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Coupling Effects in Molecular Dynamics Simulation of Polymer melts JING CAO, ALEXEI LIKHTMAN, Univ of Reading — The motion in concentrated polymer systems is described by the Rouse or reptation models, which both assume that the relaxation of each polymer is essentially independent of the other polymers. However, various experiments have shown that there is certain cooperativity in the orientational relaxation which is called coupling effects. In our simulation, we calculate orientation self- and cross-correlation functions to quantify this coupling effect for original monomer and for coarse-grained blob. We use bead-spring to investigate this effect in binary blend of unentangled and weakly entangled chains in wide range of density and chain stiffness. We found that the coupling effects are very significant: the orientational corss-correlation functions of one chain with other chains are almost the same as the auto-correlation function at late time, whereas at early time it is 5 times smaller. A universal time-dependent coupling parameter for monodisperse and bidisperse melts was introduced, and is consistent to the results in the experiments and other simulations. Based on this universal coupling parameter, we can obtain orientation self- and cross-correlation functions in binary blends by using relaxation functions in monodisperse melt of each component. This coupling parameter is also introduced for different level of coarse-graining.

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