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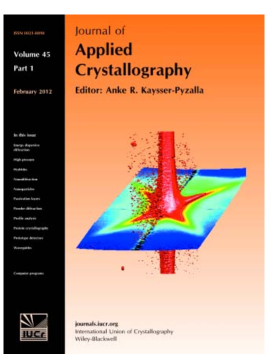

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X-ray and neutron attenuation correction factors for spherical samples

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A method is derived to calculate the attenuation correction factors for elastic or inelastic X-ray or neutron scattering experiments using a spherical sample. The method can be applied to a sphere that is either fully or partially illuminated by an incident beam of rectangular cross-sectional area. The required input parameters are the energy-dependent attenuation coefficients, the radius of the sphere and the dimensions of the incident beam. In-plane scattering is assumed.

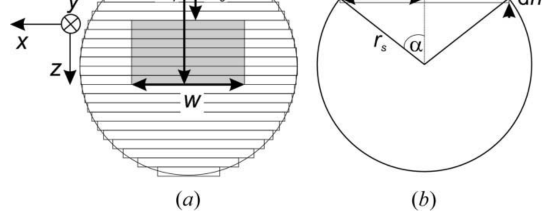
1. Introduction

X-ray and neutron scattering experiments are routinely performed on liquid and amorphous materials using levitation techniques, *e.g.* acoustic, aerodynamic, electrostatic or electromagnetic, where the sample shape is approximately spherical (*e.g.* Barnes *et al.*, 2009; Price, 2010; Hennet *et al.*, 2011; Neuefeind *et al.*, 2011; Egry & Holland-Moritz, 2011). For these experiments and also, for example, for a pair distribution function analysis of the diffraction data for polycrystalline samples (*e.g.* Egami & Billinge, 2003), it is necessary to calculate the sample attenuation correction factors if accurate results are to be obtained. Dwiggins (1975*a*,*b*) calculated the attenuation correction factors for elastic scattering for a fully illuminated sphere by first considering the attenuation correction factors for a cylinder. However, in aerodynamic levitation experiments, for example, the sphere is partly shielded by the nozzle that supplies the gas flow such that the covered part does not contribute to the scattered intensity (*e.g.* Hennet *et al.*, 2006). It is also possible to perform inelastic scattering experiments on levitated samples (*e.g.* Sinn *et al.*, 2003; Price *et al.*, 2008).

2. Method

2.1. The case when the incident beam is wider than the illuminated part of the sample

As shown in Fig. 1, a sphere can be constructed from cylinders of varying radius, r, and infinitesimally small height, dh. The path lengths for in-plane scattering of radiation by a sphere can then be found by calculating the incident and scattered path lengths L and L' through each cylinder illuminated by the incident beam and taking a weighted average. The radius of each cylinder, r, can be calculated by considering Fig. 1(*b*), in which $\cos\alpha = (r_s - h)/r_s = 1 - h/r_s$ and $\sin\alpha = r/r_s = (1 - \cos^2\alpha)^{1/2}$, where r_s is the radius of the sphere, h is the distance of the cylinder from the top of the sphere and α is the specified angle. It then follows that $r = r_s(2h/r_s - h^2/r_s^2)^{1/2}$.



(*a*) (*b*)

Figure 1
Side elevation showing (*a*) the dimensions of the incident beam (shaded grey area) and its position relative to the sphere and (*b*) the parameters describing each cylinder of radius r and height dh within the sphere.

The attenuation correction factors for a cylindrical sample placed perpendicular to the incident beam have previously been calculated. Sears (1984), following a method derived by Blake (1933), calculated them to be

$$A_{\rm cyl}(2\theta, {\rm E}) = 1/(\pi r^2)\int_0^r R\,{\rm d}R\int_0^{2\pi}\exp\left[-\mu(E_{\rm i})L - \mu(E_{\rm f})L'\right]{\rm d}\beta, \quad (1)$$

where, as shown in Fig. 2, the distance R and angle β define the position of a scattering event within the plane of the cylinder in polar coordinates, 2θ is the scattering angle, and E signifies that the calculation is in general valid for an inelastic scattering experiment. In equation (1), $\mu(E_{\rm i}) = n_{\rm s}\sigma_{\rm s}(E_{\rm i})$ and $\mu(E_{\rm f}) = n_{\rm s}\sigma_{\rm s}(E_{\rm f})$ are the attenuation coefficients for the sample at the energy of the incident and scattered radiation, $E_{\rm i}$ and $E_{\rm f}$, respectively, $n_{\rm s}$ is the atomic number density of the sample, while $\sigma_{\rm s}(E_{\rm i})$ and $\sigma_{\rm s}(E_{\rm f})$ are the total (scattering plus absorption) cross sections of the sample. In a diffraction experiment $E_{\rm i} = E_{\rm f}$ so $\mu(E_{\rm i}) = \mu(E_{\rm f})$. The incident and scattered path lengths, L and L', can be calculated by considering Fig. 2. The incident path length is given by

$$L = L_1 + L_2 = (r^2 - b^2)^{1/2} + R\cos\beta, \quad (2)$$

and the scattered path length is given by

$$L' = (L' + L_1') - L_1' = \left(r^2 - a^2\right)^{1/2} - R\cos(2\theta - \beta), \quad (3)$$

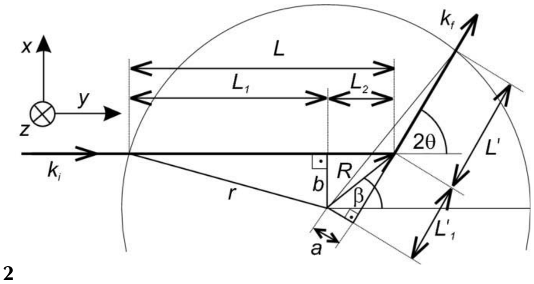


Figure 2
Plan view to show the incident and scattered path lengths, L and L', of the radiation for in-plane scattering in a cylindrical sample of radius r, where the scattering event takes place at a point with polar coordinates R and β. $k_{\rm i}$ and $k_{\rm f}$ are the magnitudes of the wavevectors for the incident and scattered radiation, respectively, and 2θ is the scattering angle.

