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Mathematical modeling of determination of "Premeltons" sites in DNA by ultra short laser pulses

A.A. Kharlamova[1]✉

[1] Northern (Arctic) Federal University named after M.V. Lomonosov, Arkhangelsk, Russia

✉ Kharlamova.anastasya2015@yandex.ru

Abstract. The article discusses a method for analyzing the structure of a molecule using ultrashort laser pulses (USP). A premelton or elongation in the structure of a molecule was chosen as a sample for theoretical modeling of the interaction of a laser pulse with a substance. A premelton is a region of a molecule in which the distance between two adjacent nitrogenous bases is increased. The study of such structures is interesting for limiting the parameters of DNA denaturation, since the process of separation of the molecule begins with the elongation region. At the moment, the study of such features of the DNA structure is difficult, electrophoresis and staining methods cannot always give an accurate result, especially on short sections of the molecule. In this paper, we theoretically model the results of the interaction of USP with a molecule in two cases, when elongation takes place and when the molecule is ideal. The results obtained show the expediency of using laser pulses as a method for determining the structure of a complex polyatomic object. _

Keywords: ultrashort laser pulses, premelton, molecule elongation, denaturation, DNA, RNA

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Математическое моделирование определения премельтонных участков в ДНК ультракороткими лазерными импульсами

А.А. Харламова[1]✉

[1] Северный (Арктический) федеральный университет им. М.В. Ломоносова, Архангельск, Россия

✉ Kharlamova.anastasya2015@yandex.ru

Аннотация. В статье рассматривается метод анализа структуры молекулы с использованием ультракоротких лазерных импульсов (УКИ). Премельтон или удлинение в структуре молекулы было выбрано в качестве объекта для теоретического моделирования взаимодействия лазерного импульса с веществом. Премельтон - это участок молекулы, в котором расстояние между двумя соседними азотистыми основаниями увеличено. Изучение таких структур интересно для определения параметров денатурации ДНК, поскольку процесс разделения молекулы начинается с области удлинения. На данный момент исследование таких участков ДНК затруднено, методы электрофореза и окрашивания не всегда могут дать точный результат, особенно на коротких участках молекулы. В этой статье теоретически смоделированы результаты взаимодействия УКИ с молекулой для двух случаев: когда в молекуле есть удлинение и когда молекула идеальна. Полученные результаты показывают целесообразность использования лазерных импульсов в качестве метода определения структуры сложного многоатомного объекта.

Ключевые слова: ультракороткие лазерные импульсы, премельтон, удлинение молекул, денатурация, ДНК, РНК

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Introduction

Of great interest are the various states of DNA. The presence of elongations in the DNA structure affects the stacking interaction in the molecule, the probability of bubble birth, the rate and time of its denaturation. Elongations were first described in 1983 [1] as a discontinuity of the stacking interaction. At the same time, the H-bonds remain intact, which complicates the theoretical and experimental modeling of an object of such a conformation. There are some calculated data linking elongations with the peculiarities of the dynamics of DNA opening. Also, the presence of elongations is indirectly confirmed by the inability to exchange H with solution molecules, but at the same time by the presence of a high activation barrier [2].

The statistics of experimental data describing such states are small. A different approach is required in modeling and studying molecules with a violation of the stacking interaction. DNA elongation is the trigger for its transition to an open state. This structure of the molecule has a great influence on a number of biochemical processes, including the transfer of the electric charge of DNA. Elongated areas may be sensitive to temperature, pH, ionic strength and other thermodynamic factors. Some studies indicate the importance of DNA elongation in the recognition of the DNA polymerase promoter [3, 4, 5].

To determine the spatial structure of a molecule with elongations, a dye is intercalated into the molecule, which stands in the place of elongation Fig. 1,*b* [3, 4]. They also use the method of X-ray diffraction analysis Fig. 1,*a*. Both methods do not accurately determine the location of the presence of elongation. The intercalation graph is blurry and approximately indicates the presence of elongation. The X-ray diffraction analysis image also does not display the elongation structure because it does not have the physical ability to work at the level of one or two nitrogenous bases of the molecule.

Today, scientists have turned to the use of ultrashort laser pulses instead of X-rays, as a tool capable of seeing the structure of a molecule at the atomic level. In this paper, we mathematically simulate the process of interaction of an ultrashort pulse with a DNA molecule having elongation in the structure and show the sensitivity of such a method to similar DNA configurations.

