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**Direct Numerical Evaluation of Plateau Modulus of Entangled Polymer Melts via Multi-Scale Molecular Dynamics(MD)** WON BO LEE, KURT KREMER, Max-Planck Institute for Polymer Research — Plateau modulus and viscosity of entangled polymer melts can be calculated by off-diagonal elements of stress tensor, which are connected by the Green-Kubo relation and tube theory. However, direct numerical evaluation of plateau modulus via stress autocorrelation function (SAF) from MD simulation is a big challenge in a computational point of view due to the following reasons: strong fluctuations, long relaxational times and large spatial scales. In the present work, SAFs of entangled polymer melts are calculated by coarse-grained MD. We find that the use of time-averaged stress helps to reduce strong noise in SAF while capturing most local chain relaxations. Plateau values by SAF are compared with plateau values predicted from the entanglement length evaluated via primitive path analysis (PPA). The importance of well equilibrated melts for such an analysis is shortly discussed.

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