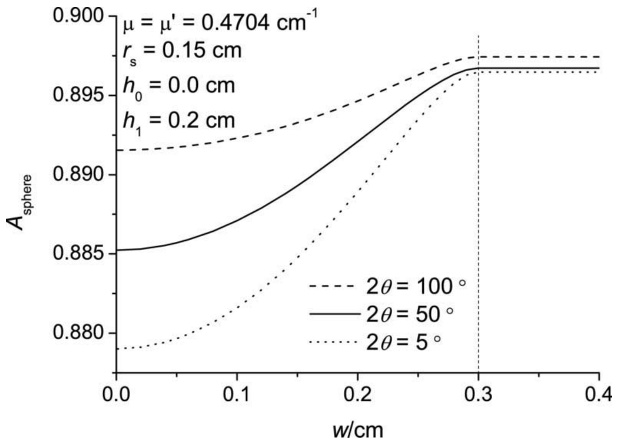


Figure 3
The dependence of the attenuation correction factor, A_{sphere}, for elastic scattering on the width of the incident beam w for scattering angles 2θ of 5, 50 and 100°. The results are presented for a spherical vanadium sample of radius $r_s = 0.15$ cm with an incident neutron wavelength of $\lambda = 0.5$ Å. For a given scattering angle, A_{sphere} is a constant for $w > 2r_s = 0.3$ cm since the sample is then fully illuminated by the incident beam.

where $a = R\sin(2\theta - \beta)$ and $b = R\sin\beta$. The attenuation correction factors for a fully or partially illuminated sphere are found by averaging over the illuminated volume:

$$A_{\mathrm{sphere}}(2\theta, \mathrm{E}) = \int_{h_0}^{h_1} A_{\mathrm{cyl}}(2\theta, \mathrm{E})\, r^2\, \mathrm{d}h \Big/ \int_{h_0}^{h_1} r^2\, \mathrm{d}h, \qquad (4)$$

where h_0 and h_1 are the upper and lower bounds of the beam illuminating the sample as shown in Fig. 1(a). Note that the attenuation correction factors for a fully illuminated sphere are equal to the attenuation correction factors for a fully illuminated hemisphere owing to the symmetry of the sample.

2.2. The case when the incident beam is narrower than the illuminated part of the sample

If $w < 2r_{\max}$, where $r_{\max}$ is the maximum radius of a cylinder within the illuminated part of the sample (see Fig. 1a), it is better for numerical reasons to perform the integration in Cartesian coordinates with the origin of coordinates placed at the top of the sphere, the x axis placed horizontally and the y axis placed in the direction of the incident beam, which is defined by the wavevector $\mathbf{k}_i$. The relations between the coordinates are given by

$$R^2 = x^2 + y^2 \quad \text{and} \quad \beta = \begin{cases} \arctan(x/y) & \text{if} \quad y > 0, \\ \arctan(x/y) + \pi & \text{if} \quad y < 0. \end{cases} \qquad (5)$$

It then follows that the attenuation correction factors for a cylinder are given by

$$A_{\mathrm{cyl}}(2\theta, \mathrm{E}) = \frac{\int_{-w/2}^{w/2} \left\{ \int_{-(r^2-x^2)^{1/2}}^{(r^2-x^2)^{1/2}} \exp\left[-\mu(E_{\mathrm{i}})L - \mu(E_{\mathrm{f}})L'\right] \mathrm{d}y \right\} \mathrm{d}x}{\int_{-w/2}^{w/2} \left[\int_{-(r^2-x^2)^{1/2}}^{(r^2-x^2)^{1/2}} \mathrm{d}y \right] \mathrm{d}x}, \qquad (6)$$

where L and L' are given by equations (2) and (3), respectively, with β and R transformed into Cartesian coordinates [equations (5)] and the beam is assumed to be symmetric around the vertical axis of the sample. These attenuation correction factors can then be inserted into equation (4) to give the attenuation correction factors for a sphere, $A_{\mathrm{sphere}}(2\theta, \mathrm{E})$. An example of the dependence of $A_{\mathrm{sphere}}(2\theta, \mathrm{E})$ on the width of the incident beam is given in Fig. 3.

In the case of elastic scattering, the calculations of $A_{\mathrm{cyl}}(2\theta, \mathrm{E})$ were checked against those obtained using the method of Paalman & Pings (1962) for $w \geq 2r$ and the method of Kendig & Pings (1965) for $w \leq 2r$. The calculations of the attenuation correction factors for a spherical sample agree with those obtained by Dwiggins (1975a,b) for elastic scattering when the whole sphere is illuminated.

3. Conclusions

The attenuation correction factors are calculated for elastic or inelastic X-ray or neutron scattering experiments using a spherical sample which is fully or partially illuminated by an incident beam of rectangular cross-sectional area, thus extending the results of Dwiggins (1975a,b) in which elastic scattering was considered for a fully illuminated sphere. The results will find application in, for example, levitation experiments.

A *Mathcad* (PTC, Needham, MA, USA) script to calculate the attenuation correction factors can be obtained by contacting the author.

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