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Molecular Dynamics Simulation on Rheological and Dyanmics Properties of Dynamically Asymmetric Binary Polymer Blends[1] WEI PENG, RAHMI OZISIK, PAWEL KEBLINSKI, Rensselaer Polytechnic Institute — The rheological and dynamic properties of dynamically asymmetric binary polymer blends are studied via Molecular Dynamics simulations. The current study is inspired by Senses et al. (Senses, E.; Isherwood, A.; Akcora, P. ACS Appl. Mater. Interfaces 2015, 7, 14682), where a reversible thermal stiffening behavior was observed in a nanocomposite, in which the matrix chains and surfactant polymer chains on the nanofillers showed 200 C difference in their glass transition temperatures (Tgs). In this work, we studied the rheological and dynamic properties of a blend system with two distinct blend morphologies: a well-mixed blend and a phase separated blend, representing dynamically coupled and dynamically confined states, respectively. The blend systems are made up of two types of bead-spring model chains with a large glass transition difference. Simulation results showed that the mixed systems were drastically stiffer than the unmixed ones – the storage modulus of the mixed blend was almost an order of magnitude greater than that of the neat matrix polymer. The effects of various parameters such as chain length and volume fraction of high-Tg chains on various static, dynamic and viscoelastic properties were further investigated to explore the mechanism of the stiffening.

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