding or filtering properties of the sample itself. Subtracting the sample holder spectrum from the sample + holder spectrum is in many cases not sufficiently accurate. This correction will be a function of the angle α of the sample to the beam, the angle θ of the scattered beam, and the energy of the scattered neutron.

Three cases are considered: that of a simple bare slab sample; that of a slab sample contained in a sample holder; and that of a metal hydride/metal sample contained in a sample holder where the scattering from the hydrogen is to be determined.

It is shown in the last section that in certain circumstances it is not necessary to carry out a measurement of the can scattering.

2. A ONE-COMPONENT SYSTEM

A one-component system is defined as a sample which is not contained in a sample holder. It is of necessity solid and the correction factor derived could typically be applied to the vanadium standard sample. It is purely a self-shielding or filtering correction and is an extension of the theory due to Birchall (1970) and Cocking (Wignall 1967).

If the monochromatic intensity incident upon the sample is I_o then the intensity I_ℓ at ℓ (see fig. 1) is given by

$$I_\ell = I_o \exp - \Sigma_s^i \ell$$

where Σ represents the total macroscopic cross-section (absorption and scattering) of the sample, the subscript s refers to the sample, and the superscript, i (initial) or f (final), refers to the energy of the neutron.

Thus the number of neutrons scattered in the elemental distance $d\ell$ into $d\Omega d\tau$ is

$$= I_o \exp(-\Sigma_s^i \ell).n_s \frac{d^2\sigma_s}{d\Omega d\tau} \, d\ell$$

where $d^2\sigma_s/d\Omega d\tau$ is the double differential scattering cross-section per atom of the sample and n_s is the number of sample atoms per cm^3.

Thus the number of these which emerge from the sample is

$$= I_o \exp(-\Sigma_s^i \ell).n_s \frac{d^2\sigma s}{d\Omega d\tau} d\ell \exp(-\Sigma_s^f x)$$

and the total intensity I_{Bs} from the whole bare sample is

$$I_{Bs} = \int_o^L I_o \exp(-\Sigma_s^i \ell).n_s \frac{d^2\sigma s}{d\Omega d\tau} d\ell \exp\left[-\Sigma_s^f (L - \ell) \frac{\sin\alpha}{\sin(\theta + \alpha)}\right]$$

$$= I_o n_s \frac{d^2\sigma s}{d\Omega d\tau} \exp\left(-\Sigma_s^f L \frac{\sin\alpha}{\sin(\theta + \alpha)}\right)\left[\frac{\exp(\Sigma_s^f \frac{\sin\alpha}{\sin(\theta+\alpha)} - \Sigma_s^i)L - 1}{\Sigma_s^f \frac{\sin\alpha}{\sin(\theta+\alpha)} - \Sigma_s^i}\right]$$

Were there to be no attenuation of the primary beam then the theoretical intensity from the sample I_{Ts} would have been

$$I_{Ts} = I_o n_s \frac{d^2\sigma_s}{d\Omega d\tau} L$$

Thus $$\underline{I_{Bs} = \phi(f) I_{Ts}}$$

where the attenuation coefficient for self-shielding is

$$\phi(f) = \exp\left(-\Sigma_s^f L \frac{\sin\alpha}{\sin(\theta+\alpha)}\right).\left[\frac{\exp(\Sigma_s^f \frac{\sin\alpha}{\sin(\theta+\alpha)} - \Sigma_s^i) L - 1}{(\Sigma_s^f \frac{\sin\alpha}{\sin(\theta+\alpha)} - \Sigma_s^i) L}\right]$$

For the special case of elastic scattering where the sample is also half-angled with respect to the scattered beam then $\alpha = \pi/2 - \theta/2$ and the factor in square brackets reduces to unity and

$$\phi(i) = \exp - \Sigma_s^i \frac{W}{\cos\theta/2}$$

where W is the thickness of the sample.

3. A TWO-COMPONENT SYSTEM

When the sample has to be held in a holder or can (eg a liquid or a powder) then this constitutes a two-component system. In order to obtain the true scattering from the sample the scattering from the can must be subtracted correctly as well as taking into account the self-shielding of the sample as in Section 2.

