Supplementary Material for "Laterally structured ripple and square phases with one and two dimensional thickness modulations in a model bilayer system"

Ananya Debnath[†] ^a, Foram Thakkar[†] ^b, Prabal K Maiti[‡], V. Kumaran[†] and K. G. Ayappa[†]

[†] Department of Chemical Engineering, Indian Institute of Science, Bangalore 560012, INDIA [‡] Centre for Condensed Matter Theory, Department of Physics, Indian Institute of Science Bangalore 560012, INDIA



Figure S1 Thickness of a larger bilayer at 283 K having the same BTMAC to SA ratio as in B3. The color bar shows that the minimum thickness between two layers is 3 nm and the maximum is 5.5 nm. The figure shows that the 2D rippling persists for the larger system size as well.



Figure S2 Thickness of 1d ripple averaged over contour along x. The plot clearly shows the 1D ripple along y direction.

present affiliation, a Indian Institute of Technology Jodhpur, Jodhpur 342011, INDIA

^b Shell India Markets Pvt. Ltd., Bangalore 560048, INDIA





Figure S3 Tilt angle superimposed on the voronoi cell areas of upper surface for bilayer B2 at (a) 283 K, (b) 330 K and for bilayer B3 at (c) 283 K, (d) 330 K. The plot shows that the cells with larger area per head group is located at the regions with lipids having higher tilt. With increasing temperature, the ripple symmetry is broken for B2 and disappears for B3. The unit of the colorbars in (a)-(d) is degree.

Figure S5 Fourier transform of thickness for bilayer B2 and B3 at two temperatures along grids on x and y. At 283 K, there are sharp peaks which are merged at higher temperature.



Figure S4 Tilt vector superimposed on the height variations of the upper surface for B2 (a) and B3 (b) at 283 K. For B2, the tilt vector points predominantly along y-axis which is the direction of the 1D ripple. For B3, the tilt vector has a predominant component along the lower height gradient of the x-axis.



Figure S6 Fourier transform of height fluctuations of the upper surface along wave vector q at different temperatures for bilayer B3. The q value corresponding to the first peak denotes the wave vector for the square phase which corresponds to 5.34 nm.