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Simulations of Coarse Grain Entangled Polymeric Systems: From Thermodynamics to Rheology ABELARDO RAMIREZ-HERNANDEZ, JUAN DE PABLO, Institute for Molecular Engineering, The University of Chicago — Coarse-grained models have been proposed for description of soft materials over length and time scales unattainable by using atomistic models. Polymeric materials present particular challenges, because characteristic length and time scales generally span several orders of magnitude. Most coarse-grained models resort to soft effective interaction potentials, with the result that important effects are lost, including those created by the non-crossability of long polymer chains. In this work we generalize a particle-based coarse-grained approach, which has been successfully used in the past to describe the structure and thermodynamics of homopolymers and block polymers, to the study of linear and non-linear rheology in polymer melts well above the entanglement molecular weight. Entanglements are represented by slip-springs introduced at the two-chain level, as fluctuating interactions between neighboring pairs of polymeric molecules. The model is shown to exhibit scaling laws for the mean square displacement and shear viscosity that are consistent with those observed in tube theories and in experiments. Comparison between simulation and experimental results shows that the model is capable of describing quantitatively the linear and non-linear rheology of homopolymer melts and blends

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