Consider the scattering from the first and second walls of the sample can separately with the sample present (see fig. 2). The intensity at t is given by

$$I_t = I_o \exp(-\Sigma_c^i t)$$

where the subscript c refers to the can. This is a similar calculation to the one carried out in Section 1, the total intensity from the first wall of the sample can being

$$I_1 = I_o n_c \frac{d^2\sigma_c}{d\Omega d\tau} \exp(-\Sigma_s^f y).\ \exp(-\Sigma_c^f z).\ \exp(-\Sigma_c^f T \frac{\sin\alpha}{\sin(\theta+\alpha)})$$

$$\times \left[\frac{\exp(\Sigma_c^f \frac{\sin\alpha}{\sin(\theta+\alpha)} - \Sigma_c^i)T - 1}{\Sigma_c^f \frac{\sin\alpha}{\sin(\theta+\alpha)} - \Sigma_c^i} \right]$$

Similarly the total intensity from the second wall is

$$I_2 = I_o n_c \frac{d^2\sigma_c}{d\Omega d\tau} \exp(-\Sigma_s^i L).\ \exp(-\Sigma_c^i T).\ \exp(-\Sigma_c^f T \frac{\sin\alpha}{\sin(\theta+\alpha)}).$$

$$\times \left[\frac{\exp(\Sigma_c^f \frac{\sin\alpha}{\sin(\theta+\alpha)} - \Sigma_c^i)\ T - 1}{\Sigma_c^f \frac{\sin\alpha}{\sin(\theta+\alpha)} - \Sigma_c^i} \right]$$

Thus the total scattering into $d\Omega d\tau$ from the sample can in the presence of the sample is

$$I_c = I_1 + I_2$$

However the total scattering from the bare can without the sample, again taking into account the self-shielding is given by

$$I_{Bc} = I_o n_c \frac{d^2\sigma_c}{d\Omega d\tau} \exp\left[-\Sigma_c^f\ 2T \frac{\sin\alpha}{\sin(\theta+\alpha)}\right] \cdot \left[\frac{\exp(\Sigma_c^f \frac{\sin\alpha}{\sin(\theta+\alpha)} - \Sigma_c^i)2T - 1}{\Sigma_c^f \frac{\sin\alpha}{\sin(\theta+\alpha)} - \Sigma_c^i} \right]$$

$$\therefore \quad I_c = \gamma(f) I_{Bc}$$

where $\gamma(f)$ = attenuation coefficient of the can scattering due to the presence of the sample and is given by

$$\gamma(f) = \left[\exp(-\Sigma_s^i L).\ \exp(-\Sigma_c^i T) + \exp(-\Sigma_s^f y).\ \exp(-\Sigma_c^f z)\right] .$$

$$\times \exp\left(\Sigma_c^f T \frac{\sin\alpha}{\sin(\theta+\alpha)}\right) .\ \left[\frac{\exp(\Sigma_c^f \frac{\sin\alpha}{\sin(\theta+\alpha)} - \Sigma_c^i)T - 1}{\exp(\Sigma_c^f \frac{\sin\alpha}{\sin(\theta+\alpha)} - \Sigma_c^i)2T - 1}\right]$$

Now consider the scattering contribution to the spectrum from the sample I_s in the presence of the can. It may be shown by a similar analysis that

$$I_s = \alpha(f) I_{Bs} = \alpha(f)\ \phi(f) I_{Ts}$$

where $\alpha(f)$ is the attenuation of the bare sample scattering I_{Bs} due to the presence of the can and is given by

$$\alpha(f) = \exp(-\Sigma_c^i T).\ \exp(-\Sigma_c^f z)$$

and I_{Ts} is the theoretical scattering from the sample in the absence of the can. The self-shielding coefficient $\phi(f)$ is given by

$$\phi(f) = \exp\left(-\Sigma_s^f \frac{\sin\alpha}{\sin(\theta+\alpha)} L\right).\ \left[\frac{\exp(\Sigma_s^f \frac{\sin\alpha}{\sin(\theta+\alpha)} - \Sigma_s^i)L - 1}{(\Sigma_s^f \frac{\sin\alpha}{\sin(\theta+\alpha)} - \Sigma_s^i)L}\right]$$

