# Molecular Dynamics Simulation of Micelle Formation in Amphiphilic Solution

Faculty of Textile Science, Kyoto Institute of Technology
Susumu Fujiwara [1], Masato Hashimoto and Takashi Itoh

溶媒分子と溶質分子（両親媒性分子）を共に粒子として陽に扱った両親媒性溶液の分子動力学シミュレーションを行った。様々な密度で形成されるミセルの構造を解析した結果、低密度では円筒状ミセルが、高密度では平面二分子層が形成されることが明らかになった。また、親水性斥力の強さが大きくなると、ミセルの大きさが小さくなることが分かった。

## 1 Introduction

Amphiphilic molecules such as lipid molecules and surfactant molecules contain both a hydrophilic "head" and a hydrophobic "tail". In aqueous or organic solvents, these molecules often spontaneously self-assemble into various structures such as spherical micelles, bilayer membranes and bicontinuous cubic structure[1]. Self-assembly of amphiphilic molecules plays an important role in many biological and industrial processes. Although numerous computer simulation studies have so far been carried out on amphiphilic solutions, little is known about the detailed molecular mechanisms of micelle formation in amphiphilic solution. With a view to investigating micelle formation in amphiphilic solution at the molecular level, we perform the molecular dynamics (MD) simulations of coarse-grained amphiphilic molecules with explicit solvent molecules and analyze the micelle formation process.

## 2 Simulation Model and Method

The computational model is based on those used in the work by Goetz *et al.*[2] and by Noguchi *et al.*[3]. An amphiphilic molecule consists of one hydrophilic particle and two hydrophobic particles which are fixed on a line and spaced equally. A solvent molecule is modeled as a hydrophilic particle. The interaction between a hydrophilic particle and a hydrophobic particle is modeled by a repulsive soft core potential and all other interactions are modeled by a 12-6 Lennard-Jones potential. The equations of motion for all particles are solved numerically using the leap-frog algorithm at constant temperature with a time step of $\Delta t^* = 0.0025$. We apply the

[1]E-mail: fujiwara@kit.ac.jp

periodic boundary conditions. The amphiphilic concentration is set to 0.05. Initially, we provide a randomly distributed configuration of 97 amphiphilic molecules in solution at high temperature ($T^* = 10$) for various number densities ($\rho^* = 0.6$, 0.65, 0.7, 0.75, 0.8, 0.85). The number of solvent molecules is 5541. The system is then quenched to $T^* = 1.3$ and MD simulations of $t^* = 2.0 \times 10^4$ ($8.0 \times 10^6$ time steps) are carried out for each number density.

## 3 Results and Discussion

We show, in Figs. 1 and 2, the snapshots of micelles formed at $\rho^* = 0.7$ and 0.75, respectively. Our simulations indicate that cylindrical micelles are formed at lower densities ($\rho^* \leq 0.7$) whereas planar bilayers are obtained at higher densities ($\rho^* \geq 0.75$). At higher densities ($\rho^* \geq 0.75$), we find that the potential energy relaxes in a stepwise manner and there are sharp bumps in the radius of gyration during coalescence of micelles. It is also found that the size of micelles becomes small as the extent of the hydrophilic repulsion increases.

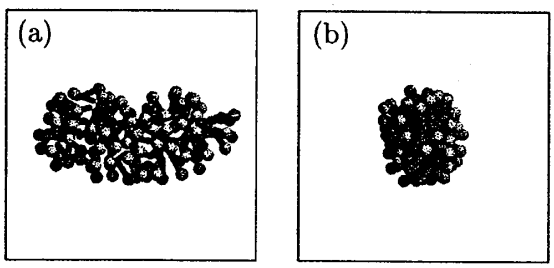


Figure 1: Snapshots of cylindrical micelles formed by amphiphilic molecules in solution at $\rho^* = 0.7$: (a) viewed along the $x$-axis (the principal axis with the largest moment of inertia) and (b) viewed along the $z$-axis (the principal axis with the smallest moment of inertia). Hydrophilic and hydrophobic groups are represented by spheres and cylinders, respectively. Solvent molecules are not shown for clarity.

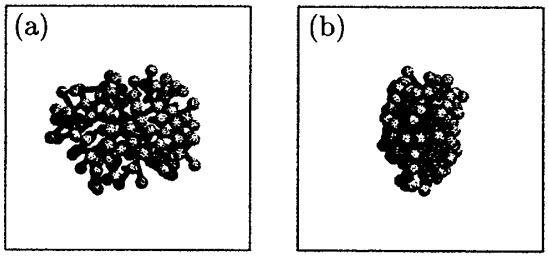


Figure 2: Snapshots of planar bilayer formed by amphiphilic molecules in solution at $\rho^* = 0.75$: (a) viewed along the $x$-axis and (b) viewed along the $z$-axis.

## References

[1] *Structure and Dynamics of Membranes*, edited by Lipowsky, R. and Sackmann, E. (Elsevier Science, Amsterdam, 1995).

[2] R. Goetz and R. Lipowsky, J. Chem. Phys. **108** (1998), 7397.

[3] H. Noguchi and M. Takasu, Phys. Rev. E **64** (2001), 041913.