

Supporting Information –

Self-assembly behaviours of primitive and modern lipid membrane solutions: a coarse-grained molecular simulation study

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Morphological phase depending on the size of simulation box

Figure S1 shows that the box-size dependence of our simulations. The vertical axis is the simulational concentration (C) of the oleic acid when the bilayer membrane and the budding from bi-layer are formed at $1.0 k_B T$, and the horizontal axis is the length (L) of a side of cubic simulation box on double-log scale. In both cases, C decreases exponentially with increasing L . The data are fitted to $C(L) = A \cdot L^B$, where A and B are constant. As a result, A and B were 117 and -0.58 in the bilayer morphology, and 130 and -0.52 in the budding from bilayer morphology, respectively. Fitting curves are almost similar, but the budding morphology has a loose curve. We estimated the concentration with an actual size by those curves.

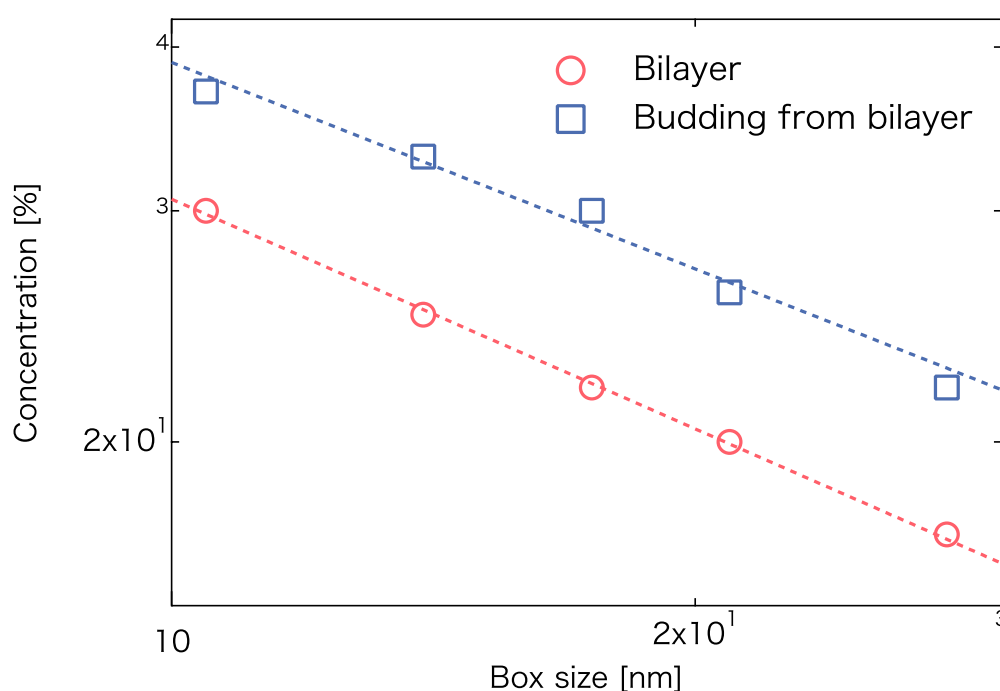


Fig. S1 The simulation box size dependence for the formations of bilayer and budding bilayer

Area density of the membrane depending on the size of simulation box

Figure S2 shows that the area density of the membrane depends on the simulation box-size. The vertical axis is the area density of the membrane (ρ_a), and the horizontal axis is the length (L) of a side of cubic simulation box on double-log scale. The area density increases exponentially with increasing L . The data is fit to $\rho_a(L) = A \cdot L^B$; the constants A and B were 2.50 and 0.42, respectively.

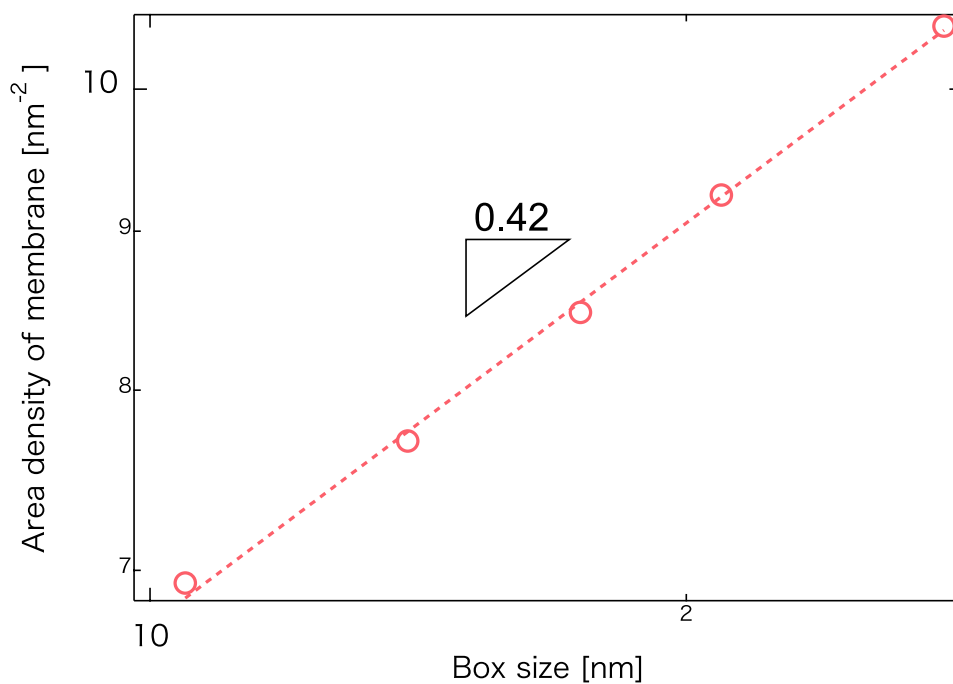


Fig. S2 The simulation box size dependence for the area density of the membrane