

Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Coarse Grained Simulations of Entangled Polymer Dynamics

ABELARDO RAMIREZ-HERNANDEZ, Argonne National Laboratory, MARAT ANDREEV, JAY D. SCHIEBER, Center for Molecular Study of Condensed Soft Matter, Illinois Institute of Technology, JUAN J. DE PABLO, Institute for Molecular Engineering, The University of Chicago — We use the Theoretically Informed Entangled Polymer Simulations (TIEPOS) approach for multicomponent polymeric systems to study the linear and non-linear rheological response of melts. In this many-chain model, the topological effect of non-crossability of polymers is described by effective fluctuating interactions, mediated by slip-springs, between neighboring pairs of macromolecules. We explore the effect of different implementations of slip-springs, namely, continuous movement of slip-springs along chains as opposite to discrete jumps between polymer segments, as well as the use of a grand-canonical approach where the total number of slip-springs fluctuates. We perform a comparison between simulation predictions and experimental data for a series of well-characterized linear polymeric melts. Our results are shown to be in quantitative agreement both in linear and non-linear rheology.

Abelardo Ramirez-Hernandez
Argonne National Laboratory

Date submitted: 15 Nov 2013

Electronic form version 1.4