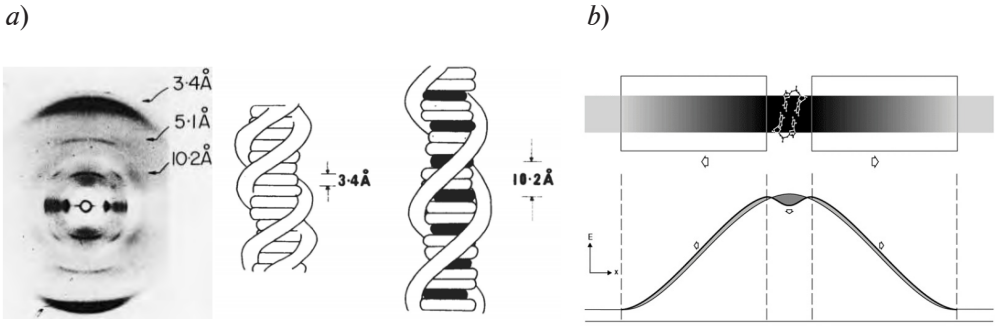

Fig. 1. Result of X-ray structural analysis of a DNA molecule whose structure contains elongations between nitrogenous bases: X-ray structural analysis of the molecule (*a*); result of analysis of the molecule by staining (*b*)

Materials and Methods

The article proposes to consider the DNA molecule as a polyatomic system on which an ultrashort laser pulse falls. The modeling of the scattering spectrum is based on the Dirac-Hartree-Fock-Slater model [6,7].

Consider a molecule with a complex polyatomic structure [8]. An ultrashort laser pulse falls on this molecule in the direction of $\mathbf{n}_0$. We assume that the duration of such a pulse τ is many times less than the characteristic atomic time τ_a. It is well known that this condition applies in the approximation of a sudden disturbance. In the approximation of a sudden perturbation of the system's own Hamiltonian, it can be neglected, since the electron in the atom does not have time to evolve under the action of the ultrashort laser pulse field. Next, we will use the electromagnetic field strength USP in a general way, $\mathbf{E}(\mathbf{r},t) = \mathbf{E}_0 h(t - \mathbf{n}_0\mathbf{r}/c)$, that is, we will consider it spatially inhomogeneous, where $\mathbf{E}_0$ is the field amplitude, $h(t - \mathbf{n}_0\mathbf{r}/c)$ is an arbitrary function defining the USP form, c is the speed of light. In the case of such pulses, in particular [9], when solving the Dirac equation, the electron wave function in the USC field with the intensity was found $\mathbf{E}(\mathbf{r},t)$.

$$\Psi(t) = \varphi_0\left(\{\mathbf{r}_a\}\right) e^{-\sum_a i \int_{-\infty}^{t} \mathbf{E}(\mathbf{r}_a,t')\mathbf{r}_a dt'}, \tag{1}$$

where $\sum$ is the summation over all electrons in complex polyatomic structures, $\varphi_0(\{\mathbf{r}_a\})$ is the initial wave function of all electrons in such a system.

To calculate the main scattering characteristics, we will use the quantum theory of USP scattering, in which there are no restrictions on the number of atoms in the system [10]. In this theory, general expressions for calculations of the main scattering characteristics are obtained. As a result, using equation ((1) and theory in [10], we obtain an expression for calculating the scattering energy ε per unit solid angle Ω_k ($\mathbf{k} = (\omega/c)\mathbf{n}$, where $\mathbf{n}$ is the direction of the scattered pulse) in a single frequency interval ω (next − spectrum)

$$\frac{d^2\varepsilon}{d\Omega_k d\omega} = \frac{\left[\mathbf{E}_0\mathbf{n}\right]^2}{(2\pi)^2} \frac{\left|\tilde{h}(\omega)\right|^2}{c^3} \left\langle \varphi_0 \left| \sum_{a,a'} e^{-i\mathbf{p}(\mathbf{r}_a - \mathbf{r}_{a'})} \right| \varphi_0 \right\rangle, \tag{2}$$

where $\tilde{h}(\omega) = \int_{-\infty}^{+\infty} h(\eta) e^{i\omega\eta} d\eta$ and $\mathbf{p} = (\omega/c)(\mathbf{n} - \mathbf{n}_0)\mathbf{n}$ has the value of the recoil pulse when the USP is scattered on the bound electron. Next, we use the well-known model of independent atoms, see, for example [11]. In this case, the problem can be solved by switching to the electron density of individual isolated atoms that make up a complex polyatomic structure. Dividing equation ((2) into two, where the first term corresponds to the summation $a = a'$, and the second term $a \neq a'$, we obtain

$$\frac{d^2\varepsilon}{d\Omega_k d\omega} = \frac{\left[\mathbf{E}_0\mathbf{n}\right]^2}{(2\pi)^2} \frac{\left|\tilde{h}(\omega)\right|^2}{c^3} \left\langle \sum_{i=1}^{s} N_{e,i} N_{A,i} \left(1 - \left|F_i\right|^2\right) + \sum_{i,j=1}^{s} \delta_{i,j} N_{e,i} N_{e,j} F_i F_j^* \right\rangle, \tag{3}$$

