Numerical modeling of denaturation of a periodic deoxyribonucleic acid molecule

Ostrik M A[1,@] and Lakhno V D[2]

[1] Leonov Moscow Region University of Technology, Gagarina Street 42, Korolev, Moscow Region 141070, Russia
[2] Institute of Mathematical Problems of Biology of the Russian Academy of Sciences, Professor Vitkevich Street 1, Pushchino, Moscow Region 142290, Russia

[@] maria.ostrik@yandex.ru

The biological aim of deoxyribonucleic acid (DNA) is to store the genetic information of a living organism at the molecular level. But DNA molecules can also be considered as structural elements of promising electronic devices [1]. Consequently, the thermodynamic behavior of DNA molecules is of both biological and technical interest. In the considered model the DNA molecule is an aperiodic one-dimensional crystal in which phase transition of the melting type is not possible, since DNA regions enriched with A–T pairs melt at a lower temperature than those enriched with G–C pairs [2]. However, it is to be expected that denaturation is similar to melting in the case of periodic interleaving of pairs A–T and G–C. A numerical realization of a helicoidal mechanical model of a DNA molecule is proposed by a tridiagonal matrix algorithm with an automatically selectable variable time step. The model is a further development of the known helicoidal DNA model [3]. The results of calculations of perturbation propagation of various types along the periodic DNA molecule are given. Molecular dynamic modeling was carried out on the basis of the developed numerical model. As a result, the denaturation temperature of the periodic DNA molecule was determined.

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