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Miscibility of PS-PI diblock copolymer by Molecular Dynamic and Mesoscopic Simulations

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Molecular dynamic and mesoscopic simulations are used to predict the morphologies of PS-b-PI diblock copolymer. Flory-Huggins interaction parameter is an intermediate parameter used to connect between both simulations. The repulsions between different beads are one of essential parameters that were calculated from the Flory-Huggins interaction parameter. The calculated repulsion is 3.79 kJ/mol. Topology parameter was calculated from polymer chain length concerning its characteristic properties. S 4 I 5 is a mesoscopic topology that was used to represent polymeric chain consisting of 50 and 44 of degree of polymerization for polyisoprene and polystyrene, respectively. The morphology at equilibrium was confirmed by free energy density and order parameters from mesoscopic simulation. The stability of obtained morphologies from the obtained pattern was confirmed. In this study, the diblock copolymers are miscible and disordered phase was obtained.

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