Chain dynamics in a semidilute polymer solution under steady shear

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Brownian Dynamics computer simulations of a bead-spring polymer model were performed in order to investigate single-chain dynamics in a semidilute solution.

In equilibrium and at small shear rates the end-to-end vector correlation function <**R**(0).**R**(t)> exhibits double-exponential relaxation. With increasing shear rate it shows oscillatory relaxation, which hints at tumbling motion previously found in dilute solutions. The change of the relaxation mode of the end-to-end vector correlation function can be correlated with shear thinning of the semidilute solution.

A real time analysis of the instantaneous values of the radius of gyration (R_g), end-to-end distance (R_d), orientation (Θ), bonding normal stress (σ^b_{xx}) and nonbonding normal stress (σ^{nb}_{xx}) reveals correlations between fluctuations of these quantities.