

The effects of copolymers on the interface in incompatible homopolymer blend : Molecular dynamics study

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Using molecular dynamics simulations the effect of copolymers as compatibilizer for reducing interfacial tension and enhancement interfacial adhesion at the interface of thermodynamic unfavorable homo-polymers blend is studied with block- and graft-copolymers. We have calculated local pressure tensor of melt polymer blend along the axis perpendicular to interface, varying bending potential energy of one part of copolymer chain to examine the effect of stiffness of surfactin molecules. The model is constructed using coarse grained bead-spring model and non-bonded potential is described with WCA potential. Here we consider symmetric diblock copolymer ( $f=1/2$ ) having  $1/2 N$  made of beads of type A and the other part made of beads of type B, and graft copolymer having main linear chain consist of  $1/2 N$  beads of type of A and branched with two side-chains consist of  $1/4 N$  beads of type B. All simulations were performed under the constant  $NP_NAT$  ensemble at  $T^*=1$ ,  $\rho^*=0.85$  for calculating interfacial tension.