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Molecular dynamics simulations of constraint release effects in entangled binary blends of linear polymers ZUOWEI WANG, RONALD G. LARSON, Department of Chemical Engineering, University of Michigan, Ann Arbor, MI 48109-2136 — We present extensive molecular dynamics simulations of the dynamics of entangled binary blends consisting of long test chains diluted in shorter chain matrix. The ratio between the long and short chain lengths is varied by a factor of ten covering the crossover from the chain reptation regime to the tube Rouse relaxation regime. Consistent with Neutron Spin Echo experiments, the dynamic structure factor of the long chains is found to decay faster in the matrix with shorter chain lengths, owing to the stronger constraint release effect. Correspondingly the monomers and centers of mass of the long chains show a faster time-dependent diffusivity than that expected from pure reptation. The simulation results for the diffusion properties agree qualitatively with the predictions based on constraint release Rouse motion model at long time scales, but show deviations from the theoretical predictions in the intermediate time regime. Our preliminary analysis of diffusion of the matrix chains in the tube-region of the long chains indicates that this discrepancy results from neglect of the broad distribution of the lifetimes of constraint release events in the theoretical treatment.

Zuowei Wang
University of Michigan - Ann Arbor

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