Direction-dependent self-absorption calculation of plate-like geometry samples

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A calculation of the direction-dependent transmission factor and scattering corrections for highly absorbing samples of finite thickness with a plate-like geometry.

WHY

The absorption of radiation of a sample is something which is not always avoidable. Thus, this calculation sets out to show the effects on the scattered intensity of a highly absorbing sample with plate-like geometry. Capillary geometry will have similar absorption effects as a *maximum*, for scattering in the direction of the capillary axis.

DEFINITIONS

Incoming radiation with intensity I_0 is partially absorbed by a sample of thickness D, exiting with intensity I_T. Scattered radiation at an angle 2θ has intensity I_l (c.f. Figure 1).

We are interested in determining I_l, which (assuming D is much smaller than the sample-to-detector distance) is the sum of all scattering contributions to 2θ from throughout the entire width D of the sample (c.f. Figure 2). A scattering event occurring at distance t in the sample will scatter with an intensity I_{0t}, travel through distance l through the sample (and being slightly aborbed), exiting with an intensity I_{lt}. The sum (or integral) of I_{lt} for all contributions for $0 \leq t \leq D$ is $I_l(\theta)$. It is important to note that $I_{0t} = I_0(t)P(2\theta)$ where $P(2\theta)$ is the scattering probabiltiy, and $I_0(t)$ the intensity of the

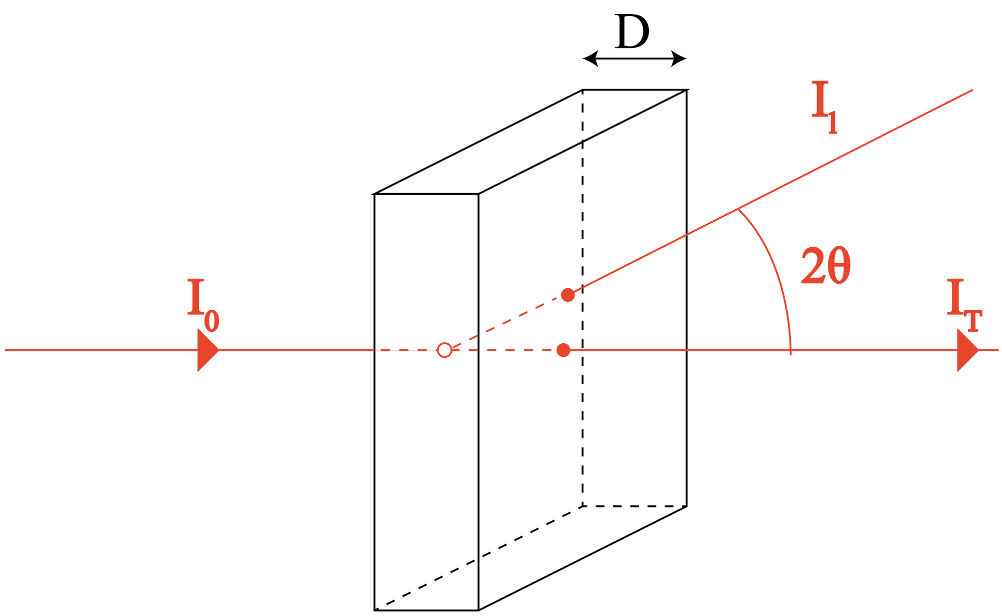

FIG. 1. Definitions of parameters to calculate the angle-dependent transmission through a sample with plate geometry, macro scale.

unscattered beam at point t.

DERIVATIONS

What we are ultimately interested in is the correction factor C_{plate} due to the sample geometry. This can be defined as:

$$C_{\mathrm{plate}} = \frac{T_l}{T} = \frac{I_{lt}/I_{0t}}{I_T/I_0} \tag{1}$$

Where T is the transmission factor of the direct beam, T_l the transmission factor of the scattered radiation. The transmission factor of the direct beam is defined by the Lambert-Beer law:

$$\frac{I_T}{I_0} = \exp(-\alpha D) \tag{2}$$

Where α is the absorption coefficient of the sample.