Now the experimentally measured spectrum from the sample in the can I_{s+c} is made up of the scattering from the can in the presence of the sample and from the sample in the presence of the can, ie:-

$$I_{s+c} = I_s + I_c$$

$$= \alpha(f) I_{Bs} + \gamma(f) I_{Bc}$$

$$= \alpha(f)\ \phi(f) I_{Ts} + \gamma(f)\ I_{Bc}$$

$$\therefore \quad I_{Ts} = \frac{I_{s+c} - \gamma(f) I_{Bc}}{\alpha(f)\ \phi(f)}$$

Thus by measuring I_{s+c} and I_{Bc} and calculating the attenuation coefficients α, ϕ, and γ the theoretical scattering from the sample I_{Ts} can be obtained.

Note, for use in Section 4, that the scattering from the bare sample without taking into account the self-shielding is given by

$$I_B = \frac{I_{s+c} - \gamma(f) I_{Bc}}{\alpha(f)} \qquad \ldots\ldots\ (1)$$

4. A THREE-COMPONENT SYSTEM

As an example of a three-component system take the case of a metal hydrogen system enclosed in a sample can. Measurements are normally made with and without the hydrogen present and the two spectra subtracted. However this is only correct in one special case. In all other cases a separate spectrum from the can also needs to be measured.

From the theory in section 3 correction for the presence of the sample can may be effected by applying equation (1) to the bare can and can + sample spectra giving I_{BM} and I_{BMH}, the theoretical intensity from the bare metal and bare metal hydride respectively without the attenuation coefficient for the self-shielding being applied. This latter factor must be evaluated. The system is shown in fig. 3.

To calculate the scattering from the bare metal hydride I_{BMH}, the scattering from the metal in the presence of hydrogen $I_{M/H}$ and the scattering from the hydrogen in the presence of metal $I_{H/M}$ must be determined separately. It is found that

$$I_{M/H} = I_o n_M \frac{d^2\sigma_M}{d\Omega d\tau} \exp - (\Sigma_M^f + \Sigma_H^f)L \frac{\sin\alpha}{\sin(\theta+\alpha)} \left[\frac{\exp\left[(\Sigma_M^f + \Sigma_M^f)\frac{\sin\alpha}{\sin(\theta+\alpha)} - (\Sigma_M^i + \Sigma_H^i)\right] L - 1}{(\Sigma_M^f + \Sigma_M^f)\frac{\sin\alpha}{\sin(\theta+\alpha)} - (\Sigma_M^i + \Sigma_H^i)} \right]$$

$$= I_o n_M \frac{d^2\sigma_M}{d\Omega d\tau} \rho(f)$$

and

$$I_{H/M} = I_o n_H \frac{d^2\sigma_H}{d\Omega d\tau} \rho(f)$$

$$\therefore \quad I_{BMH} = I_{M/H} + I_{H/M}$$

$$= I_o \rho(f) \left[n_M \frac{d^2\sigma_M}{d\Omega d\tau} + n_H \frac{d^2\alpha_H}{d\Omega d\tau} \right]$$

If there were no self-shielding, all nuclei in the sample would see I_o then:

$$I_{TMH} = I_o \left[n_M \frac{d^2\sigma_M}{d\Omega d\tau} + n_H \frac{d^2\sigma_H}{d\Omega d\tau} \right] L \quad = \frac{I_{BMH} L}{\rho(f)}$$

or

$$I_{TMH} = \frac{I_{BMH}}{\phi_{MH}(f)} \qquad \ldots\ldots\ldots (2)$$

where $\phi_{MH}(f)$ is the self-shielding or filtering factor for the metal hydride.

