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Simulation of single molecule stretching experiments on denatured ssDNA[1]

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We have performed simulations of stretching denatured ssDNA using a bead-spring model to compare with recent single molecule experiments. Each bead represents a singly charged base or monomer in the ssDNA. The salt and counterions are explicitly treated. An equal and opposite force is applied to the two terminal beads, and the force-extension curves are calculated at a range of forces. In denatured ssDNA, the bases of ssDNA are blocked from pairing making the flexible polyelectrolyte model applicable. The recent single molecule stretching experiments[2] on denatured ssDNA have studied the effect of added salt treating both 1:1 and 2:1 salts. These experiments found force-extensions curves exhibit two regimes: at low forces, the extension $R \sim f^{\gamma}$, where $\gamma = 0.60 - 0.69$ and a high force regime where $R \sim \log f$. The force-extension curves can be scaled to produce overlap for the salt dependence. The force at the crossover between the two regimes f_c scales as $c_s^{1/2}$ for 1:1 salt, but as I^3 for 2:1 salt, where is I is the ionic strength. The simulation data reproduce the experimental overlap for both salt cases. The two regimes including the logarithmic behavior at large forces are present in the simulation results. The simulation results imply that the behavior is due to a competition between electrostatics, entropy and the applied force and that other molecular interactions can be neglected. Thus, the standard theoretical methods are not missing an important term in the free energy, although approximation level may be an issue. We will present simulation data on the conformations as a function of applied force and discuss the implications for analytic theory.

[1]This work was performed, in part, at the Center for Integrated Nanotechnologies, a U.S. Department of Energy, Office of Basic Energy Sciences user facility. Sandia National Laboratories is a multi-program laboratory operated by Sandia Corporation.

[2]McIntosh and O.A. Saleh, Macromolecules **44**, 2328 (2011).