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Diffusion and Friction Coefficients of Athermal Polymer Melts
NENAD STOJILOVIC, Physics Department, John Carroll University, JUTTA LUETTMER-STRATHMANN, Departments of Physics and Chemistry, The University of Akron — The dynamics of polymer chains in polymer melts depends on mobility of polymer segments and entanglement effects and, at present, it is a challenge to separate these two effects in simulation studies. We study chain dynamics of athermal polymer melts using Monte Carlo simulations and extract diffusion and friction coefficients. We compare results of two different Shaffer's bond-fluctuation models. In the first model, bonds between polymer segments are allowed to cross each other and as a result chains do not entangle; in the second model, bond crossings are forbidden and entanglement effects play important role. Both models exhibit similar static properties allowing us to separate local friction and entanglement effects. We perform simulations for three different densities and a range of chain lengths and investigate connections between static and dynamic properties of athermal polymer melts.

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