Relationship between Hydration Induced DNA Dynamical Transition and DNA-sequence Dependent Deformability

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Flexibility of DNA structure is important for protein-DNA recognition. Molecular dynamics simulations and inelastic neutron scattering experiments were conducted on two hydrated DNA dodecamers with distinct deformability; 5'CGCGAATTCGCG3' and 5'CGCGTTAACGCG3'. Molecular dynamics simulation study showed that the former is rigid and the latter is flexible [1]. To investigate the relationship between DNA dynamics dependent on the sequence and the hydration water dynamics, MD simulations and INS experiments were carried out with changing the temperature from cryogenic to room temperature. The mean-square displacements of both DNA dodecamers exhibit so-called dynamical transition around 200-240 K and hydration water also exhibits the abrupt increase in the mean-square displacement at the same temperature. The fluctuation amplitude of the central tetramer AATT is smaller, and its relaxation time longer, than that observed on TTAA, suggesting that the AT step is kinetically more stable than the TA step. The sequence dependent DNA base pair step fluctuations appear above the dynamical transition temperature. Therefore, we concluded that the hydration water induces the DNA dynamical transition, and this enhanced motion by hydration is related to the deformability of DNA structure.

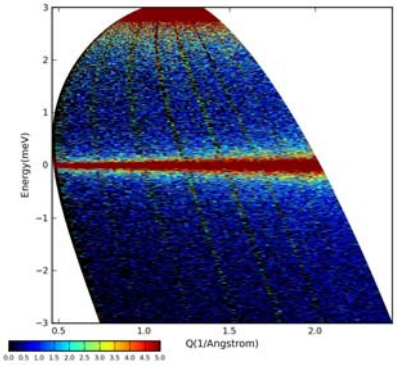

Fig. 1
Neutron inelastic spectra of the DNA with sequence of "CGCGAATTCGCG" at 300 K.

References

[1] Yonetani, Y., and H. Kono, Biophys. J., 97, 1138-1147 (2009).