Theoretical analysis of gyrotropy and absorption of terahertz electromagnetic waves in layer of DNA molecules

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Abstract. Certain type of low-frequency DNA molecular oscillations was analysed within the self-consistent phonon approximation. There were calculated dispersion relationship, exiting the oscillations by electromagnetic wave and corresponding contribution to the absorption spectrum of ensemble of parallel DNA molecules. The dependence of the DNA spectral characteristics on the length and period of the DNA duplex structure is revealed. The method of experimental check of obtained results is suggested. If the described model is confirmed by experiment, the obtained results available to reconstruct the length and duplex period of the DNA in a sample by its absorption spectrum.

1. Introduction

Chemical properties and functions of big complex bio molecules, such as DNA and proteins, are determined by their spatial structure – so-called conformation. Conformational state of many biological molecules can change without any chemical reaction, just by thermal motion. So investigation of conformations needs non-invasive methods. Electron and atomic force microscopy, traditionally used for the molecular visualisation, works only with adsorbed molecules, but adsorption can influence on the conformation itself [1]. Roentgen structural analysis excels at spatial resolution but this method works well only with molecular crystals but not solutions of molecules.

The terahertz (THz) spectroscopy is considered as perspective method to get information on structure and dynamics of biological molecules [2,3,4,5,6]. THz spectroscopy enables measurements of bio molecules *in situ*, in aqueous solution. Instead of roentgen, THz irradiation is non-ionizing and is suspected to be non-invasive for bio molecules [2,3,4,5,6], at least if the power of the irradiation lies below some threshold. Unfortunately, today there are no well established methods of interpreting molecular spectra in the THz frequency range. This work is aimed at simulation of dependence of DNA absorption spectra on the length and the period of the DNA duplex. If the experimental data confirm the model predictions, the algorithm of interpreting the absorption spectra is suggested.

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2. Model description.

The dynamics of the DNA molecule was analysed within the self consistent phonon approximation [7,8]. The DNA molecule was described as a chain of coupled oscillators having the same partial frequency. Each oscillator presents a pair of nucleotides which have opposite charges, different masses and can oscillate along the line perpendicular to the molecules axis. Each nucleotide is springily connected with its neighbors (as shown on Fig. 1). A direction of oscillations is not the same for all nucleotide pairs but it turns by the same small angle for each next oscillator which is used to simulate the duplex structure of DNA molecule. The DNA layer was simulated as parallel duplexes placed in isotropic and spatially uniform dielectric medium.

The two Cartesian coordinate systems were used. The equations of motion of each nucleotide were write in a 'local' coordinates, where the axis x_n is parallel to the hydrogen bond in the nth base pair (as shown on Fig. 2) and the axis z_n is perpendicular to the plane of the nth base pair. The 'global' coordinates correspond to the DNA film: the z axis is parallel to the helix axes of DNA molecules and the axes x and y lie in the plane of the film.

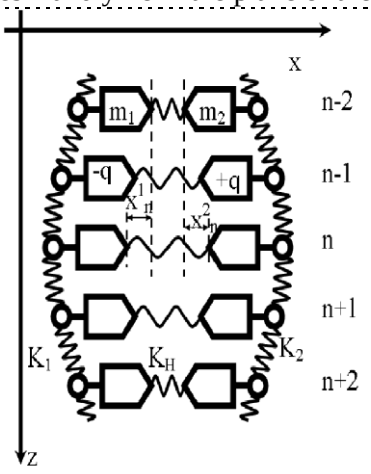

Figure 1. The model of the DNA molecule. Helix structure is omitted on the picture.

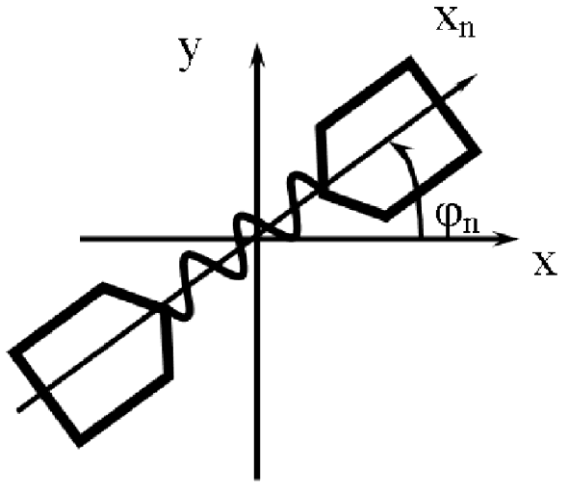

Figure 2. The local and global Cartesian coordinates in the model.

