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Microscopic theory of the tube confinement potential and relaxation of entangled needle liquids under stress
DANIEL SUSSMAN, KEN SCHWEIZER, University of Illinois at Urbana-Champaign — We have developed a first-principles theory of the transverse confinement potential in an entangled needle fluid based on exactly enforcing uncrossability at the two-rod level while self-consistently renormalizing many-particle effects [Sussman & Schweizer PRL 107, 078102 (2011); J. Chem. Phys. 135, 131104 (2011)]. The predicted tube radius and long-time diffusion constant are consistent with the asymptotic reptation scaling laws under quiescent conditions, but in contrast with the usual tube model strong anharmonicities soften the confinement potential in a manner that quantitatively agrees with experiments on heavily entangled F-actin solutions. This weakening of entanglement constraints has multiple dramatic consequences under applied deformation: tube dilation, accelerated reptation, reduction of the transverse entropic barrier, and a critical stress or strain beyond which tube localization is destroyed. The degree-of-entanglement-dependent competition between reptative and transverse-hopping relaxation is established as a function of stress and strain. A mapping between rigid rods and flexible chain systems is also proposed, allowing predictions to be made for the tube diameter, entanglement onset, and transport properties of chain polymer liquids.

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