

# Supporting Information for “Self-assembly of rod-coil diblock copolymer-nanoparticle composites in thin film: Dissipative particle dynamics”

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## 1. Nanoparticle behavior as a function of nanoparticle fraction

In this paper, the fraction of nanoparticles within the nanoparticle-diblock copolymer blends is fixed to 0.05. To observe the effect of nanoparticle fraction, additional simulations with different nanoparticle fractions were performed. When the nanoparticles consist of 19 bead, decreasing the fraction to 0.025 did not change the tendency of the distribution and seems to show linear regimes due to their repulsion constant dependent property. Increasing the fraction to 0.1 with large size nanoparticles derives the defect included structure as shown in Fig. S1(c). The increasing number of low mobility nanoparticles hinders the formation of the smectic lamellar phase.

In the case of small nanoparticles, (NP size: 4) density distribution analysis was available in the 0.1 nanoparticle fraction since the small nanoparticles have more mobility than large nanoparticles. As shown in Fig. S1(a) and Fig. 4(a), increasing nanoparticle fraction with small size nanoparticles does not change the tendency of density distribution since the translational entropy of nanoparticles is dominant in both system. On the other hand, comparing Fig. S1(b) and Fig. 4(a) decreasing fraction to 0.025 in small nanoparticle size condition displays different behavior. The nanoparticles have less dispersed distribution as the nanoparticle fraction decreases to 0.025. As the number of nanoparticles decreases, the entropic effect becomes less dominant and the resulting distribution gets a less dispersed shape.

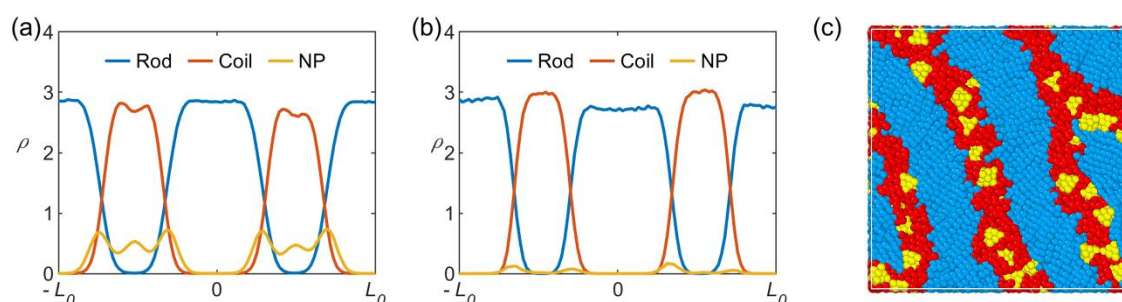


Fig. S1. (a) The density distribution of 0.1 nanoparticle fraction system ( $a_{rod-NP}=100.0$ , NP size: 4) (b) The density distribution of 0.025 nanoparticle fraction system ( $a_{rod-NP}=100.0$ , NP size: 4) (c) Defect example in the 0.1 fraction nanoparticle system with large size nanoparticles

## 2. The effect of repulsion constant between nanoparticles

In the experiment, there are coated or grafted polymers in the surface of the nanoparticle. The polymers located at the nanoparticle surface can attract surroundings and show steric effects due to their occupied space. However, representing coated polymers or grafts in the nanoparticle surface to the coarse-grained beads increases the size of the nanoparticle and increases the relaxation time of the system. To run DPD simulation in the appropriate time scale, these polymers should be removed and steric effect should be expressed as an effective repulsion between nanoparticles.

The interactions between polymer matrix and grafts (or coated polymers) were replaced by the interaction between polymer matrix and nanoparticle surface. However, for  $a_{NP-NP}=100.0$  which is the same as the repulsion constant between two coils or two rods, nanoparticles are relatively attractive to each other which results in the aggregation of nanoparticles as shown in Fig. S2.

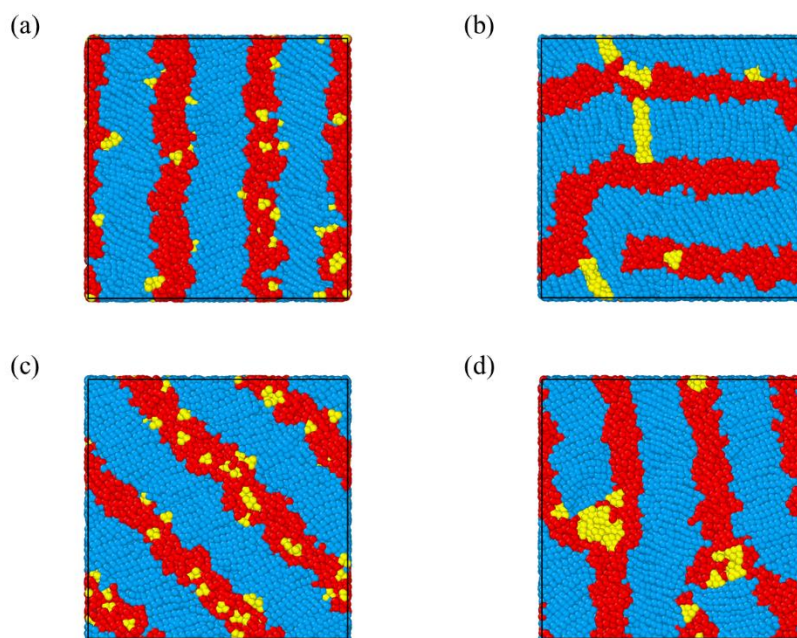


Fig. S2. The vertical view of final snapshot in the  $a_{NP-NP}=100.0$  condition. (a)  $a_{rod-NP}=100.0$ , NP size: 4 (b)  $a_{rod-NP}=100.0$ , NP size: 19 (c)  $a_{rod-NP}=105.0$ , NP size: 4 (d)  $a_{rod-NP}=105.0$ , NP size: 19

For smaller nanoparticles, nanoparticle aggregation can be decreased by dispersion from nanoparticle entropy. (Fig. S2(a) and (c)) On the other hand, as nanoparticle size increases, (Fig. S2(b) and (d)) the aggregations between nanoparticles are clearly observed and generate defects with distorting smectic lamellar phase. As coarse-grained nanoparticles cannot reflect the steric effect of grafts or coated polymers,  $a_{NP-NP}=100.0$  cannot prevent the aggregation. To resolve this problem, we set the  $a_{NP-NP}=120.0$  to block the aggregation of nanoparticles and to disperse the nanoparticles.