Promotion of Microphase Separation in Core-Shell Bottle Brush Polymer System : A Monte Carlo Study

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The self-assembly behavior of core-shell bottle brush (CSBB) copolymers were investigated by using Monte Carlo (MC) simulations. CSBB represents the bottle brush polymer that has AB diblock copolymer as side chains with terminal B block. The self-assembly of bottle brush polymers were simulated by updating bead positions of bottle-brush bead-spring chains through a dynamic Metropolis Monte Carlo (MMC) method. Simulating the morphological structures of molten CSBB, the microphase separation transitions were investigated as a function of the degree of incompatibility (χN) and the number of the backbone segments (M) which was compared to the result of linear diblock copolymers. To interpret the architecture effect, the investigation of order-disorder transition (ODT) behavior were extended to a general bottle brush architecture expressing in terms of grafting position along the side chain. The ODT curves in the χN -M space show the promotion of ordered phase as the backbone length increases. Results suggest the enhancement of ordering of short building block via controlling chain architecture.