

FIG. 2: (Color) Dynamic simulations of a microscopic model accommodating U, M, B and S forms of DNA [11]. Here we show microscopic configurations (vertical axis) as a function of time (horizontal axis) from an illustrative simulation of a 300-basepair fragment of λ -DNA at 21°C and salt concentration 150 mM, extended at 1000 nm/s. The molecule possesses one free end, permitting unpeeling. White indicates B-DNA, red indicates unhybridized DNA (unpeeled or molten), and blue indicates S-DNA. The spatial scale indicates molecular length. The maximum force attained is 90 pN (central dotted line). At forces in excess of about 50 pN, S-form DNA is themodynamically unstable with respect to unpeeled DNA. However, unpeeling takes time to proliferate, and S-DNA is seen to be transiently stable even near forces of about 90 pN. The step-by-step processivity of unpeeling confers upon overstretching an anomalous kinetics that, we argue, rationalizes several nontrivial experimental observations [16–18].