Abstract Submitted
for the DFD09 Meeting of
The American Physical Society

Entangled chain dynamics of polymer knots in extensional flow
LOUISE WILKIN, DEMOSTHENES KIVOTIDES, THEO THEOFANOUS, University of California, Santa Barbara — We formulate a coarse grained molecular dynamics model of polymer chains in solution that includes hydrodynamic interactions, thermal fluctuations, nonlinear elasticity, and topology-preserving solvent mediated excluded volume interactions. The latter involve a combination of potential forces with explicit geometric detection and tracking of chain entanglements. By solving this model with numerical and computational methods, we study the physics of polymer knots in strong extensional flow (Deborah number, $De = 1.6$). We show that knots slow down the stretching of individual polymers by obstructing via entanglements the "natural", unraveling, flow-induced chain motions. Moreover, the steady state polymer length and polymer-induced stress values are smaller in knotted chains than in topologically trivial chains. We indicate the molecular processes via which the rate of knot tightening affects the rheology of the solution.

Demosthenes Kivotides
University of California, Santa Barbara

Date submitted: 31 Jul 2009 Electronic form version 1.4