Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Statistical Mechanical Theory of Coupled Slow Dynamics in Glassy Polymer-Molecule Mixtures RUI ZHANG, KENNETH SCHWEIZER, University of Illinois at Urbana-Champaign — The microscopic Elastically Collective Nonlinear Langevin Equation theory of activated relaxation in one-component supercooled liquids and glasses is generalized to polymer-molecule mixtures. The key idea is to account for dynamic coupling between molecule and polymer segment motion. For describing the molecule hopping event, a temporal casuality condition is formulated to self-consistently determine a dimensionless degree of matrix distortion relative to the molecule jump distance based on the concept of coupled dynamic free energies. Implementation for real materials employs an established Kuhn sphere model of the polymer liquid and a quantitative mapping to a hard particle reference system guided by the experimental equation-of-state. The theory makes predictions for the mixture dynamic shear modulus, activated relaxation time and diffusivity of both species, and mixture glass transition temperature as a function of molecule-Kuhn segment size ratio and attraction strength, composition and temperature. Model calculations illustrate the dynamical behavior in three distinct mixture regimes (fully miscible, bridging, clustering) controlled by the molecule-polymer interaction or chi-parameter. Applications to specific experimental systems will be discussed.

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Date submitted: 07 Nov 2016 Electronic form version 1.4