The definition of T_{lt} is slightly less straightforward. We begin by determining the pathlength the scattered radiation has to travel through after scattering. This scattered intensity will travel a length l through the sample. This length is:

$$l = \frac{D - t}{\cos(2\theta)} \tag{3}$$

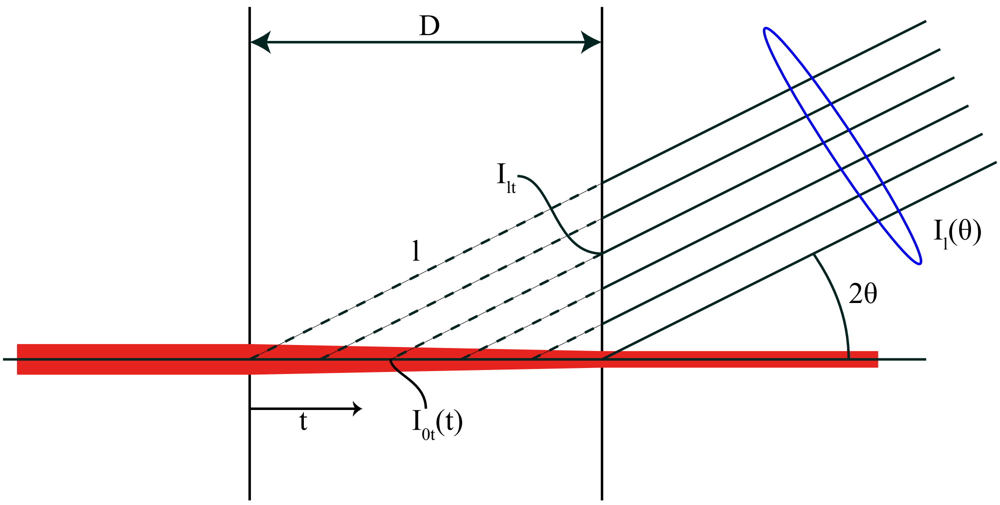

FIG. 2. Definitions of parameters to calculate the angle-dependent transmission through a sample with plate geometry, micro-scale.

When at point t, the sample scatters to an angle of 2θ, The intensity I_{lt} then becomes:

$$\begin{aligned} I_{lt} &= I_{0t}\exp(-\alpha l) \\ &= P(2\theta)I_0\exp(-\alpha t)\exp(-\alpha\tfrac{D-t}{\cos(2\theta)}) \\ &= P(2\theta)I_0\exp\left\{-\tfrac{\alpha}{\cos(2\theta)}\left[t\cos(2\theta)+(D-t)\right]\right\} \end{aligned} \tag{4}$$

Throughout the sample, the radiation will be absorbed by different lengths of material, and thus we need to integrate over all points along $0 \leq t \leq D$, assuming equal scattering probability and switching to transmission, we get from Mathematica:

$$\begin{aligned} T_l = I_{lt}/I0t &= \int_0^D \tfrac{1}{D}\exp\left\{-\alpha t-\alpha\tfrac{D-t}{\cos(2\theta)}\right\}\mathrm{d}t \\ &= \tfrac{-\exp(-\alpha D)+\exp(-\alpha D/\cos(2\theta))}{\alpha D-\alpha D/\cos(2\theta)} \end{aligned} \tag{5}$$

which for $2\theta = 0$ resolves to equation 2.

C_{plate} then becomes the ratio between equation 5 and 2:

$$C_{\mathrm{plate}} = \exp(\alpha D)\frac{-\exp(-\alpha D)+\exp\left(-\alpha D/\cos(2\theta)\right)}{\alpha D-\alpha D/\cos(2\theta)} \tag{6}$$

THE EFFECTS

Computing C_{plate} for some heavy absorptions result in only mild deviations at high scattering angles, not even amounting to a percent at 2θ=10 degrees for a sample absorbing 50% of the radiation (c.f. Figure 3). For a sample absorbing 75% of the radiation, a percent deviation is just reached (c.f. Figure 3).

