Validity of the bead-spring model for describing the linear viscoelastic properties of single-strand DNA under strongly denaturing conditions

SEMANT JAIN, RONALD LARSON, University of Michigan — Using a normal mode analysis, we predict the infinite dilution linear viscoelastic properties of single-strand-DNA molecules and compare the results to the linear viscoelastic data of Shusterman et al. (Shusterman, Alon, Gavrinyov, and Krichevsky, 2004) obtained by monitoring the diffusion of a fluorescently labeled terminus of the molecule. To compute the overall best global fit, we constrain the hydrodynamic interaction parameter, $h^*$, equilibrium rms spring extension, $b$, and the number of Kuhn steps per spring, $N_{K,S}$, to be equal for the strands compared. The fits using the bead-spring model for all but 23100 base ss-DNA strands match the experimental data at long times with significant deviations at intermediate and short times. However, parameters fitted separately to all individual strand lengths predict results well. The best-fits to data for 2400 and 6700 base pairs yield $N_{K,S} \sim 12$ and $h^* = 0.12$. These values are similar to those found for conventional polymers such as polystyrene which have been successfully modeled with $N_{K,S} \sim 7$ and $h^* = 0.15$, indicating ss-DNA and polystyrene exhibit analogous hydrodynamic behavior.