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Rouse and Entangled Dynamics in Coarse Grain Polymeric Systems[1] ABELARDO RAMIREZ-HERNANDEZ, DARIN PIKE, Department of Chemical and Biological Engineering, University of Wisconsin-Madison, USA, FRANCOIS DETCHEVERRY, Universite Lyon 1 and CNRS, France, JUAN DE PABLO, Department of Chemical and Biological Engineering, University of Wisconsin-Madison, USA — The understanding of the kinetics of microphase ordering of block copolymers is important for controlling the morphology of these polymeric materials. Much of our current understanding of the equilibrium morphologies of block copolymers has emerged from studies using Self-Consistent Field Theory (SCFT), in which the effect of non-crossability of chains is not taken into account. In this work, we use a particle-based coarse grain model of block copolymers, and introduced elastic slip-links to model the effect of entanglements on the dynamics of the melts. These effects can be important when the self-assembly occurs in non-equilibrium conditions. We show that our model is able to reproduce both Rouse and Entangled dynamical behavior for a homopolymeric melt. We apply our computational approach to block copolymer systems under equilibrium and non equilibrium (shear flow) conditions.

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