Theoretical Study of Anisotropy Polymer Solution Composed of Mn3O4 and Polystyrene via Coarse-Grained Molecular Dynamics

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Anisotropic particles can be used in a wide range of applications, such as catalysts and sensors, and sedimentation of components within particles can be a method of formation of anisotropic particle. In this study, sedimentation of polymer solution on SiO2 wall was investigated using coarse-grained molecular dynamics to understand the formation of anisotropic particles. Wall and vacuum were introduced with polymer solution, which were composed of polystyrene (PS), Mn3O4 nanoparticle (NP) and chloroform, to confirm the evaporation of solvent and sedimentation of polymer solution. Mn3O4 NP was stabilized with surfactants, which were oleic acid (OA) and oleylamine. We showed that the sedimentation of Mn3O4 NPs occurred faster than PS and the interaction between Mn3O4 NPs and PS acted to pull down PS towards the wall while Mn3O4 NPs were settling. Strong interaction sites were identified to be carboxyl group of OA and backbone of PS. Furthermore, fast settlement by gravitational force and large sedimentation with high concentration of Mn3O4 NPs were confirmed. More aggregated Mn3O4 NPs increased the interactions between aggregates and PS.