§39. Dissipative Particle Dynamics Simulation of Phase Behavior and Molecule Bending in Bolaamphiphilic Splution

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Investigation of the self-organization in nonequilibrium and nonlinear systems attracts much interest. To gain insights into the universal self-organizing properties in nature, we study the self-organization in model systems such as amphiphilic molecules. With a view to investigating the structure formation of bolaamphiphilic molecules, we perform the dissipative particle dynamics (DPD) simulations of coarse-grained bolaamphiphilic molecules and analyze the phase behavior of bolaamphiphilic solution. The purpose of this study is to clarify the phase behavior of bolaamphiphilic solutions. Bolaamphiphilic molecules are modeled as ABA trimers in water. We perform DPD simulations on coarse-grained bolaamphiphilic molecules with explicit solvent molecules and analyze the formation processes of micelles and mesophases [1)]

In our simulation, we use modified Jury model molecule that is composed of a hydrophilic particle (A) and a hydrophobic particle (B) [1),2)]. Water molecules are modeled as particles W. In our model, we introduce five kinds of forces :conservative, dissipative and random forces between particles, bond stretching force between neighboring particles, and bending force in the molecules [1),2)]. The number density of particles ρ is set to 5. Total number of particles $N \equiv 3N\mathrm{ABA} + N\mathrm{W}$ is fixed to $N = 5000$, where NABA is the number of modeled bolaamphiphilic molecules ABA and NW is the number of water particles. The simulation box is set to cubic. The dimensionless length of the box L is $L = (N/\rho)^{1/3} = 10.0$. We use periodic boundary conditions in simulation.

First, we set the bending force in the ABA molecule to be zero, we obtained phase diagrams which is shown in Figure 1a). The ordinate denotes the intensity α of the conservative force and the abscissas represent the concentration. The obtained molecular configurations are classified into four phases: the isotropic micellar (symbol ×), the micellar (trianbles), the rod-shaped micellar (squares), and the hexagonal (circles). Next, setting the bending force to be nonzero, we obtained phase diagrams which is shown in Figure 1b). Tow new configurations are obtained. One is the network-structure (open squares), and the other is the lamellar phases (rhombuses).

We investigate the distributions of the distortion angle of the ABA molecules and find that the majority of the molecules are strongly bended when the bending potential is excluded, whereas they are weakly bended when the bending potential is included.

In conclusions, our simulations show that there are six kinds of phases, and that the strength of the restoring potential of bolaamphiphilic molecules decides the property of the formation of the mesophases.

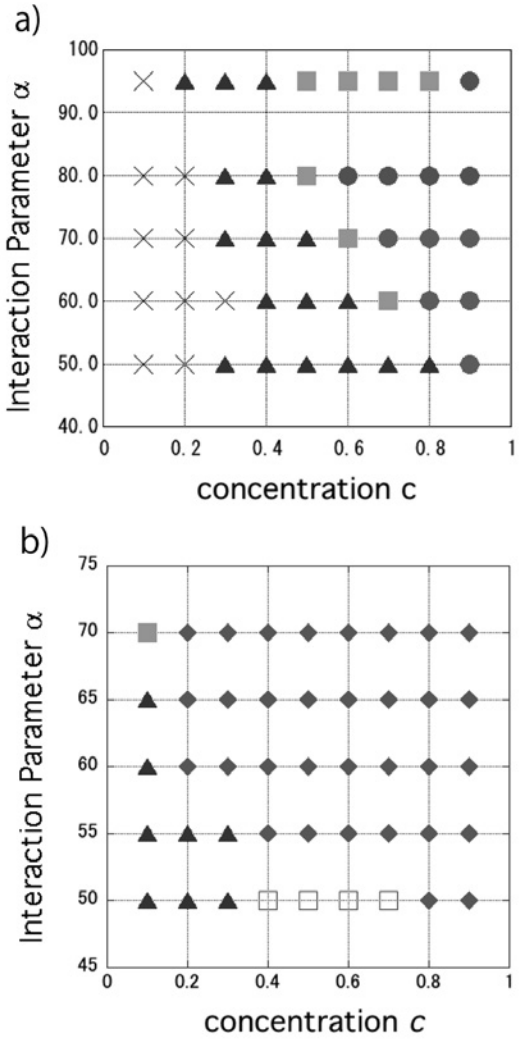

Fig. 1. Phase diagrams of ABA solution. In Fig. a), the strength of the bending force a_{BM} is set to $a_{BM} = 0.0$. In Fig. b), $a_{BM} = 10.0$. The dimensionless temperature T is set to T=1.0. The ordinate denotes the intensity coefficient of the interaction α between the water particle and the hydrophobic particle and the abscissa represents the concentration c. Symbol × , triangles, squares, circles, open squares, and rhombuses represent the isotropic micellar, the micellar phase, the rod-shaped micellar phase, the hexagonal phase, the network-structure phase, and the lamellar phase, respectively.

1) R. Shirasaki, Y. Yoshikai, H. Qian, S. Fujiwara, Y. Tamura, H. Nakamura, *Plasma Fusion Res*. 6, 2401116 (2011).
2) S. Jury, P. Bladon, M. Cates, S. Krishna, M. Hagen, N. Ruddock and P. Warren, *Phys. Chem. Chem. Phys*. 1, 2051 (1999).