Now the scattering from the metal is just the result of the one-component system, ie

$$I_{TM} = \frac{I_{BM}}{\phi_M(f)} \qquad \ldots\ldots\ldots (3)$$

where $\phi_M(f)$ is the self-shielding factor for the metal given by

$$\phi_M(f) = \exp(-\Sigma_M^f L \frac{\sin\alpha}{\sin(\theta+\alpha)}) \cdot \left[\frac{\exp(\Sigma_M^f \frac{\sin\alpha}{\sin(\theta+\alpha)} - \Sigma_M^i)L - 1}{(\Sigma_M^f \frac{\sin\alpha}{\sin(\theta+\alpha)} - \Sigma_M^i)L}\right]$$

Thus the theoretical scattering from the hydrogen in the metal, ie the final corrected spectrum is given by the difference of equations (2) and (3).

$$I_H = \left[\frac{I_{BMH}}{\phi_{MH}(f)} - \frac{I_{BM}}{\phi_M(f)}\right]$$

or, substituting in equation (1)

$$I_H = \left[\frac{I_{MH+c} - \gamma_{MH}(f) I_{Bc}}{\alpha(f)\phi_{MH}(f)} - \frac{I_{M+c} - \gamma_M(f) I_{Bc}}{\alpha(f)\phi_M(f)}\right]$$

For the special case of elastic scattering where the sample is half-angled with respect to the scattered beam then

$$\alpha(i) = \exp(-2\Sigma_c^i \frac{W}{\cos\theta/2})$$

where W is the wall thickness of the can

$$\gamma_{MH}(i) = \exp -(\Sigma_M^i + \Sigma_H^i) \frac{W}{\cos\theta/2}$$

$$\gamma_M(i) = \exp -\Sigma_M^i \frac{W}{\cos\theta/2}$$

$$\phi_{MH}(i) = \exp -(\Sigma_M^i + \Sigma_H^i) \frac{W}{\cos\theta/2}$$

and

$$\phi_M(i) = \exp -\Sigma_M^i \frac{W}{\cos\phi/2}$$

Now it can be seen that $\gamma_{MH}(i) = \phi_{MH}(i) \equiv \beta(i)$

$$\text{and } \gamma_M(i) = \phi_M(i) \equiv \delta(i)$$

$$\therefore \quad I_H = \frac{1}{\alpha(i)} \left[\frac{I_{MH+c}}{\beta(i)} - \frac{I_{M+c}}{\delta(i)} \right]$$

Thus for this special case only there is no need to make separate measurement of the scattering from a bare can.

5. REFERENCES

Birchall J H L, PhD thesis, University of Birmingham (1971)

Cocking S J, in Wignall G D, AERE Report M1928 (1967).

