

Non-Equilibrium Simulation of Polymer Shear Flow via Dynamic Monte Carlo Simulation

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The use of an on-lattice Monte Carlo simulation to predict melt rheological properties of polymers is explored and has been demonstrated to have considerable utility. The methodology employed consists of the cooperative motion algorithm of Pakula and a derived biasing technique based on previous studies of Binder and Baushnagel. Chain correlation functions demonstrate that Rousian dynamics are obtained. In shear flow, a uniform linear velocity profile is obtainable for low molecular weight chains for all values of the biasing parameter. However, for larger chain lengths the velocity profile becomes distorted; this distortion is eliminated if the value of the biasing parameter is reduced. Use of the Kramers form for entropic springs allows for the calculation of stress in the simulation, providing a means for exploring rheological properties, including viscosity and normal stress differences. Results are in excellent agreement with well-established experimental facts; a shear thinning viscosity is obtained, the first normal stress difference increases with shear rate, and the first normal stress coefficient decreases with shear rate. For higher molecular weight chains under strong shearing flows, a non-monotonic stress as a function of shear rate is observed. This phenomenon is demonstrated to be due to a stacking of polymer chains such that an excess of chain ends is observed in the middle of the shear plane. These simulations provide insight into important industrial polymer processing operations in which “melt fracture” phenomena are observed, and into viscosity reductions observed when nanoparticles are added to polymer melts.