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Dynamics of Polystylen (PS) Melts: Multi-Scale Molecular Dynamic(MD) Approach WON BO LEE, VAGELIS HARMANDARIS, DOMINIK FRITZ, KURT KREMER, Max-Planck Institute for Polymer Research — Multi-scale approaches provide a systematic way to simulate much longer time and bigger systems, which allows us to study both large space and time scale problems. Dynamics of entangled polymer melts is one of those problems since it is always related to long time scales and large system sizes. Coarse- grained potentials of PS are obtained by multi-scale (atomistic to coarse-grained) MD approach. Time mapping (connection between atomistic and coarse-grained time units) is performed via matching mean square displacements of chain center of mass from both atomistic and coarse-grained simulations. One of interesting dynamic properties is stress autocorrelation functions (SAF) since they are directly related to physical properties of entangled polymer melts such as moduli, viscosities and entanglement lengths. SAF's of PS melts are evaluated by MD simulations. In order to reduce strong noise in SAF, we use time-averaged stresses, where averaging time is small enough to capture local chain relaxations.

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