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Composition Distributions and Effective Concentration of Miscible Polymer Blends Probed by MD Simulation WENJUAN LIU, RALPH COLBY, Department of Materials Science and Engineering, The Pennsylvania State University, DMITRY BEDROV, Department of Materials Science and Engineering, University of Utah, DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING, THE PENNSYLVANIA STATE UNIVERSITY TEAM, DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING, UNIVERSITY OF UTAH TEAM — Using molecular dynamics we simulate the effects of thermally-driven concentration fluctuations and chain connectivity on segmental dynamics of miscible weakly interacting polymer blends. These naturally lead to local variations in glass transition temperature and hence, a distribution of segmental relaxation times. The self-concentration and pure component limits naturally truncate the Gaussian distribution of compositions surrounding a given segment. The most-probable composition differs considerably from the mean-field estimation of Lodge and McLeish for blend compositions that differ from 50/50, when we consider chain connectivity effects for all chains in the control volume.

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