

Abstract Submitted  
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**Dynamics of Entangled Polymers: Role of Attractive Interactions**

GARY S. GREY, JASON KOSKI, Sandia National Laboratories — The coupled dynamics of entangled polymers, which span broad time and length scales, govern their unique viscoelastic properties. Numerical simulations of highly coarse grained models are often used to follow chain mobility from the intermediate Rouse and reptation regimes to the late time diffusive regime. In these models, purely repulsive interactions between monomers are typically used because it is less computationally expensive than including attractive interactions. The effect of including the attractive interaction on the local and macroscopic properties of entangled polymer melts is explored over a wide temperature range using large scale molecular dynamics simulations. Attractive interactions are shown to have little effect on the local packing for all temperatures  $T$  and chain mobility for  $T$  higher than about twice the glass transition  $T_g$ . For lower  $T$ , the attractive interactions play a significant role, reducing the chain mobility compared to the repulsive case. As  $T$  approaches  $T_g$  breakdown of time-temperature superposition for the stress autocorrelation function is observed. Sandia National Labs is a multiprogram laboratory managed and operated by Sandia Corporation, a Lockheed-Martin Company, for the U.S. Dept of Energy under Contract No. DEAC04-94AL85000.

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