

Abstract Submitted
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Entanglement of Semiflexiible Polymers: A Brownian Dynamics

Study SHRIRAM RAMANATHAN, DAVID MORSE, University of Minnesota — We report extensive Brownian dynamics simulations of very tightly entangled solutions of semiflexible rods, of length L comparable to their persistence length L_p , at concentrations comparable to those in recent experiments on Fd-virus and filamentous actin. We find a clear crossover with increasing number concentration c from a regime of loosely entangled rods, in which rotational diffusion is hindered by topological constraints but transverse bending fluctuations are not, to a tightly entangled regime in which bending fluctuations are also restricted, and can relax only by reptation along a wormlike tube. This crossover occurs at a dimensionless concentration $c^{**}L^3 \sim 500$ for chains with $L = L_p$. The tube radius R_e is found to depend upon c and L_p with the predicted scaling relation $R_e \propto c^{-3/5}L_p^{-1/5}$ for $c > c^{**}$. The dynamic modulus $G(t)$ has been obtained from simulations of the relaxation of stress after a small amplitude step extension of the simulation unit cell. An elastic plateau in $G(t)$ that is absent at lower concentrations also appears for $c \geq c^{**}$.

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