1 Absorption Correction

This section derives a formula to correct the absorption effect due to the sample. The idea follows Yufeng's thesis, chapter 6.

Within each domain, there is no x-ray absorption due to lipids or water. Let the domain size be L_z and thickness t. $t = NL_z$, where N is the total number of domains. Let $I_{meas} = NI_0$ represent the measured intensity at the detector. Here, I_0 is equal to the x-ray intensity due to each domain. Assume that x-rays travel to the middle of each domain and scatter. The path length of x-ray within the top most domain is given by $L_z/\sin\theta$, $3L_z/\sin\theta$ within the second domain, and $(2i+1)L_z/\sin\theta$ within the ith domain. Then, the measured intensity is given by

$$\begin{aligned} I_{meas} &= \sum_{i=0}^{N-1} I_0 \exp\left\{-\frac{(2i+1)L_z}{x_a \sin\theta}\right\} \\ &= I_0 \sum_{i=0}^{N-1} ar^i \\ &= I_0 a \frac{1-r^N}{1-r}, \end{aligned} \tag{1}$$

where $a = \exp\{-L_z/(x_a \sin\theta)\}$ and $r = a^2$. Since $I_{meas} = AI_{ideal} = ANI_0$, the absorption correction, A_c is given by

$$A_c = \frac{1}{A} = \frac{N}{a}\frac{1-r}{1-r^N} \tag{2}$$

$$= \frac{t/L_z}{\exp(-\frac{L_z}{x_a \sin\theta})} \frac{1-\exp(-\frac{2L_z}{x_a \sin\theta})}{1-\exp(-\frac{2t}{x_a \sin\theta})}. \tag{3}$$

In the NFIT program, a convenient quantity called scaling factor denoted by ϕ is defined via $I_{meas} = \phi(q_z)S(\mathbf{q})$. Then, $\phi(q_z) = A|F(q_z)|^2/q_z$. $\phi(q_z)$ is calculated by NFIT and input to the SDP program. The SDP program then converts $\phi(q_z)$ to $|F(q_z)|$. These two quantities are related by

$$|F(q_z)| = \sqrt{q_z A_c \phi(q_z)} \tag{4}$$

In the SDP program, L_z is assumed to be 2000 Å. $\sin\theta$ is related to q_z by

$$\sin\theta = \frac{q_z \lambda}{4\pi}, \tag{5}$$

where λ is the wavelength. This relation assumes that scattering of the interest is at $q_r = 0$, which is not a bad approximation for LAXS analysis. Also, note that the derived formula for absorption correction works well for specular scattering, in which the incident angle is the same as the outgoing angle. A more refined theory that takes diffuse scattering into account will be considered in the next section.

2 Absorption Correction 2

In this section, a slightly more accurate theory will be derived for the absorption effect. It will involve an explicit integration over the incident angle, ω, which is necessiated by the sample rotation during an x-ray exposure. The procedure is to write down an absorption factor, A_ω, for a given incident angle, and then integrate over ω. For each ω, A_ω will have explicit dependence on q_z because x-rays hitting different CCD pixels travel different paths through the sample. Note that we ignore q_x dependence.

Assume that all the x-rays enter the sample from the top surface. The total scattering angle is given by 2θ. See Figure. Let z-axis point downward. At the top surface (air-sample interface), $z = 0$. For x-rays that travel to z and then scatter, the total path length within the sample is given by

$$L_{tot} = \frac{z}{\sin\omega} + \frac{z}{\sin(2\theta - \omega)} = zg(\omega, \theta), \tag{6}$$

where $g(\omega, \theta) = (\sin\omega)^{-1} + (\sin(2\theta - \omega))^{-1}$. For each ray, the intensity is attenuated by the sample. If non-attenuated intensity is equal to I_0, then the attenuated intensity is

$$I = I_0 \exp\left(-\frac{L_{tot}}{\mu}\right) \tag{7}$$

Then, the observed intensity from a sample fixed at ω is given by

$$\begin{aligned} I_{\text{obs}}(\omega, \theta) &= \int_0^t I(z)dz = I_0 \int_0^t \exp\left(-\frac{g(\omega, \theta)}{\mu} z\right) dz \\ &= I_0 \mu \frac{1 - \exp\left(-\frac{t}{\mu} g(\omega, \theta)\right)}{g(\omega, \theta)}. \end{aligned} \tag{8}$$

Since, for a given ω, $I_{\mathrm{obs}}(\omega,\theta) = A(\omega,\theta) t I_0$,

$$A(\omega,\theta) = \frac{\mu}{t} \frac{1 - \exp\left(-\frac{t}{\mu} g(\omega,\theta)\right)}{g(\omega,\theta)}, \tag{9}$$

which is the absorption factor for x-ray scattering with the total scattering angle of 2θ for a given angle of incidence. Note that q_z dependence is through θ in $g(\omega,\theta)$ because

$$\theta = \arcsin\left(\frac{q_z \lambda}{4\pi}\right). \tag{10}$$

The total intensity including the sample rotation is given by

$$I_{\mathrm{total}}(\theta) = \int_0^{2\theta} \mathrm{d}\omega I_{\mathrm{obs}}(\omega,\theta), \tag{11}$$

so that the total absorption factor is equal to

$$A(\theta) = \frac{\mu}{2\theta t} \int_0^{2\theta} d\omega \frac{1 - \exp\left(-\frac{t}{\mu} g(\omega)\right)}{g(\omega)}. \tag{12}$$

If μ is taken to infinity (no absorption), A goes to 1 as expected. Here, it is important to note that $1/2\theta$ factor in the above equation is normally called Lorentz polarization factor, which is usually approximated as $1/q_z$ for LAXS analysis. Since the SDP program applies this correction factor in addition to the absorption correction, we remove this factor in the formula for A_c. Therefore, the final result for the total absorption correction is

$$A_c(\theta) = \frac{1}{2\theta A(\theta)} = \frac{t}{\mu} \left[\int_0^{2\theta} d\omega \frac{1 - \exp\left(-\frac{t}{\mu} g(\omega)\right)}{g(\omega)} \right]^{-1}$$

with $g(\omega) = 1/\sin\omega + 1/\sin(2\theta - \omega)$.