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Conformations of double stranded DNA: the effect of breathing bubbles AIQUN HUANG, ANIKET BHATTACHARYA, University of Central Florida — A double stranded DNA (dsDNA) is a natural semi-flexible biopolymer with persistence length ≈ 50 nm, while a single stranded (ss) DNA is very flexible whose persistence length is one order of magnitude smaller (3-5 nm). Depending on the temperature and sequence, the two strands in a dsDNA can locally denature into two single strands and form bubbles along the polymer chain, i.e. dsDNA exists in the form of a combination of double strands and single strands, exhibiting a heterogeneity of bending rigidity. In our study, we adopt a coarse grained model of dsDNA developed by Kim *et al.* [J. Y. Kim, J. H. Jeon, and W. Sung, J. Chem. Phys. **128**, 055101 2008] and further improve it by incorporating excluded volume effect and sequence heterogeneity. In this model, a dsDNA is described as two semi-flexible chains paired with each other by hydrogen bonding, the stacking interaction is designed such that the persistence length of the paired chains interpolates 3 nm and 50 nm depending on the fraction of the melted base pairs. By performing Langevin dynamics simulation we study the bubble statistics as a function of temperature and sequence and how the bubbles affect local bending rigidity and the chain conformations. We compare our results with those from WLC model.

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