SUPPLEMENTARY MATERIAL

Lipid bilayer structure determined by the simultaneous analysis of neutron and x-ray scattering data

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Experimental Form Factors

Experimental form factors $F(q)$ were obtained from the measured scattering intensities $I(q)$ for both neutrons and x-rays using

$$|F(q)| = \sqrt{I(q)P_{LC}(q)/P_{TS}(q)}\,, \qquad (1.)$$

where $P_{LC}(q)$ is the Lorentz correction, and is equal to q for oriented bilayers and q^2 for ULVs, while $P_{TS}(q)$ represents the difference between oriented and ULV bilayers. In the case of oriented bilayers, $P_{TS}(q)$ is a constant, but in the case of ULVs it describes their "sphericity" and "polydispersity" (1) as follows

$$P_{TS}(q) = \frac{8\pi^2(z+1)(z+2)}{s^2}\left\{1-\left(1+\frac{4q^2}{s^2}\right)^{-\frac{z+3}{2}}\cos\left[(z+3)\arctan(2q/s)\right]\right\}, \qquad (2.)$$

where $s = R_m/\sigma_R^2$ and $z = R_m^2/\sigma_R^2 - 1$ are the products of the ULV's mean radius R_m and the system's polydispersity σ_R. Despite its complicated form, P_{TS} is constant over the entire experimental range (q > 0.03 Å^{-1}) in the case of a typical ULV system characterized by R_m=300 Å and σ_R =75 Å (Figure 1A). What this means is that when the Lorentz correction is applied, theoretically there is no difference between the calculated form factors for oriented and spherical bilayers (Figure 1B).

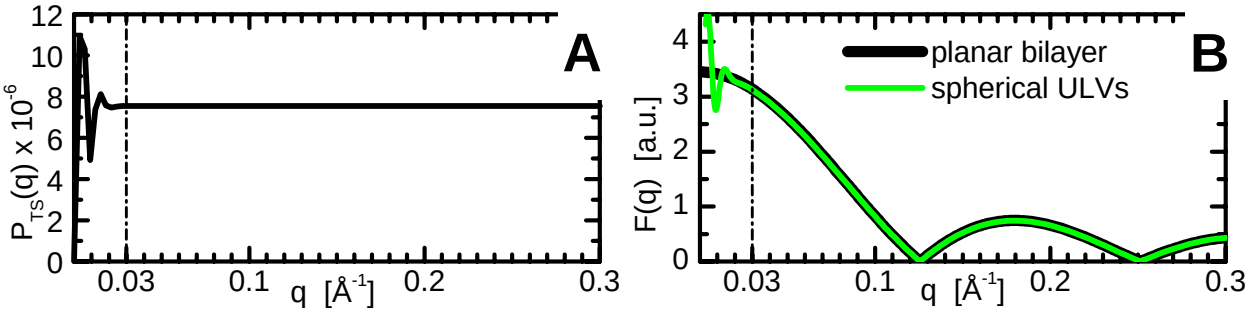

Figure 1: Panel A shows $P_{TS}(q)$ function across the experimentally achievable range of q values as calculated for a typical ULV system (R_m=300 Å and σ_R =75 Å). Panel B then compares P_{TS} correction included ULV form factors to form factors calculated for a planar bilayer, both corrected with P_{LC}. Broken lines emphasize the lower limit of q range used in this study.

In addition to this theoretical evaluation, we have addressed the differences in structure between oriented and spherical bilayers experimentally using both neutron and x-ray scattering in (2). Our study concluded no difference between the two for x-ray and neutron scattering data collected above q = 0.03 Å^{-1}.

References

1. Pencer,J., S.Krueger, C.P.Adams, and J.Katsaras. 2006. Method of separated form factors for polydisperse vesicles. *J. Appl. Crystallogr.* 39:293-303.
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