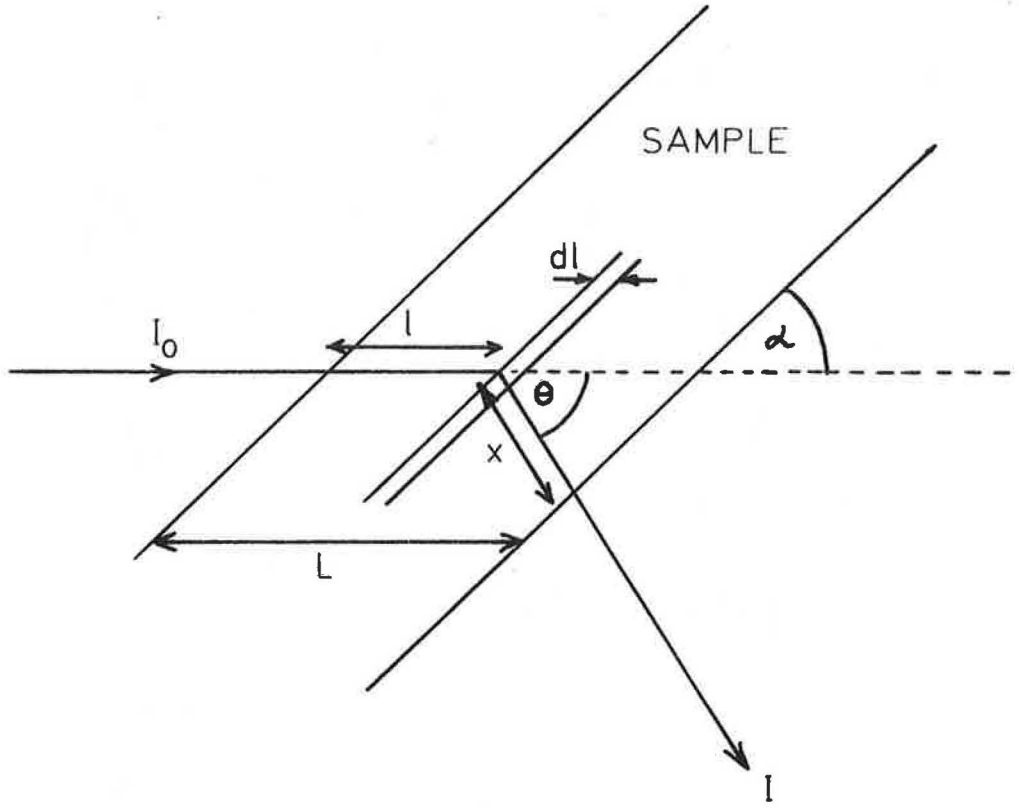

FIG 1 ONE COMPONENT SYSTEM

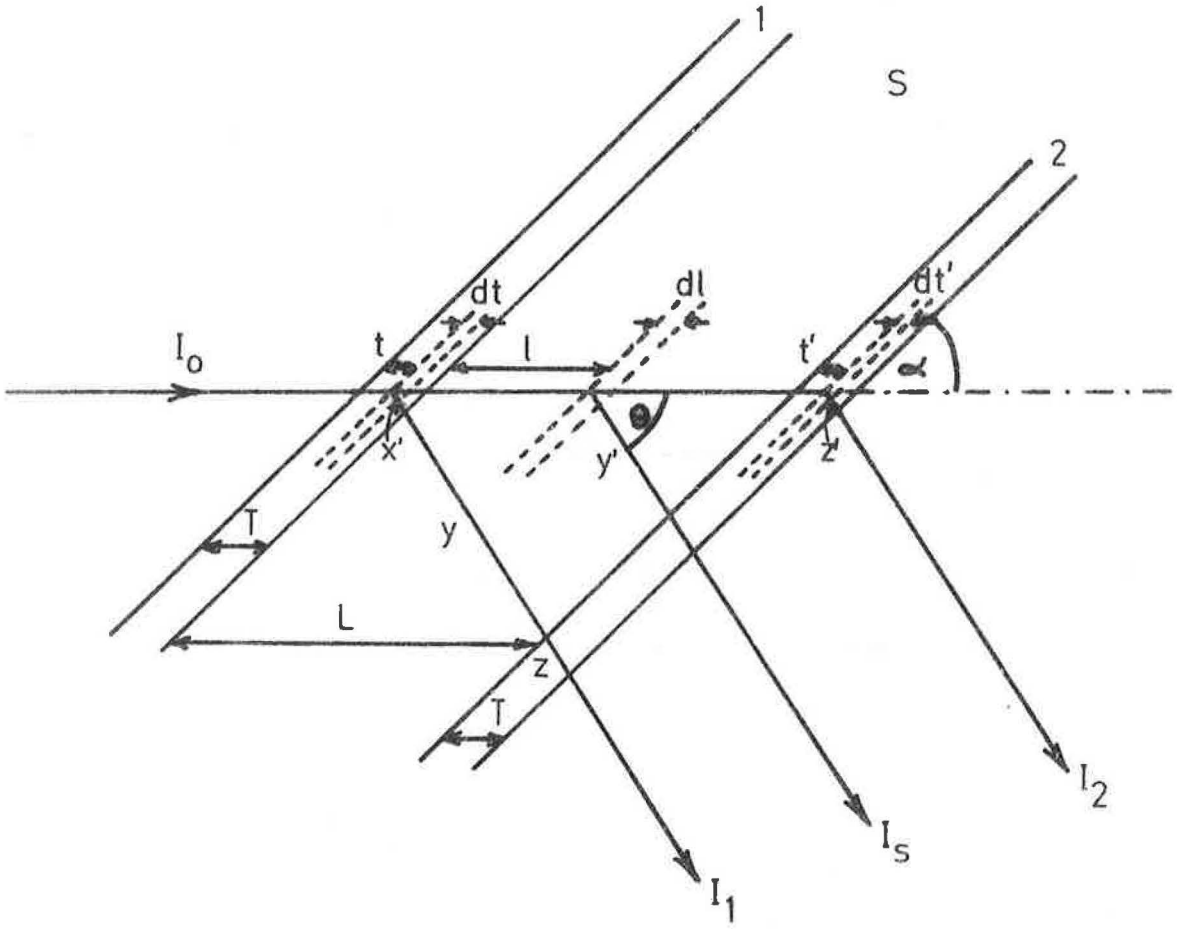

