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Dynamics in a polymeric melt: coupling the standard model to a slip-link model FRANCOIS DETCHEVERRY, LPMCN, Claude Bernard University , DARIN PIKE, JUAN DE PABLO, Chemical and Biological Engineering, University of Wisconsin-Madison — We present a coarse grain approach to simulate the chain dynamics in a polymeric melt. The starting point is a particle-based implementation of the standard model of polymers, where chains are represented by a collection of beads interacting through soft pairwise potentials. A Langevin dynamics provides a realistic description for the behavior of short, unentangled polymers. To take into account at a coarse-grained level the entanglements that are important at high molecular weight, the model is supplemented with slip-links. We describe the specifics of our implementation, which, in contrast to some previous works, induces coupling between different chains. For the simple case of a homopolymeric melt, we characterize the motions of slip-links, the dynamics of the chain and the relaxation of stresses. The approach is also tested on diblock copolymers.

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