

Structure Formation in Binary Mixtures of Surfactants: Self-Assembly, Vesicle Division, and Rupture to Octopus-like Micelles

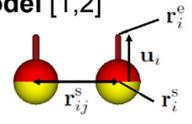
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Structure formation in binary surfactant mixtures is studied using coarse-grained molecular simulations. It is found that the rupture of two-component vesicles leads to formation of bicelles (disk-shaped micelle), cup-like vesicles, and octopus-like micelles depending on the surfactant ratio and critical micelle concentration (CMC). The obtained octopus shape of micelles agrees with those observed in the cryo-TEM images. Self-assembly dynamics into bicelles and detergent-adsorption-induced vesicle division are also investigated.

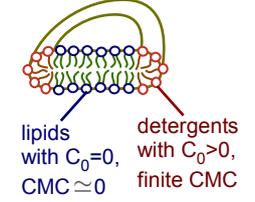
Solvent-free molecular model [1,2]

$$\frac{U}{k_B T} = \sum_{i < j} U_{rep}(r_{ij}^e) + \sum_i \epsilon_i U_{int}(\rho_i) + \frac{k_{int}}{2} \sum_{i < j} [(u_i \cdot r_{ij}^s)^2 + (u_j \cdot r_{ij}^s)^2] w_{cv}(r_{ij}^e) + \frac{k_{bend}}{2} \sum_{i < j} (u_i - u_j - C_{bd}^{ij} r_{ij}^s)^2 w_{cv}(r_{ij}^e) + \epsilon_{AB} \sum_{\langle N_A, N_B \rangle} U_{AB}(r_{ij}^e)$$

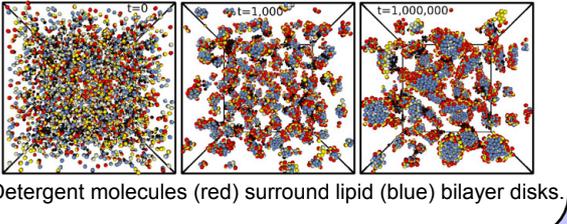
monolayer spontaneous curvature $C_0 \simeq C_{bd}/2\sigma$
 interaction between different molecules $\epsilon_{AB} > 0$ repulsion, $\epsilon_{AB} < 0$ attraction



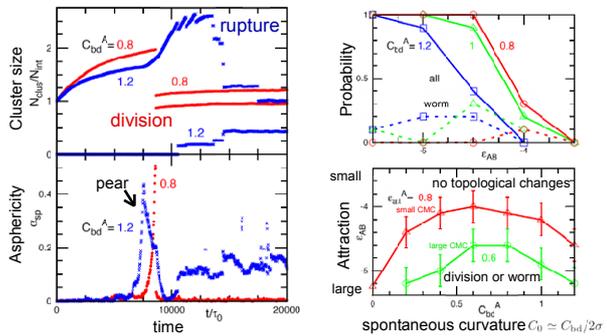
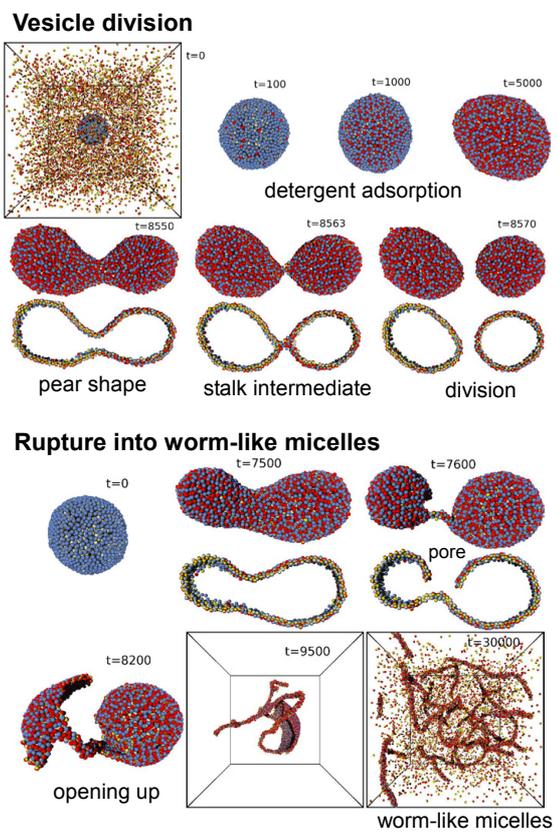
bicelle (disk-shaped micelle)



