Understanding the phase behavior of disk-coil block copolymers under cylindrical confinement: Role of curvature-induced frustrations

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In this work, we explore the self-assembly behavior of disk-coil block copolymers (BCPs) confined within a cylinder using molecular dynamics simulations. As functions of the diameter of the confining cylinder and the number of coil beads, concentric lamellar structures are obtained with a different number of alternating disk-rich and coil-rich bilayers. Our work focuses on the curvature-induced structural behavior in the disk-rich domain of a self-assembled structure, which is investigated by calculating the local density distribution $P(r)$ and the orientational distribution $G(r,\theta)$. In the inner layers of cylinder-confined disk-coil BCPs, both $P(r)$ and $G(r,\theta)$ show characteristic asymmetry within a bilayer which is directly contrasted with the bulk and slab-confined disk-coil BCPs. We successfully explain the structural frustration of disks arising from the curved structure due to packing frustration of disks and asymmetric stretching of coils to the regions with different curvatures in a bilayer. Our results are important to understand the self-assembly behavior of BCPs containing a rigid motif in a confined structure, such as a self-assembled structure of bacteriochlorophyll molecules confined by a lipid layer to form a chlorosome, the photosynthetic antennae complex found in nature.

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References

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