DNA helicity and elasticity explained on the nanoscale

December 5 2013

A simple mechanical model to effectively implement the well-known double-stranded structure and the elasticity of DNA on a nano-meter scale has been developed by Jae-Hyung Jeon and Wokyung Sung of Pohang University of Science and Technology in the Republic of Korea, in an effort to more comprehensively explore the nucleic acid containing genetic material of cells. The model was published in Springer's *Journal of Biological Physics*.

Ever since Watson and Crick first described the basic structure of DNA in 1953, a number of quantum chemical calculations to describe it on an atomistic scale or small molecule level have been developed. So far, however, these have proved too computationally demanding or analytically unfeasible to adequately describe the nanoscale DNA conformation and mechanics probed by modern single molecule experiments. At micron scales, on the other hand, the wormlike chain model has been instrumental to analytically describe DNA mechanics and elasticity. It however lacks certain molecular details which are essential to describe the hybridization, nanoscale confinement, and local denaturation or structural changes in DNA caused by extreme conditions.

To fill this fundamental gap, the Korean researchers set about to develop a workable and predictive mesoscopic model of double-stranded DNA, where the nucleotides beads constitute the basic degrees of freedom.

Using the model, the Korean researchers studied how a DNA duplex self-assembles into the helix structure due to the stacking interaction modelled by interaction between diagonally opposed bases, and also how the helix is deformed against the stretching force in comparison with related single molecule experiments. They found that an overstretching transition with the force plateau, as shown in typical force-extension experiments, can be induced by the coexistence of helix and ladder structures at a critical force close to the experimental value. This plateau occurs due to the transition between the helical state and ladderlike state of DNA.

The research duo also showed analytically how a wormlike-chainlike elastic model, frequently used in DNA mechanics, can be derived by using their new model. It is used to explain the bending and twist stiffness in terms of basic interactions in their model and DNA geometrical constants, in reasonable agreement with corresponding experimental values.

"This basic model and its extension, used together with further analytical calculations and numerical simulations, provides new possibilities with which to study a variety of single DNA phenomena from nano to micron length scales," writes Jeon and Sung. "It can, for instance, be used to study the effects of sequence heterogeneity, ionic solutions, and torsional constraints on mechanics and, furthermore, various phenomena such as DNA local denaturation and protein-DNA interaction."

More information: Jeon, J-H. & Sung, W. (2013). An effective mesoscopic model of double-stranded DNA, *Journal of Biological Physics*. DOI: 10.1007/s10867-013-9333-9

Provided by Springer