Dynamics of Entangled Polymers: Role of Attractive Interactions
GARY S. GREST, 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 reper-
tation 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 dynam-
ics 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
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