Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Microscopic theory for tube confinement and self-diffusivity of entangled needle liquids in presence of hard spherical obstacles UMI YAMAMOTO, KENNETH SCHWEIZER, University of Illinois, Urbana-Champaign — A microscopic theory for the motion of topologically entangled, non-rotating needles in presence of spatially fixed, hard sphere inclusions has been formulated. Exact two-body dynamical uncrossability constraints are imposed, and an effective Brownian evolution equation at two-needle level is self-consistently constructed. The needle transverse localization length (effective tube diameter) and long-time diffusivity are determined as a function of its length and concentration, the sphere diameter and volume fraction, and needle-sphere liquid pair structure. In contrast to single-component entangled needle liquids, the transverse and longitudinal diffusivity become coupled, and reptation is increasingly suppressed with sphere volume fraction in a manner that depends on the relative sphere-needle size. The slow dynamics also depends on needle concentration, reflecting a competition between inter-needle topological uncrossability constraints and needle-sphere excluded volume interactions. The effective tube diameter is a monotonically decreasing function of the sphere density, consistent with the suppression of polymer translational diffusion. Extension to treat entangled flexible chains, and comparison with recent simulations and experiments, are under study.

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Date submitted: 05 Nov 2012 Electronic form version 1.4