

Effect of molecular rigidity on micelle formation in amphiphilic solution

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The spontaneous formation of structures in plasmas has been intensively studied in order to improve plasma confinement. Such creation of order, self-organization, is a universal nature in non-equilibrium and nonlinear systems interacting with environments. In order to explore the universal self-organizing properties in nature, we investigate the self-organization in other systems such as amphiphilic systems. Amphiphilic molecules such as lipids and surfactants contain both a hydrophilic part and a hydrophobic part. In aqueous solvents, these molecules spontaneously self-assemble into various structures such as micelles, bilayer membranes and bicontinuous cubic structures [1]. Self-assembly of amphiphilic molecules plays an important role in many biological and industrial processes. Although several computer simulations have so far been carried out in relation to the effect of molecular rigidity on structure formation of polymers, few simulation studies have been done systematically with respect to the effect of molecular rigidity on micelle formation in amphiphilic solution. With a view to investigating the effect of molecular rigidity on micelle formation in amphiphilic solution at the molecular level, we perform the molecular dynamics simulations of coarse-grained amphiphilic molecules with explicit solvent molecules and analyze the micelle formation process.

The computational model is similar to that used in the previous work [2-4], which is based on the model of Goetz *et al.* [5]. An amphiphilic molecule is a flexible or semiflexible chain which consists of one hydrophilic particle and three hydrophobic particles. A solvent molecule is modeled as a hydrophilic particle. We consider bond-stretching and bond-bending potentials as bonded potentials. As for non-bonded potentials, 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 Lennard-Jones potential. The molecular rigidity is controlled by the bending modulus in the bond-bending potential. The equations of motion for all particles are solved numerically using the velocity Verlet algorithm at constant temperature and volume. The amphiphilic concentration is set to 0.06. Initially, we provide a randomly distributed configuration of amphiphilic molecules in solution at high temperature for various bending moduli. The system is then quenched to lower temperature.

Our simulations show that the micellar shape changes from a sphere into a cylinder, and then into a disc as the hydrophilic interaction increases. We also find that a threadlike micelle changes into a cylindrical or disc micelle as the molecular rigidity increases. This fact indicates that the micellar shape can be affected by the molecular rigidity.

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