Dissipative Particle Dynamics simulation of bottlebrush copolymers with incompatible side chains: effect of brush configuration

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In present study, we examine self-assembly behavior of ABC-type bottlebrush copolymers with different molecular architecture using Dissipative Particle Dynamics (DPD) simulation. Solvophobic A and solvophilic B homopolymer brushes are grafted on backbone chain C in different topology: C-g-(A-r-B) type (brushes A and B are randomly grafted on backbone chain C) and C-g-(A-b-B) (brushes A are grafted on the first half of the backbone chain C and brushes B are grafted on the second half of the backbone chain C) type. DPD simulation confirms that backbone chains of bottlebrush random copolymer in self-assembled structure are located along the core-corona interface, while those of bottlebrush block copolymer are located normal to core-corona interface. Hence, domain size of bottlebrush random copolymer primarily follows the length scale of side chains, while bottlebrush block copolymer primarily follows the length scale of backbone chains. This study suggests that grafting topology of bottlebrush copolymer can be key factor to control self-assembly structure.