An interaction of DNA molecule with electromagnetic field was considered as interaction of charged nucleotides with plane spatially uniform monochromatic electromagnetic wave, propagating along the DNA helix axis. The equations of motion are given below (1):

$$m_{1,2}\frac{\mathrm{d}x_n^{1,2}}{\mathrm{d}t} = \pm K_H\left(x_n^2 - x_n^1\right) - K_{1,2}\left(2x_n^{1,2} - x_{n-1}^{1,2} - x_{n+1}^{1,2}\right) - m_{1,2}\gamma\frac{\mathrm{d}x_n^{1,2}}{\mathrm{d}t} \mp qE_{xn}\mathrm{e}^{ikz_n - i\omega t} \quad (1)$$

where $x_n^{1,2}$ and $m_{1,2}$ are coordinates and masses of nucleotides, K_H and $K_{1,2}$ are rigidities of hydrogen and chemical bonds correspondingly, γ is damping coefficient and $E_{xn}\mathrm{e}^{ikz-i\omega t}$ is the projection of the electric field vector on the axis x_n in the local coordinates. Indexes 1 and 2 correspond to the "left" and "right" strand of the DNA molecule on the Fig. 1, index n corresponds to the number of base pair.

The masses of nucleotides were calculated from their chemical structure while rigidities of bonds were adjustable parameters.

3. The simulation results.

3.1. Eigen modes.

There are two types of eigen modes of the DNA model (1): acoustic and optic (fig.3). The acoustic modes correspond to in-phase oscillations of nucleotides in each bas pair while the optic modes correspond to anti-phase oscillations. The frequencies of eigen modes is written below (2):

$$\omega_{\kappa\, a,o}{}^2 = 0.5\left(\omega_{H1}{}^2 + \omega_{H2}{}^2\right) + 2\left(\omega_1{}^2 + \omega_2{}^2\right)\sin^2(\pi\kappa/2N) \mp \\ \mp\left[\left(0.5\left(\omega_{H1}{}^2 - \omega_{H2}{}^2\right) + 2\left(\omega_1{}^2 - \omega_2{}^2\right)\sin^2(\pi\kappa/2N)\right)^2 + \omega_{H1}{}^2\omega_{H2}{}^2\right]^{1/2} \quad (2)$$

where $\omega_{H1,2}{}^2 = K_H/m_{1,2}$; $\omega_{1,2}{}^2 = K_{1,2}/m_{1,2}$; N is the number of base pairs (b.p.) in the DNA molecule and κ is an integer number, determining the spatial structure of oscillations (3). For the κ eigen mode the spatial structure of oscillations is written below:

$$x_n^{1,2} = A^{1,2}\cos\left(\frac{\pi\kappa}{N}(n+1/2)\right)e^{-i\omega t} \quad (3)$$

where $A^{1,2}$ is amplitudes of eigen modes.

