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The nonlinear elasticity of alpha helical polypeptides: Analytical and Monte Carlo studies BUDDHAPRIYA CHAKRABARTI, ALEX LEVINE, Department of Physics, University of Massachusetts, Amherst — We study a minimal extension of the worm-like chain model to describe polypeptides having alpha-helical secondary structure. In this model presence/absence of secondary structure enters as a scalar variable that controls the local chain bending modulus. Using this model we analytically compute the extensional compliance of an alpha-helix under tensile stress, the bending compliance of the molecule under externally imposed torques, and the nonlinear interaction of such torques and forces on the molecule. We find that, due to coupling of the "internal" secondary structure variables to the conformational degrees of freedom of the polymer, the molecule has a highly nonlinear response to applied stress and bending torques. In particular we demonstrate a sharp lengthening transition under applied force and a buckling transition under applied torque. We use perturbative calculations and a mean field analysis to obtain these results. We also carry out Monte Carlo simulations of this model. The numerical results agree well with the mean-field and perturbative calculations where they are expected to do so. The Monte Carlo simulations allow us to examine the response of the chain to large forces and torques where the perturbative approaches fail. In addition we extend our mean-field analysis by studying the fluctuation dominated regime at the force-induced denaturation transition.

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