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Going up in time and length scales in modeling polymers

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Polymer properties depend on a wide range of coupled length and time scales, with unique macroscopic viscoelastic behavior stemming from interactions at the atomistic level. The need to probe polymers across time and length scales and particularly computational modeling is inherently challenging. Here new paths to probing long time and length scales including introducing interactions into traditional bead-spring models and coarse graining of atomistic simulations will be compared and discussed. Using linear polyethylene as a model system, the degree of coarse graining with two to six methylene groups per coarse-grained bead derived from a fully atomistic melt simulation were probed. We show that the degree of coarse graining affects the measured dynamic. Using these models we were successful in probing highly entangled melts and were able reach the long-time diffusive regime which is computationally inaccessible using atomistic simulations. We simulated the relaxation modulus and shear viscosity of well-entangled polyethylene melts for scaled times of 500 s. Results for plateau modulus are in good agreement with experiment. The long time and length scale is coupled to the macroscopic viscoelasticity where the degree of coarse graining sets the minimum length scale instrumental in defining polymer properties and dynamics. Results will be compared to those obtained from simple bead-spring models to demonstrate the additional insight that can be gained from atomistically inspired coarse grained models. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energys National Nuclear Security Administration under contract DE-AC04-94AL85000.