

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Interplay of cooperativity and entanglements in polymer melt dynamics: insights from theory and simulations¹ MARINA GUENZA, IVAN LYUBIMOV, University of Oregon — Dynamical heterogeneities in polymer melts generate cooperative motion, which results in subdiffusive center-of-mass mean-square displacement at times shorter than the longest Rouse relaxation time. This behavior is described by our Generalized Langevin Equation for cooperative dynamics, which is found to be in agreement with data from simulations and from Neutron Spin Echo experiments. We present a study of the interplay between cooperative dynamics and polymer confinement due to the presence of entanglements. Semi-flexibility, which is specific to the chemical structure of the polymer, and intermolecular interactions, which generate dynamical cooperativity and entanglements and are functions of the degree of polymerization, are explicitly included in the theory.

¹We acknowledge support from NSF, grant DMR-0804145

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Date submitted: 18 Nov 2009

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