The mechanism of collapse of heterogeneous lipid monolayers

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Supporting material

Table S1. Summary of simulations performed

C	T, K	γ_m, mN/m	γ_{m0}, mN/m	t, μs	phase	collapse
DPPC: POPG: DOPC 3:1:1	310	23	30*	5	LE	-
		0	23	10x2	LE	+
		-1	23	10	LE	+
		eq	-1	5	LE	-
		15	eq	10	LE	+
	290	1	5*	10x2	LE+LC	-
		0	5*	10x2	LE+LC	+
		-1	5*	10	LE+LC	+
		eq	0; -1	10x2	LE	-
		15	eq	10	LE	+
		10	eq	10	LE	+
	270	23	20*	10	LE+LC	-
		0	23	10	LE+LC	-
		-1		10	LE+LC	+
		-2		10	LE+LC	+
		eq	-2; -3	25x4	LE+LC	-
		20	eq	10	LE+LC	+
		15	eq	10x2	LE+LC	+
		10	eq, 15	10x2	LE+LC	+
		5	eq, 10	10x2	LE+LC	+
DPPC: DOPC: cholesterol 5:3:4	290	4	30*;5*	10	Ld+Lo	+
		3		10x2	Ld+Lo	+
		2		10x2	Ld+Lo	+
		1		10	Ld+Lo	+
		eq	1; 2	25x4	Ld+Lo	-
		15	eq	10x2	Ld+Lo	+
		10		10	Ld+Lo	+
		5		10	Ld+Lo	+
POPG: DOPC 1:1	290	3	23	10x2	LE	-
		2		10	LE	+
	270	2	23	10x2	LE	-
		1		10	LE	+
DOPC	290	2	23	10x2	Ld	-
		1		10	Ld	+

Here C is the monolayer composition, T is temperature, γ_m is surface tension, γ_{m0} is surface tension in the starting configuration, eq corresponds to the equilibrium surface tension of a monolayer in coexistence with bilayer folds (see Table 3), t is simulation time; +/- indicates whether monolayer collapse was observed on the simulation time scale; phase corresponds to the monolayers and is as follows: LE - liquid-expanded, LC – liquid-condensed, Lo – liquid-ordered, Ld - liquid-disordered. *Simulations from ref. (56), 25 μs long each.

Table S2. Equilibrium surface tensions

C	T, K	monolayer phase	bilayer phase	γ_{eq}, mN/m
DPPC:POPG:DOPC 3:1:1	310	LE	LE	21.7±0.6
	290	LE	LE	21.4±0.6
	270	LC+LE	LE	21.5±0.3
		LC+LE	LC+LE	25.4±0.4
DPPC:DOPC: cholesterol 5:3:4	290	Lo+Ld	Ld	21.3±0.7
		Lo+Ld	Lo+Ld	23.0±0.2

Here C is the monolayer composition, T is temperature, γ_{eq} is the equilibrium surface tension.

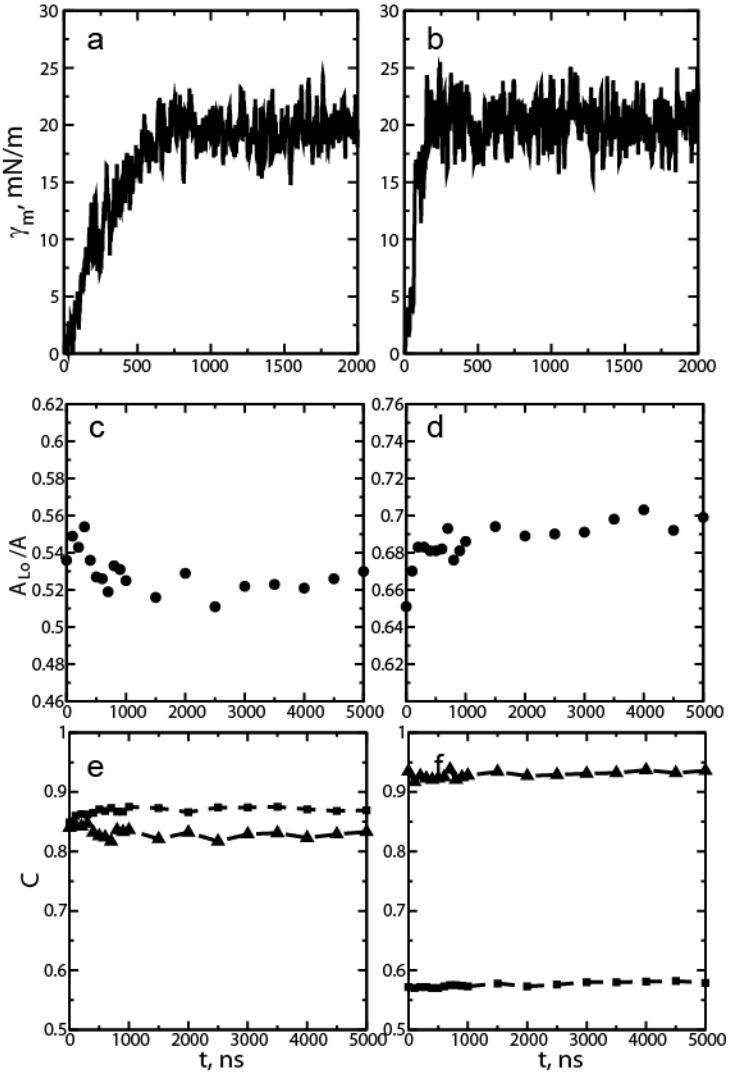

Figure S1. The monolayer properties as a function of time during equilibration with bilayers at constant interfacial area, for mixtures of 3:1:1 DPPC: POPG: DOPC at 270 K (left panel) and 5:3:4 DPPC: DOPC: cholesterol at 290 K (right panel). Surface tension (a,b), area fraction of the ordered phase (LC or Lo) (c,d), DPPC fraction forming the ordered phase, triangles (e,f), and DPPC concentration in the ordered phase, squares (e,f), are shown.