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Entropy-driven hysteresis in a model of DNA overstretching STEPHEN WHITELAM, University of Warwick, SANDER PRONK, PHILLIP GEISSLER, UC Berkeley — When pulled along its axis, double-stranded DNA elongates abruptly at a force of about 65 pN. Two physical pictures have been developed to describe this overstretched state. The first proposes that strong forces induce a phase transition to a molten state consisting of unhybridized single strands. The second picture instead introduces an elongated hybridized phase, called S-DNA, structurally and thermodynamically distinct from standard B-DNA. Little thermodynamic evidence exists to discriminate directly between these competing pictures. Here we show that within a microscopic model of DNA we can distinguish between the dynamics associated with each. In experiment, considerable hysteresis in a cycle of stretching and shortening develops as temperature is increased. Since there are few possible causes of hysteresis in a system whose extent is appreciable in only one dimension, such behavior offers a discriminating test of the two pictures of overstretching. Most experiments are performed upon nicked DNA, permitting the detachment ('unpeeling') of strands. We show that the long-wavelength motion accompanying strand separation generates hysteresis, the character of which agrees with experiment only if we assume the existence of S-DNA.

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