FIG 2 TWO COMPONENT SYSTEM

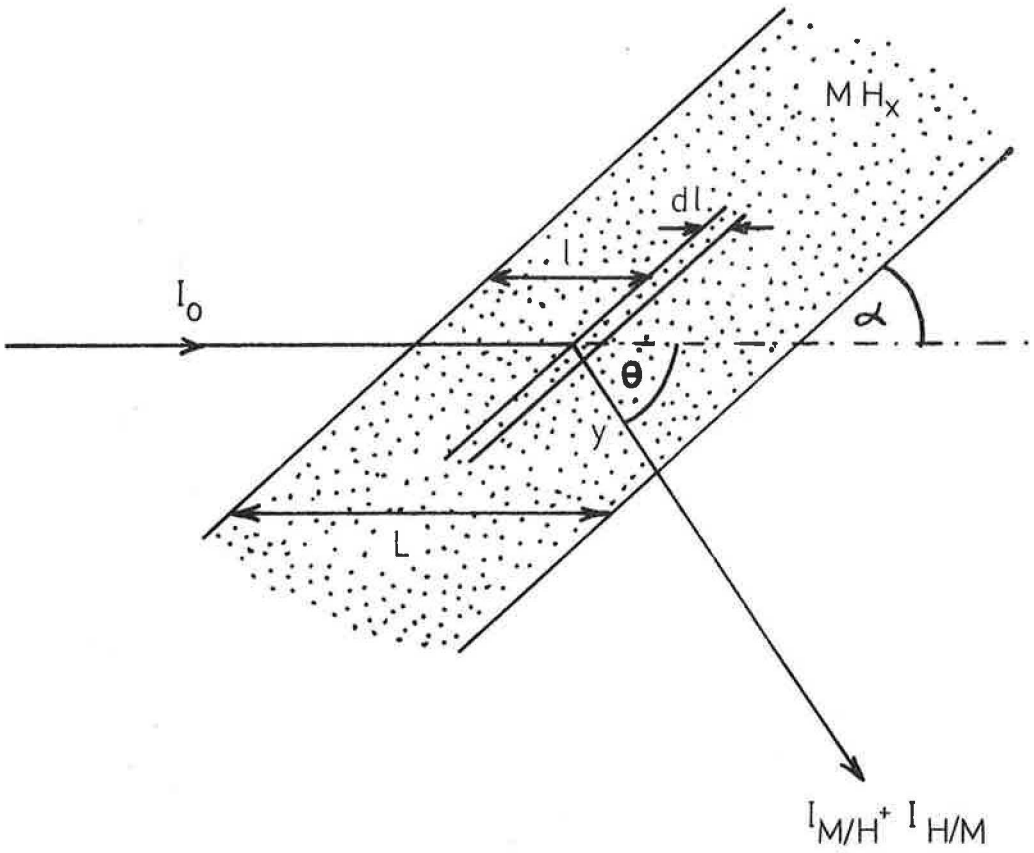

FIG 3 METAL HYDROGEN SYSTEM