Title:	Hysteresis and nonequilibrium work theorem for DNA unzipping
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Abstract:	We study by using Monte Carlo simulations the hysteresis in unzipping and rezipping of a double stranded DNA (dsDNA) by pulling its strands in opposite directions in the fixed force ensemble. The force is increased at a constant rate from an initial value g 0 to some maximum value g m that lies above the phase boundary and then decreased back again to g 0. We observed hysteresis during a complete cycle of unzipping and rezipping. We obtained probability distributions of work performed over a cycle of unzipping and rezipping for various pulling rates. The mean of the distribution is found to be close (the difference being within 10%, except for very fast pulling) to the area of the hysteresis loop. We extract the equilibrium force versus separation isotherm by using the work theorem on repeated nonequilibrium force measurements. Our method is capable of reproducing the equilibrium and the nonequilibrium force-separation isotherms for the spontaneous rezipping of dsDNA.
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