where $N_{e,i}$ is the number of electrons in the atom of the i-variety; $N_{A,i}$ is the number of atoms of the I-variety; $F_i = \frac{1}{N_{e,i}} \int \rho_{e,i}(\mathbf{r}) e^{-i\mathbf{p}\mathbf{r}} d^3\mathbf{r} = 1$ is a form factor of the atom of the i-variety with an electron density $\rho_{e,i}(\mathbf{r})$. Coefficient $\delta_{i,j} = \sum_{Ai,A'j} e^{-i\mathbf{p}\left(\mathbf{R}_{Ai} - \mathbf{R}_{A'j}\right)}$ depends only on the coordinates of atoms of the i-variety (with A_i number), the position of which is determined by the radius vector $\mathbf{R}_{A_i}$. Eq. (3) is analytical, which contributes to a fairly simple calculation of spectra. The calculation of the electron density is difficult here. To find it, we use the method described in [12].

Results and Discussion

As an object of research, we take a small fragment of DNA with the bases cytosine, cytosine, guanine, cytosine between which there was an elongation (Fig. 2,*b*).

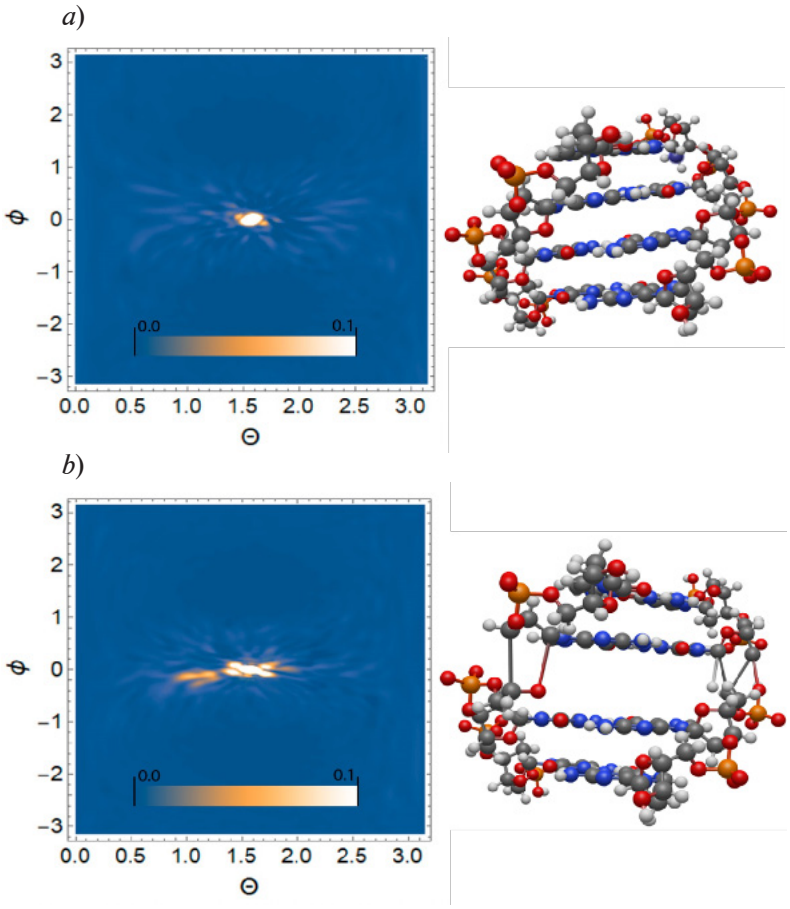

Fig. 2. Perfect DNA fragment (*a*) DNA fragment with elongation or 'premelton' (*b*)

We compare it with the same DNA fragment, but of an ideal shape, without elongation (Fig. 2,*a*).

As a result of mathematical modeling of the interaction of USP with elongated DNA, a radiation spectrum was obtained, which we can compare with the spectrum of interaction from ideal DNA in Fig. 2 where θ the angle between the spiral axis and the scattering direction **n**, φ is the angle between the *x*-axis and the projection **n** on a plane perpendicular to the axis of the spiral.

Conclusion

As can be seen from the obtained contour graph, a change in the distance between the nitrogenous bases leads to a change in the scattering angle, which is reflected in the form of elongated spots. This suggests that the resulting theory is able to respond to changes in the spatial position of atoms in the object of study.

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THE AUTHOR

KHARLAMOVA Anastasya A.
kharlamova.anastasya2015@yandex.ru
ORCID: 0000-0002-8192-615X

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