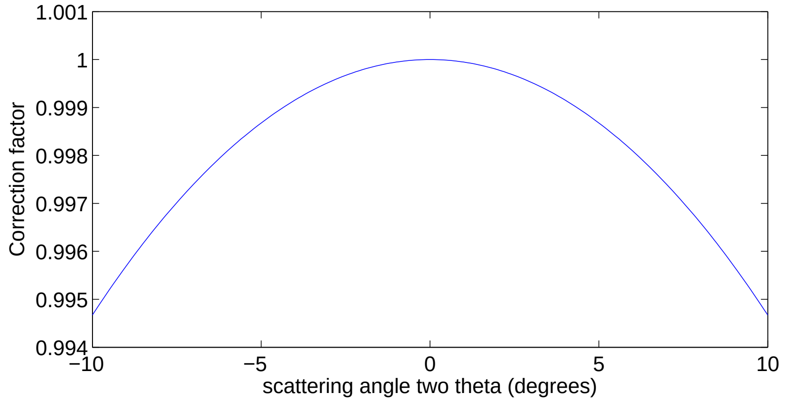

FIG. 3. Absorption due to sample geometry for a sample with 50 percent absorption of the direct beam

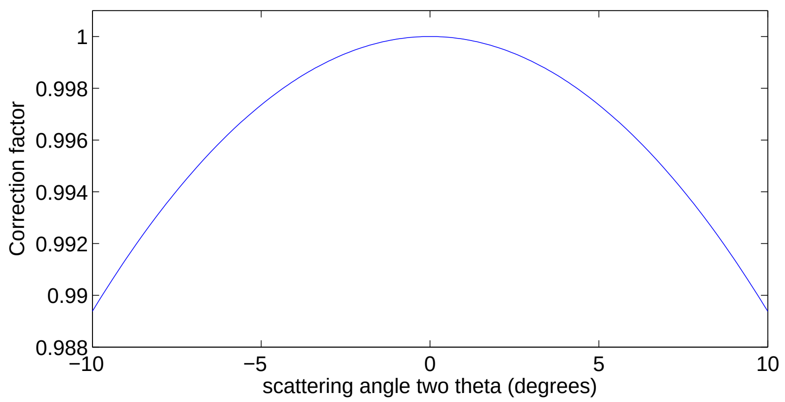

FIG. 4. Absorption due to sample geometry for a sample with 75 percent absorption of the direct beam

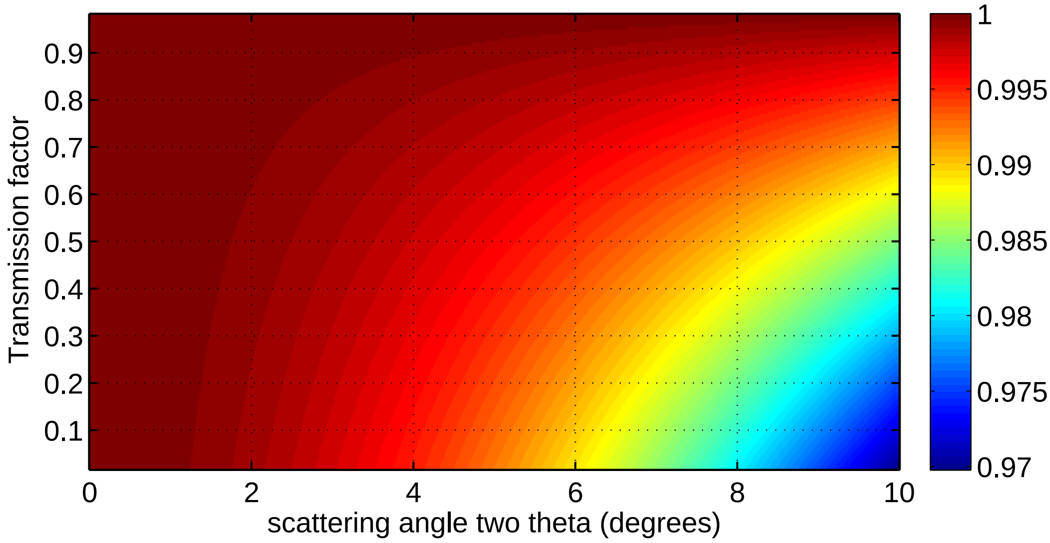

FIG. 5. Absorption due to sample geometry for a sample for a range of absorptions