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A predictive model for the thermomechanical melting transition of double stranded DNA

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By extending the classical Peyrard-Bishop model, we are able to obtain a fully analytical description for the mechanical response of DNA under stretching at variable values of temperature, number of base pairs and intrachains and interchains bonds stiffness. In order to compare elasticity and temperature effects, we first analyze the system in the zero temperature mechanical limit, important to describe several experimental effects including possible hysteresis. We then analyze temperature effects in the framework of equilibrium statistical mechanics. In particular, we obtain an analytical expression for the temperature-dependent melting force and unzipping assigned displacement in the thermodynamical limit, also depending on the relative stability of intra vs inter molecular bonds. Such results coincide with the purely mechanical model in the limit of zero temperature and with the denaturation temperature that we obtain with the classical transfer integral method. Based on our analytical results, explicit analysis of the phase diagrams and cooperativity parameters are obtained, where also discreteness effect can be accounted for. The obtained results are successfully applied in reproducing the thermomechanical experimental melting of DNA and the response of DNA hairpins. Due to the generality of the model, exemplified in the proposed analysis of both overstretching and unzipping experiments, we argue that the proposed approach can be extended to other thermomechanically induced molecular melting phenomena.

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