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Fermeture/ouverture de bulles de dénaturation dans l'ADN en solution

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Summary

The issue of the nucleation and slow closure mechanisms of non-superhelical-stress-induced denaturation bubbles in DNA is addressed by using coarse-grained MetaDynamics simulations. A minimal mesoscopic model is proposed, where the double helix is made of two interacting bead-spring rotating strands, with a prescribed realistic torsional modulus in the duplex state. The timescales for the nucleation and closure of an approximately 10 base-pair bubble are shown to be in agreement with experimental available values, and are associated with the crossing of free-energy barriers of 22 kBT and 13 kBT, respectively, at room temperature. MetaDynamics allows us to highlight the limiting step, a collective twisting, that controls the nucleation/closure mechanism, and to access opening time scales on the millisecond range. A special emphasis will be made between these long-lived equilibrated denaturation bubbles (with a lifetime on the microsecond time-scale) and much more short-lived breathers, which survive less than a nanosecond.

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