Phase separation of ternary mixtures incorporating bottlebrushes: A Dissipative Particle Dynamics approach

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Abstract

Perfluoropolyether (PFPE) is used as a type of liquid lubricant. Due to its chemical inertness, it is non-toxic and environmentally friendly. Recently a bottlebrush with PFPE tails was shown to modify polymer membrane surface with oil repellency[1]. The bottlebrush architecture allows an extensive structural tunability and controllable self-assembly[2] compared to linear polymers, leading to a number of applications in electronic and photonic materials[3], strain-adaptive stiffening materials[4], and thermal stabilization of enzymes[5]. Herein we develop a coarse-grained model of this amphiphilic bottlebrush using dissipative particle dynamics (DPD) approach. The architectures of the bottlebrushes are chosen based on our concurrent experimental studies. We validate our model with respect to the prior Molecular Dynamics simulations and experimental studies. We focus on dynamics of phase separation in the ternary system that consists of bottlebrushes, solvent, and polymer matrix with different affinities to the backbones. The affinities between different moieties and relative volume fractions are chosen to match corresponding experimental studies. We characterize domain growth dynamics and an evolution of a number of contacts between different species on the surface of growing domains. We isolate the effects of bottlebrush rigidity and an affinity between the backbones and matrix on phase separation morphology. We compare our simulation results with the corresponding experimental findings.

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