§29. Dissipative Particle Dynamics Simulation of Bolaamphiphilic Solution

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Investigation of self-organization in nonequilibrium and nonlinear systems is very important to improve plasma confinement. To gain insights into the universal self-organizing properties in nature, we study the self-organization in model systems such as amphiphilic molecules. Amphiphilic molecules contain hydrophilic and hydrophobic parts. In aqueous solvents, amphiphilic molecules often self-assemble spontaneously into various structures. The purpose of this study is to clarify the phase behavior of bolaamphiphilic solutions using dissipative particle dynamics (DPD) simulations. The bolaamphiphilic molecule contains a hydrophobic stalk and two hydrophilic ends.

a_{ij}	W	A	B
W	25	25	α
A	25	25	α
B	α	α	25

Table I: Coefficients a_{ij}, where i and j denote the kinds of particles W, A, and B. α is varied from 50 to 90 in simulations.

In our simulation, we use modified Jury model molecule that is composed of a hydrophilic particle (A) and a hydrophobic particle (B)[1]. The random dissipative forces are introduced in this model. Water molecules are modeled as particles W. The mass of all particles are assumed to be unity. The number density of particles ρ and total number of particles $N \equiv 3N_{\rm ABA} + N_{\rm W}$ are fixed, where $N_{\rm ABA}$ is the number of modeled bolaamphiphilic molecules ABA and $N_{\rm W}$ is the number of water particles.

The simulation box is set to cubic and the dimensionless length of the box L is $L = (N/\rho)^{1/3}$. We use periodic boundary conditions in simulation. The interaction coefficients a_{ij} are presented in Table I. The coefficient of the interaction between A and B is written by a variable α. The strength of the interaction between W and B is set to be equal to that of the interaction between A and B. The interaction parameter of the bond-stretching potential $a_{\rm B}$ is adopted as $a_{\rm B} = 100$. We use the dimensionless time-interval as $\Delta t = 0.06$.

In the initial configuration, all molecules and water particles are located randomly and the velocity of each particle is set under Maxwell distributions with dimensionless temperature T. We prepare ABA solutions of various concentrations ($0.1 \leq c = 3N_{\rm ABA}/N \leq 0.8$) and DPD simulations of 1.0×10^7 time intervals are carried out for each run.

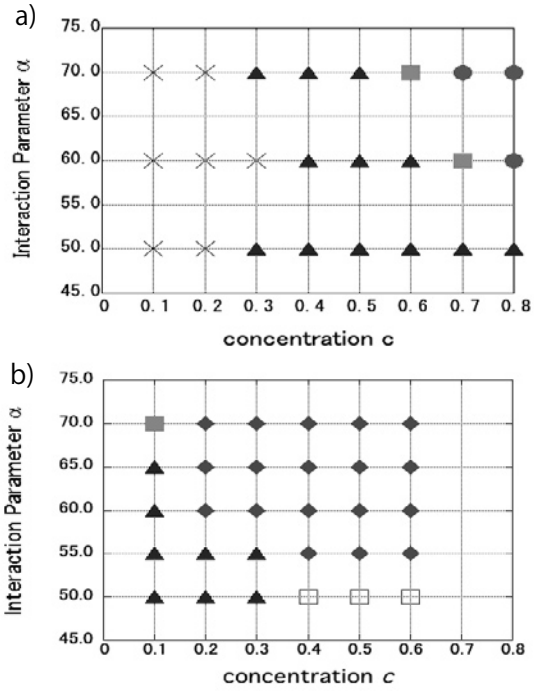

Fig. 1: Phase diagrams of ABA solution. T is set to 1.0. a) $a_{\rm BM}$ is set to 0. b) $a_{\rm BM}$ is set to 10. In these figures, the abscissa represents the concentration c. Symbol $\times$, triangles, squares, circles, open squares, and rhombuses represent the isotropic micellar, the micellar, the rod-shaped micellar, the hexagonal, the network-structure, and the lamellar phase, respectively.

We found that four kinds of phases (isotropic micellar, micellar, rod-shaped micellar, and hexagonal phase) were formed when the interaction parameter of bond bending potential $a_{\rm BM}$ is zero. When $T \geq 1.0$, the isotropic micellar phase is observed at lower concentrations, whereas the hexagonal phase is observed at high concentrations. In the case of $a_{\rm BM} = 10.0$, two new phases appear, namely, the network-structure phase and the lamellar phase. The isotropic micellar phase and the hexagonal phase disappear. The phase behavior of the bolaamphiphilic solutions is obtained for $a_{\rm BM} = 0$ and $a_{\rm BM} = 10.0$ in Figs. 1a) and 1b), respectively. It would be very interesting to know if these phase behaviors can be observed experimentally. A detailed examination is future problem.

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[1] H. Nakamura, Mol. Simulation, **30**, 941 (2004).