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Anomalous Behaviors of Block Copolymers at the Interface of an Immiscible Polymer Blend¹ JI HO RYU, WON BO LEE, Seoul Natl Univ — We investigate the effects of structure and stiffness of block copolymers on the interface of an immiscible polymer blend using coarse-grained molecular dynamics (CGMD) simulation. The diblock and grafted copolymers, which are described by Kremer and Grest bead spring model, are used to compare the compatibilization efficiency, that is, reduction of the interfacial tension. It is found that, overall, the grafted copolymers are located more compactly at the interface and show better compatibilization efficiency than diblock copolymers. In addition, it is noted that an increase in the stiffness of one block of diblock copolymer causes inhomogeneous interfacial coverage due to bundle formation among the stiff blocks and orientational constraint on bundled structures near the interface, which makes copolymers poor compatibilizers. The dependence of anomalous orientational constraint on the chain length of homopolymers is also investigated.

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