Adsorption of PEO-PPO-PEO Triblock Copolymers on Lipid Surface using Coarse Grained Simulation

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粗視化分子シミュレーションにより、親水性及び疎水性の表面が両親媒性トリブロックコポリマーの自己集合形態に与える影響を調べた。トリブロックコポリマーの振る舞いは設置された壁表面の種類に大きく依存し、多様な集合形態を示した。次にシステムを発展させ、トリブロックコポリマーのリン脂質2分子膜への吸着現象の観察を行い、脂質膜の安定性に関する考察を行った。

We investigated the conformation of the polyethylene oxide-polypropylene oxide-polyethylene oxide (PEO-PPO-PEO) tri-block copolymers solution near surface using a coarse grained molecular simulation. PEO-PPO-PEO tri-block copolymers are non-ionic surface active agents commonly known as Pluronic® (trade mark by BASF Corp.) which are widely used for industrial applications, such as detergents, stabilizers, emulsifiers, and drug delivery systems [1, 2, 3].

It is of great interest to study the interaction of the copolymers with biological membrane in relation to drug delivery system. It is necessary to observe the conformation of the copolymers and biological membrane at the molecular level. It is, however, computationally not yet feasible to study directly the complex interaction between Pluronics and biomembranes or other wall systems in atomistic detail. Therefore, as a first step we study the interaction of the copolymers with simple artificial walls using a coarse grained model. Secondly, we also investigate the interaction between the copolymers and a DPPC (Dipalmitoyl phosphatidylcholine) bilayer. DPPC is an abundant phospholipid and its bilayers are widely used as biomembrane models.

The coarse grained model of Pluronics is based on the methods derived for lipids by Marrink et al. [4], in which we model PPO monomers as hydrophobic superatoms, whereas PEO are hydrophilic superatoms and wall particles are simple hydrophilic or hydrophobic interaction superatoms as well.

Snapshots of various systems are shown in Figure 1. Even under the same conditions, including temperature, pressure, and concentration, the polymer conformation is changeable

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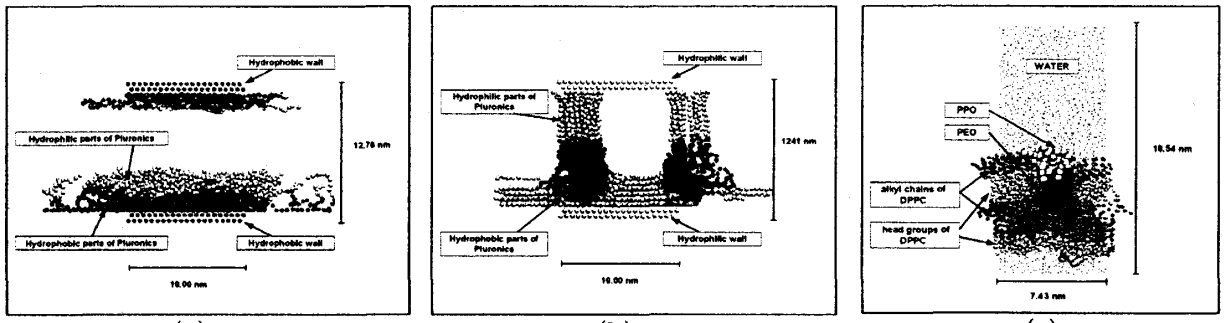

(a) (b) (c)

Figure 1: Snapshots of Pluronics. PPO monomers are shown in black and PEO in white, water is not shown for clarity at (a) and (b). Periodic boundary condition is applied. (a): Pluronics and hydrophobic walls, (b): Pluronics and hydrophilic walls, (c): Pluronics and DPPC bilayer.

depending on the type of walls. If there are hydrophobic walls, the copolymers are adsorbed and distributed evenly over the surface. The copolymers are, however, not distributed in hydrophilic walls system, but making hydrophobic cores near the surface and stretched between walls. Regarding the interaction of copolymers with DPPC bilayer, Pluronics copolymers are embedded into the bilayer, although they are not fully embedded but their hydrophobic parts are inside and hydrophilic parts attache to the water surface.

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