

How thick should my sample be?

Cautionary remarks

The most common answer to the question "How thick should my sample be?", or more generally "What should be the dimensions of my sample?", is that the sample should be a "10% scatterer", which presumably means that 10% of the neutrons that enter the sample are scattered at least once (or does it mean that 10% of the neutrons are scattered once and then leave without being absorbed or scattered again?) The argument is that a "10% scatterer" scatters roughly 10% of the scattered neutrons a second time (and ~10% of those neutrons yet again), and that this amount of multiple scattering is in some sense acceptable.

The fact that a sample is a "10% scatterer" does not necessarily imply that ~10% of the scattered neutrons are scattered again before they exit the sample. For example, Wuttke (Physica B **292**, 194 (2000)) has shown that a thin annular sample whose transmission is 96% for a tightly collimated beam, and ~94% for a beam that fully illuminates the sample, scatters ~10% of the scattered neutrons a second time. This implies that a "10% scatterer", meaning a sample with little absorption and a transmission of about 90% (depending how it is measured), scatters something like 15-25% of the neutrons a second time.

An experimentalist sometimes has to decide the dimensions of his or her sample using a calculated value for the transmission. This implies that the macroscopic scattering and absorption cross sections are known. The number density can generally be calculated quite well, and the microscopic cross sections are generally obtained from a compilation such as that of Sears in Neutron News **3** (3), 26 (1992). This approach can be quite misleading, especially for hydrogenous materials. This is discussed below, under the heading "Scattering cross sections". See also a forthcoming article entitled "Total neutron scattering cross sections" by J.R.D. Copley, to be published in Neutron News.

Calculating the scattering probability given the dimensions of a sample

Given the proposed geometry (we shall consider slabs, cylinders and annular samples), and the relevant macroscopic scattering and absorption cross sections, Σ_S and Σ_A respectively, the scattering probability, S , can be calculated. Note that S is the probability of scattering at least once (followed by escape, absorption or additional scattering).

For a *slab sample* of thickness t , whose normal is at an angle α to the beam,

$$S = \frac{\Sigma_S}{\Sigma_T} [1 - \exp(-\Sigma_T t \sec \alpha)].$$

For a fully illuminated *cylindrical sample* of radius R , with axis normal to the beam,

$$S = \frac{\Sigma_S}{\Sigma_T} \frac{1}{2R} \int_{-R}^R dy [1 - \exp(-2\Sigma_T d(y))]$$

where $d(y) = \sqrt{R^2 - y^2}$.

For a fully illuminated *annular sample* with inner and outer radii R_1 and R_2 respectively (annular thickness $t = R_2 - R_1$), whose axis is normal to the beam,

$$S = \frac{\Sigma_s}{\Sigma_T} \frac{1}{2R_2} \int_{-R_2}^{R_2} dy \left[1 - \exp(-2\Sigma_T \{d_2(y) - d_1(y)\}) \right]$$

where $d_2(y) = \sqrt{R_2^2 - y^2}$, $d_1(y) = \sqrt{R_1^2 - y^2}$ if $y < R_1$, and $d_1(y) = 0$ if $y \geq R_1$.

Calculating the dimensions of a sample given its scattering probability

For a *slab sample* normal to the beam, the value of t can be directly obtained from the single scattering probability expression:

$$t = -\frac{1}{\Sigma_T} \ln \left[1 - \frac{S\Sigma_T}{\Sigma_s} \right].$$

There is no solution if $S > \Sigma_s / \Sigma_T$.

For the general case of an *annular sample* there is no analytical solution so the integral must be calculated numerically. An approximate solution (which is only valid if $t \ll R_{1,2}$) is based on the approximate result

$$S = \frac{\Sigma_s}{\Sigma_T} \left[1 - \exp(-\pi\Sigma_T t) \right]$$

which yields

$$t = -\frac{1}{\pi\Sigma_T} \ln \left[1 - \frac{S\Sigma_T}{\Sigma_s} \right].$$

Again there is no solution if $S > \Sigma_s / \Sigma_T$.

For the general case of a *cylindrical sample* there is no analytical solution. The integral can be calculated numerically as a function of the dimensionless magnitude $\Sigma_T R$.

Scattering cross sections

In general the macroscopic total scattering cross section Σ_s is not the same as the macroscopic bound atom scattering cross section Σ_B ; Σ_s depends on much more, including the temperature, the incident neutron energy, and the physics and chemistry, indeed the structure and dynamics of the sample. (Think about the ideal gas, a rigid crystalline solid, graphite, beryllium, water, the ammonium halides, etc.)

The *macroscopic bound atom scattering cross section* Σ_B may be calculated as follows:

$\Sigma_B = \sum_k \rho_k \sigma_k$ with $\rho_k = \rho_N n_k$, $\rho_N = \frac{\rho N_A}{M}$ and $M = \sum_k n_k m_k$. In these expressions, ρ_k is the number density of atoms of element k , σ_k is the total (coherent plus incoherent)

bound atom scattering cross section of element k , ρ_N is the number density of scattering units, n_k is the number of atoms of element k per scattering unit, ρ is the mass density, N_A is Avogadro's number, M is the mass ("molecular weight") of a scattering unit, and m_k is the atomic mass of element k .

The *macroscopic total scattering cross section* Σ_s , which appears in the expressions for S given above, may be written as

$$\Sigma_s = \int_0^\infty \int_{4\pi} \frac{d^2\Sigma}{d\Omega dE_f} d\Omega dE_f,$$

where $(d^2\Sigma/d\Omega dE_f)$ is the macroscopic differential cross section for scattering into solid angle Ω and scattered energy E_f .

The need to distinguish between Σ_s and Σ_B is particularly important when working with hydrogenous materials. For example Σ_B for water is roughly 170 b/molecule whereas Σ_s at 9 Å (1 meV) is ~240 b/molecule. On the other hand Σ_s at 1.8 Å (25 meV) is about 100 b/molecule.

The *macroscopic total cross section* is defined as the sum of the macroscopic total scattering cross section and the macroscopic absorption cross section.