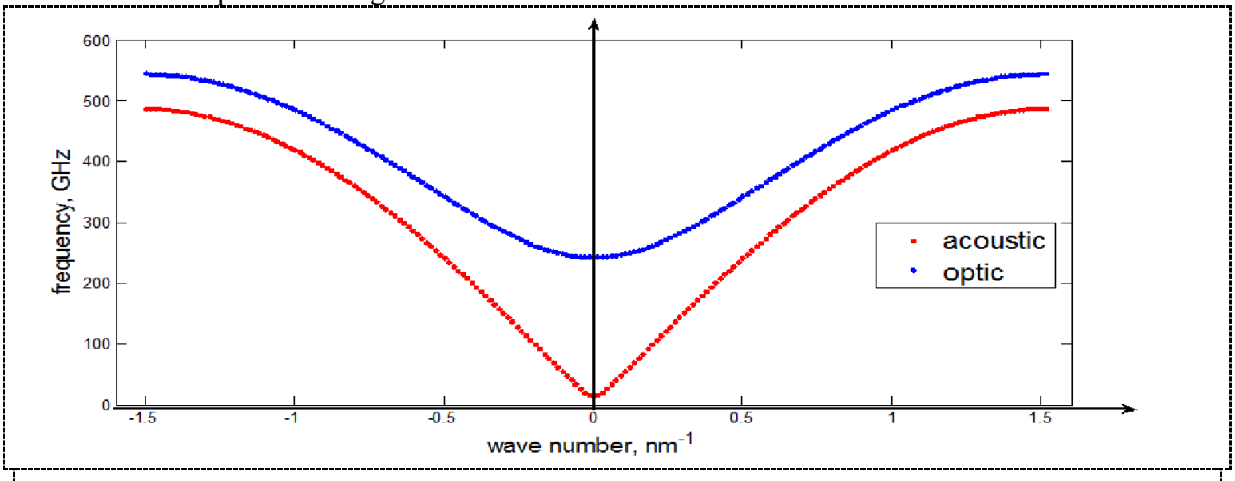

Figure 3. Dispersion relationship for both types of eigen modes of the DNA. The lowest frequency of the acoustic branch is equal to 0; the lowest frequency of the optic branch is determined by the properties of hydrogen bonds

The stationary solution of the equation (1) is written below (2):

$$p_\kappa(\omega) = \frac{qE_\kappa}{m_1 m_2}\frac{4(K_1+K_2)\sin^2(\pi\kappa/2N) - (\omega^2 + i\gamma\omega)(m_1+m_2)}{\left((\omega^2+i\gamma\omega) - \omega_{\kappa a}{}^2\right)\left((\omega^2+i\gamma\omega) - \omega_{\kappa o}{}^2\right)} \quad (4)$$

where $p_\kappa(\omega)$ and E_κ is coefficients of Fourier finite transformation (5):

$$p_n = \sum_{\kappa=0}^{N-1} p_\kappa(\omega)\cos\left(\frac{\pi\kappa(n+1/2)}{N}\right)e^{-i\omega t} \\ E_{xn}e^{ikz} = E_0\cos(\phi_n)e^{ikz} = \sum_{\kappa=0}^{N-1} E_\kappa\cos\left(\frac{\pi\kappa(n+1/2)}{N}\right) \quad (5)$$

where p_n is a projection on the nth base pair dipole moment on the axis x_n and ϕ_n is the angle between the electric field vector and the nth nucleotide pair.

The absorption of the DNA-containing media is proportional to the electrical field work on the excitation the molecular oscillations (6):

$$abs \propto \sum_{n=0}^{N-1} E_{xn} p_n^*$$
$$abs \propto \sum_{\kappa=0}^{N-1} \frac{q|E_\kappa|^2}{m_1 m_2} \frac{4(K_1+K_2)\sin^2(\pi\kappa/2N) - (\omega^2 + i\gamma\omega)(m_1+m_2)}{((\omega^2+i\gamma\omega)-\omega_{\kappa a}{}^2)((\omega^2+i\gamma\omega)-\omega_{\kappa o}{}^2)} \quad (6)$$

where *abs* is absorption coefficient.

There are two factors, determining the $p_\kappa(\omega)$: frequency and spatial structure. First, $|p_\kappa(\omega)|^2$ is maximum if the frequency of the wave is close to the eigen frequencies $\omega_{\kappa a,o}$. Second, E_κ and correspondingly $p_\kappa(\omega)$ strongly depend on the number κ. For the regular DNA duplex with the period N_{hel} E_κ can be estimated as (6):

$$|E_\kappa|^2 \propto \begin{cases} \left(1+(\kappa-\kappa_{hel})^2\right)^{-1}, & |\kappa-\kappa_{hel}| << N \\ 1/N^2, & |\kappa-\kappa_{hel}| \propto N \end{cases} \quad (6)$$

where $\kappa_{hel} = \frac{2N}{N_{hel}} + kaN$ and a is the distance between neighbor nucleotide pairs in the DNA.

The absorption spectra of the DNA molecule calculated in the context of the presented model are shown on the fig. 4 (a, b). The lines of absorption correspond to the frequencies of the eigen modes. The frequency of the maximum absorption depends on the helix period of DNA molecule.

