

Supplement 4 - Geometric broadening

Supplementary information for:

Order parameters and areas in fluid-phase oriented lipid membranes using wide angle x-ray scattering

Thalia T. Mills, Gilman E. S. Toombes, Stephanie Tristram-Nagle, Detlef-M. Smilgies, Gerald W. Feigenson, and John F. Nagle

Geometric broadening is spreading of the scattering intensity over a range of q values due to the non-negligible size of the sample in comparison with the sample to detector distance. Fig. S4.1 diagrams the lipid sample and considers the scattering which arrives at the detector a distance $S \tan \theta$ from the beam center. Scattering from the upstream part of the sample will arrive at a different point on the detector than scattering from the downstream end (closer to detector) of the sample, causing scattering peaks to broaden. Fig. S4.1 also takes into account the finite width of the x-ray beam, b .

On the detector, a peak that would be at $S \tan 2\theta$ neglecting geometric broadening will be spread over a distance $b + f \tan 2\theta$, where b (~ 0.3 mm) is the size of the beam and f is the sample footprint (always 5 mm in our experiments). In the small angle approximation, the following equation gives the geometric broadening, Δq , in terms of the fraction of the scattering wavevector magnitude, q :

$$\frac{\Delta q_{\text{geom}}}{q} \approx \frac{b + f \tan 2\theta}{S \tan 2\theta} \quad (\text{S4.1})$$

Assuming $q = 1.4 \text{ \AA}^{-1}$ (a common value for the lipid WAXS peak), we obtain $\Delta q_{\text{geom}}/q = 0.053 = 5.3\%$ for February 2006 D-1 setup and $\Delta q_{\text{geom}}/q = 0.040 = 4.0\%$ for the October 2006 G-1 setup. Other experimental factors which can broaden the peak are the energy dispersion ($\sim 1.1\%$ at G-1 in October 2006; 0.6% at D-1 in February 2006) and the beam divergence ($\Delta \theta_{\text{div}}^{\text{rad}} = 10^{-4}$ radians). The broadening due to the energy dispersion is:

$$\frac{\Delta q_{\text{energy}}}{q} = \frac{\Delta E}{E} = 0.01 = 1\% \quad (\text{S4.2})$$

The broadening due to the beam divergence is given by:

$$\frac{\Delta q_{\text{div}}}{q} \approx \frac{1}{q} \left(\frac{4\pi}{\lambda} \Delta \theta_{\text{div}}^{\text{rad}} \right) \quad (\text{S4.3})$$

With $q = 1.4 \text{ \AA}^{-1}$, $\Delta q_{\text{div}}/q < 0.001$ (or $\Delta q_{\text{div}}/q < 0.1\%$), which is negligible in comparison with the effects of geometric broadening and the energy dispersion. The total resolution is given by:

$$\frac{\Delta q_{\text{tot}}}{q} = \sqrt{\left(\frac{\Delta q_{\text{geom}}}{q} \right)^2 + \left(\frac{\Delta q_{\text{energy}}}{q} \right)^2} \quad (\text{S4.4})$$

For the G-1 setup, $\Delta q_{\text{tot}}/q = 0.041 = 4.1\%$. For the D-1 setup, $\Delta q_{\text{tot}}/q = 0.054 = 5.4\%$.

Assuming the samples are well aligned, geometric broadening is the main artifact causing smearing of the WAXS peak (the energy dispersion was much less in both setups). To reduce the effect of geometric broadening, the sample footprint could be shortened, although trimming the sample more would probably increase mosaic spread. Also, with a larger detector, the sample-to-detector distance can be increased, as it was for the experiment at G-1 in October 2006. Since the samples in this experiment for the most part have very wide WAXS peaks and we are most interested in trends in the data, the $\sim 5\%$ effect of geometric broadening does not pose a large problem in interpreting the WAXS data. We can compare our calculated value for the resolution to the full width at half maximum (FWHM) for the DPPC gel phase equatorial (2,0) peak, which should be a sharp peak (see Fig. 1A in main text). For this sample: $\text{FWHM}/q = 0.04 \text{ \AA}^{-1} / 1.48 \text{ \AA}^{-1} = 3\%$. The 5% resolution calculated for the February 2006 D-1 experiment is actually somewhat larger than the broadening we observed in the DPPC gel-phase peak. This could be due to absorption of the x-rays by the sample that effectively reduces the sample footprint and the geometric broadening that is the major contributor to q_r resolution.

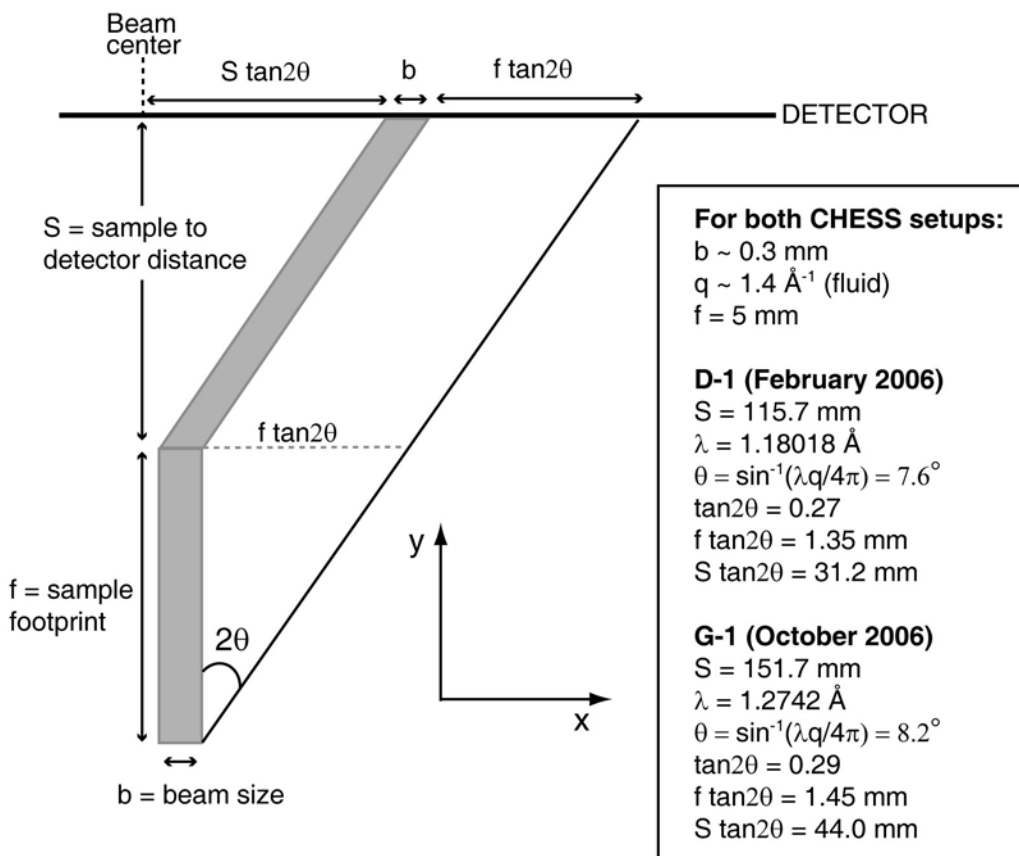


Figure S4.1. Schematic showing the effect of geometric broadening on the scattering which arrives at the detector.