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Dynamics of PEO-PMMA diblock copolymers. JAVIER SACRISTAN, CHUNXIA CHEN, JANNA MARANAS, Department of Chemical Engineering, The Pennsylvania State University, University Park, Pennsylvania 16802 — The structure and dynamics of a poly(ethylene oxide)–poly(methyl methacrylate) diblock copolymer (PEO-PMMA) are studied by molecular dynamics simulation using a united atom model, with emphasis on the junction point effect. These results are compared to those from a homopolymer blend. The intermolecular pair distribution function reveals that the internal packing of unlike segments is enhanced in the copolymer with respect to the blend. Thus the effective concentration of both PEO and PMMA decay towards the bulk faster as a function of local volume size in the copolymer than in the blend. The mean square displacement (MSD) illustrates differing mobilities of PEO and PMMA in both systems. In the copolymer, their mobilities are separated by less than in the blend. The junction point accelerates motion of PMMA up to a distance of 5A. In contrast, on both systems PEO mobility reach the average value close to the junction point. In spite of the different PMMA effective concentration on both systems copolymer and blend its dynamics are not affected by changes in local packing. In contrast PEO dynamics are strongly influenced by the differences on its effective concentration.

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