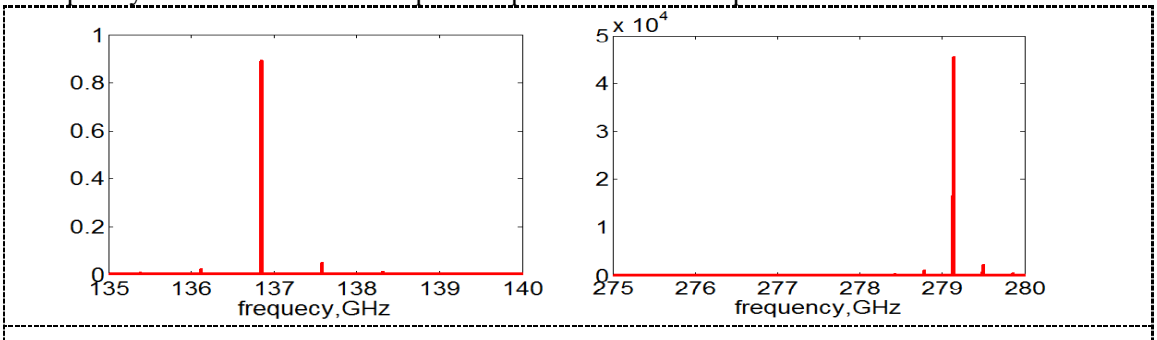

Figure 4a. Absorption of the DNA molecule with the length 1002 b.p. and helix period 11 b.p.

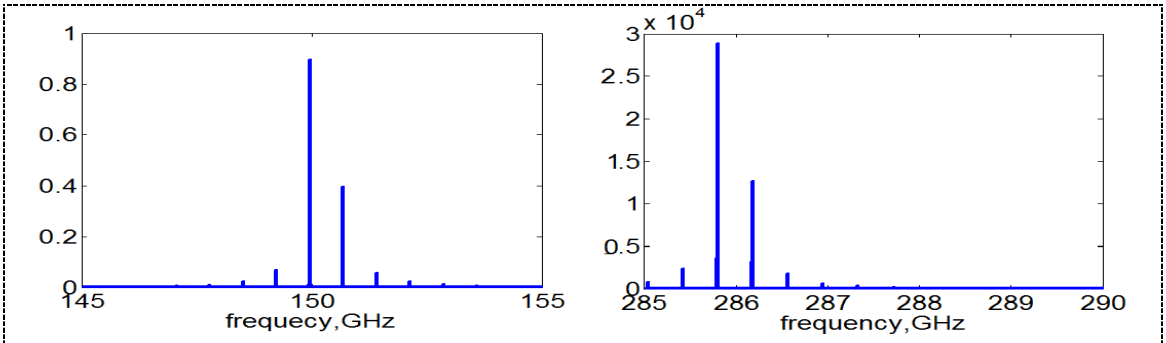

Figure 4b Absorption of the DNA with the length 1002 b.p. and helix period 10 b.p.

4. Conclusion

In the self-consistent phonon approximation the eigen modes and absorption spectra of the layer of identical parallel DNA molecules were calculated. The absorption spectra contain two series of lines corresponding to the acoustic and optic branches of the dispersion relationship. Each series presents one big central (major) line and few satellites. The frequency of the major line in the both series depends on the DNA helix period while the distance between the major line and its neighbour satellites depends on the length of the DNA molecules. It's interesting, that the distance between the lines in the absorption spectra doesn't depend on the helix structure of the DNA molecule and *vice versa*, the frequency of the major lines doesn't depend on the length of the molecule according to the model.

These results can be simply checked by comparing absorption spectra of DNA molecules with different length or different helix structure.

The results can be important for practical applications. It is possible to-determine the helix structure of the DNA molecules in the sample from the THz absorption spectra. If somebody measures the both major absorption lines, predicted by the model, and two satellites for each major line, he can calculate such parameters as K_H, $K_{1,2}$, N and N_{hel} from the frequencies of the measured lines. Also somebody can put together absorption spectra of DNA molecules alter by length but with the same duplex structure (or *vice versa*) and then compare the spectrum of an unknown sample with these standard spectra. If the frequency of the mayor line in the unknown sample is similar with the standard sample, the helix structures of the both samples are identical. Also if the distances between lines in the absorption spectra of the samples are equal, the length of the DNA molecules in the samples are equal.

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5. References

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