Self-assembly into bicelles [3]

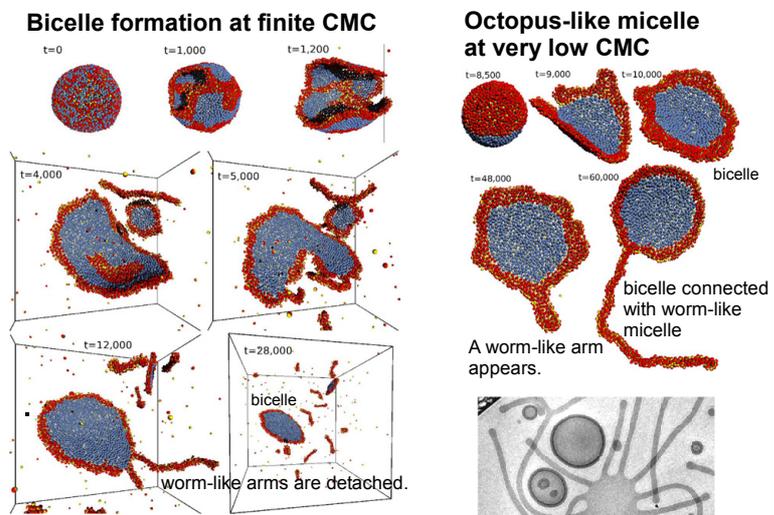


Detergent-adsorption into a lipid vesicle [3]



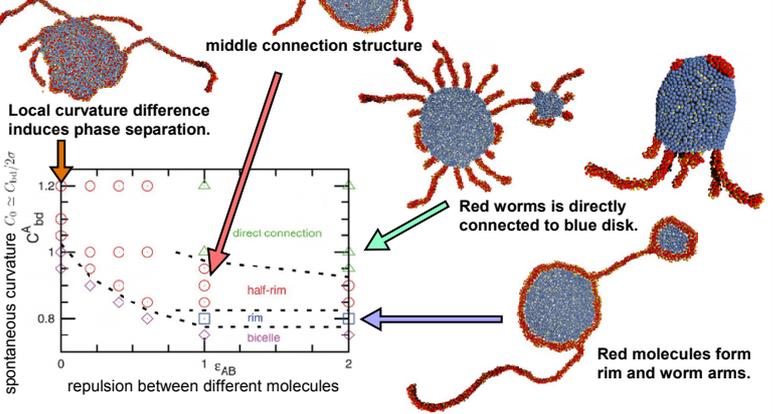
Detergent adsorption induces effective spontaneous curvature of the bilayer, thereby leading to vesicle division or rupture into worm-like micelle formation.

Vesicle opening-up into bicelles or octopus-like micelles [2]



At finite CMC (detergents), octopus-like micelles appears only as temporal structure. cryo-TEM image of binary mixture of diblock copolymers [4] 100 nm

Phase diagram at very low CMC



Octopus-like micelles are formed at very low CMC even with no direct repulsion between different molecules. Two types of connection structures are found.

[1] H. Noguchi, J. Chem. Phys. 134, 055101 (2011). [4] S. Jain and F. S. Bates, Macromolecules 37, 1511 (2004).
 [2] H. Noguchi, Soft Matter 8, 8926 (2012).
 [3] H. Noguchi, J. Chem. Phys. 138, 024907 (2013).