Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Single molecule dynamics of self-associating polymers
CHARLES SING, ALFREDO ALEXANDER-KATZ, Massachusetts Institute of Technology — Recent progress has been made experimentally in understanding the importance of reversible interactions in polymer systems, with systems such as stimuli-responsive gels demonstrating tunable properties. We extend these ideas to single molecules, since this type of behavior is especially important in biological polymers where molecular interactions can be both reversible and long-lived. We have developed simulation models where a Bell-like association model is incorporated into a Brownian Dynamics simulation, so that we represent a self-associating polymer in a coarse-grained fashion. We find that there are exciting implications of these binding properties on the dynamics of polymers both in and out of equilibrium. The introduction of this extra time scale to a dynamic polymer system manifests itself in drastic changes in polymer properties under dynamic loading; in particular, self-associating polymers in shear flow demonstrate large non-monotonic effects and single-molecule pulling scenarios demonstrate pulling behaviors reminiscent of biological molecules. This thus represents a physical model that has intriguing implications in both biological and synthetic polymer systems.

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Date submitted: 04 Nov 2011 Electronic form version 1.4