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DNA overstretching transition and the biophysical properties of S-DNA

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DNA double helix undergoes an "overstretching" transition in a narrow tensile force range slightly above 60 pN. Overstretched DNA is about 1.7 times longer than B-DNA. Despite numerous studies the basic question of whether the strands are separated or not remains controversial. Our recent experiments show that two distinct transitions are involved in DNA overstretching: a slow hysteretic strand-unpeeling transition to strand separation from free DNA ends or nicks, and a fast, non-hysteretic B-to-S transition to an elongated double helix called "S-DNA". We find that the relative fraction of these two overstretched forms is sensitive to factors that affect DNA base pair stability. Under conditions when S-DNA is stable, we characterize its force-extension curve and compare it with that of single-stranded DNA. We find that the S-DNA is 0.01 - 0.02 nm/bp shorter than that of a nucleotide of single-stranded DNA in the force range 75 - 110 pN. Under conditions when S-DNA is less stable than single-stranded DNA, a slow force increase leads to direct strand separation from B-DNA, while a quick force jump to greater than 70 pN leads to a quick formation of the S-DNA first, followed by a slow secondary transition which is a strand separation from S-DNA. From the secondary transition, the extension difference between S-DNA and single-stranded DNA can be directly calculated, which is found in perfect agreement with that computed from the force-extension curves. Finally, we show that DNA in between a pair of small GC-rich segments is biased toward B-to-S transition. This result also demonstrates that in the absence of nicks and free ends, torsion-unconstrained DNA still undergoes the overstretching transition but only through the B-S transition pathway.