Influence of monomer sequence on microstructure of nonadditive hard chain copolymers: simulation and equation of state.

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Abstract

Influence of copolymer structure on self-assembly of the copolymer was investigated by introducing nonadditive size interactions among different type segments in copolymers composed of touching hard spheres. The copolymer structures investigated are diblock, alternating, multiblock, and random. The copolymers were simulated using discontinuous mol. dynamics simulation. Equations of state of the different model copolymers were developed using the TPT1 theory. Diblock copolymers self assemble readily at high values of the nonadditivity parameter Δ and at high densities. Multiblock and random copolymers self assembled to a smaller extent and the alternating copolymer self-assembled only at very high Δ and densities. The TPT1 equation of state provided good prediction of the compressibilities of the different copolymer systems at neg. and small pos. values of Δ. Deviations between the model and simulation results were obsd. at high Δ and high densities. Deviations were assocd. with self-assembly of the copolymers.