Supplementary material

High-resolution structure of coexisting nanoscopic and microscopic lipid domains

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1. Testing the model on DOPC bilayers

Our complex model for the analysis of coexisting L_O/L_D domains can be simplified to the case of a homogeneous bilayer by setting Φ_D and p_D equal to 1. This allowed us to test its capabilities on the well-studied system of DOPC. Figure S1 shows the SAXS data obtained at 20 °C and Figure S2 the corresponding distribution functions of the structural components and the electron density profile.

Structural results, reported in Tab. S1 show that the obtained $d = 62.3$ Å is in a good agreement with $d = 62.0$ Å reported for oriented DOPC multibilayers [1] at the same temperature, but also with $d = 63.1$ Å obtained for MLVs at 30 °C, considering temperature induced swelling [2]. Qualitatively, a similar trend can be observed for $\eta = 0.0551 \pm 2.0$ as compared to $\eta \sim 0.1$ at 30 °C [3,4]. However, additionally also an improvement in data quality and modeling precision needs to be considered, which leads apparently to lower η values.

A comparison of A to literature values is given in the main text. The thickness of the hydrocarbon layer D_C is coupled to A, see Eq.

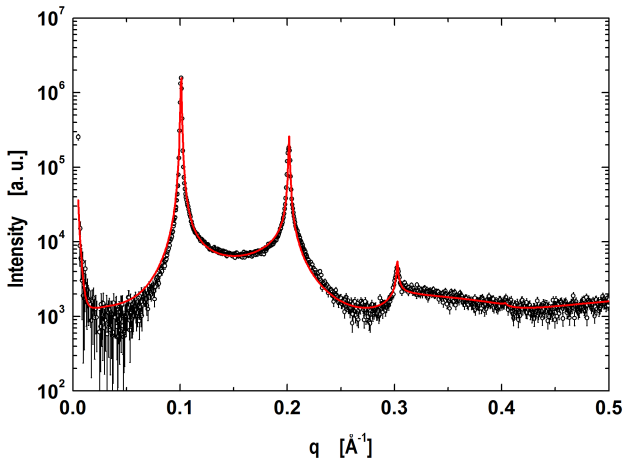

Fig. S1 The SAXS curve of DOPC MLVs at 20 °C and the corresponding model fit (red line).

Tab. S1 Structural parameters of DOPC MLVs. Parameter uncertainties are $< 2\%$.

Parameter	DOPC
d [Å]	62.3
η [10^{-2}]	5.51
Δ^*_{fl} [Å]	4.65
N_{bil}	29.46
A [Å^2]	64.3
D^*_C [Å]	15.0
z_{GC} [Å]	15.75
z_{PCN} [Å]	19.75
σ_{CH_3} [Å]	3.0

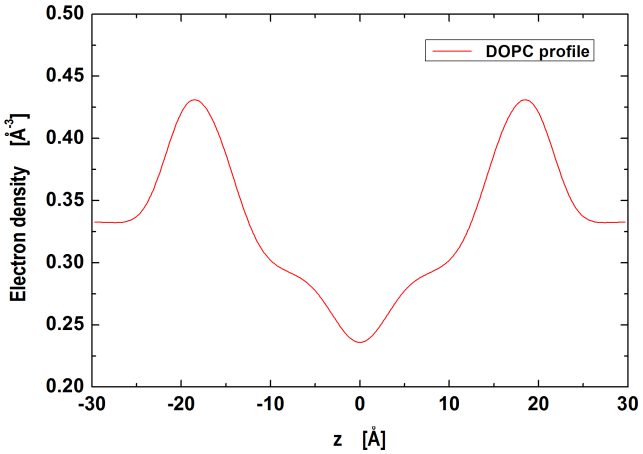

Fig. S2 The DOPC electron density profile corresponding to the fit on Fig. S1.

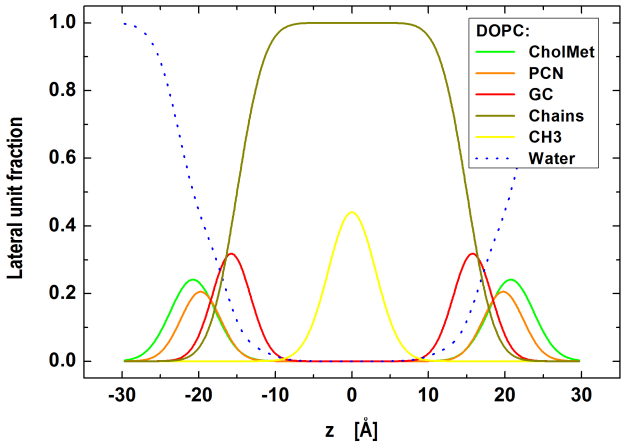

Fig. S3 The DOPC component group structure (B) corresponding to the fit on Fig. S1.

2. Structure factor polydispersity

The number of spatially correlated bilayers in the whole system (nanoscopic regime) or separately in L_D- and L_O-dominated bilayer stacks (microscopic regime) was described by Schulz-Flory distribution

$$f_{Schulz}(N;N_{mean}) = \frac{1}{N_{mean}} \exp\left(-\frac{N}{N_{mean}}\right), \tag{1}$$

where N_{mean} is a mean number of spatially correlated bilayers in a given kind of stacks. The corresponding averaged structure factor $S(q) = \langle S(q;N)\rangle_N$ was calculated as follows

$$S(q) = \langle S(q;N)\rangle_N = \frac{1}{C_{norm}} \cdot \sum_{m=2}^{N_{max}} f_{Schulz}(m;N_{mean}) S(q;m), \tag{2}$$

with

$$C_{norm} = \sum_{m=2}^{N_{max}} f(m;N_{mean}), \tag{3}$$

where $N_{max} > 100$.

3. Internal model parameters values

Tab. S2 Supplied internal model parameters values used during fitting. γ_i's are isobaric thermal expansivities used to calculate the corresponding molecular volumes of CH and CH_2 groups for t = 22 ℃ (see ref. 6 for further details).

Parameter	Value
V_{GC} [Å^3]	135.71[a]
σ_{GC} [Å]	2.47[a]
V_{PCN} [Å^3]	95.99[a]
σ_{PCN} [Å]	2.63[a]
V_{ChoMet} [Å^3]	99.3[a]
σ_{ChoMet} [Å]	2.98[a]
σ_{HC} [Å]	2.44[a]
$V_{CH_2}(L_D)$ [Å^3]	27.42[b]
$\gamma_{CH_2}(L_D)$ [K^{-1}]	118.4[b]
$V_{CH}(L_D)$ [Å^3]	22.17[b]
$\gamma_{CH}(L_D)$ [K^{-1}]	71.0[b]
$V_{CH_2}(L_O)$ [Å^3]	27.42[c]
$V_{Chol}(L_D)$ [Å^3]	628[d]

References:
[a] See ref. 5.
[b] See ref. 6.
[c] See ref. 7.
[d] See ref. 8.

References

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