Dependence on the length of localization of G4 DNA molecule to temperature and electric field

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Abstract. The charge transport property of G4 DNA molecule that represented mathematically by using Hamiltonian tight binding approach has been studied. Charge transport property in the model of 102 base pairs long G4 DNA is studied from localization length under influence of electric field and temperature. Electric field affects electron hopping constants in G4 DNA molecule, while temperature leads to DNA structural disorder. Localization length is calculated by using transfer matrix method and using gram-schmidt orthonormalization method to reduce calculation errors. The result show, the increment of electric field and temperature decreases localization length, so that G4 DNA molecules becomes less conducting.

Keywords: DNA, DNA G4, Localization Length, Electric Field, Temperature

1. Introduction
The research progress has been bringing physicists to examine and study electrical properties of various biological materials, for instance DNA molecule. DNA molecule is an active element candidate that interesting to be studied because DNA can be passed by electric current along π-way [1]. DNA molecule has self-assembly and recognition properties. Self-assembly property is the ability of molecules to spontaneously assemble themselves. Recognition property is the ability of molecule to form selective bond with other molecules. These ability make DNA to be a promising candidate for used in molecular electronics [2].

DNA structure has been frequently modified in order to improve its effectiveness in transporting charges. Ones found structures such as single stranded DNA (ss-DNA), double stranded DNA (ds-DNA) and G-quadruplexes DNA (G4 DNA). Recently, G4 DNA has been investigated extensively because it has unique structure and self-assembly property [3]. Theoretical and experimental results show G4 DNA is efficient for long distance charge transport and more stable than ss-DNA and ds-DNA [3,4]. G4 DNA structural disorder is smaller than ds-DNA so that its conduction property is better [4]. Structural disorder can be caused by thermal agitation such as twisting motion [5].

In this report, DNA G4 model is studied in the presence of electric field along its symmetrical axis. This report will be focused on electron localization length which measures the distance spanned by an electron wave function. The localization length of DNA model was calculated by considering that electric field affect electron hopping constants of DNA molecule [6]. In the model, environment temperature is also taken into account. Temperature influences charge transport so that localization length decreases.

2. Theoretical model
G-quadruplexes also known as G4-DNA is a helix structure containing guanine tetrad where four
Localization length can be calculated using transfer matrix

\[ L = \sum_{n=1}^{N} \sum_{\tau=1}^{4} \left( e^t + \delta^\tau \right) |n, \tau\rangle \langle n, \tau| + t_{n,n+1}^{t,\tau} |n, \tau\rangle \langle n+1, \tau| + h.c \]  

The parameter in equation (1) has been described in paper [8]. Electric field is applied parallel to DNA symmetrical axis (axis-Z). The direction of electron flows is opposite to the direction of electric field. Electric field leads to changes in the value of electron hopping constant from site \( i \) (initial state) to site \( i+1 \) (final state) according to Miller-Abrahams formula [6]. In this report, the electron hopping constant can be written as

\[ t_{i,i+1} = t_0 \exp \left\{ -eE \left( \frac{Z(i+1) - Z(i)}{k_B T} \right) \right\} \]  

In equation (1) and equation (2), \( t_{i,i+1} \) is electron hopping constant from initial state \( i + 1 \) to final state \( i \) and \( t_{i,i-1} \) is electron field affected electron hopping constant from initial state \( i - 1 \) to final state \( i \). \( t_0 \) is electron hopping constant in the absence of electric field, \( e \) is electron charge, \( Z(i) \) is the position of site- \( i \) along the z axis of DNA. \( k_B \) is Boltzmann constant and \( T \) is temperature. The effect of temperature is considered in this study following procedure in reference [5].

2.1. Localization length

Localization length is the size of room in length that might be traveled by charge in the system. Localization length can be calculated using transfer matrix method. Tight binding Hamiltonian
approach can be used to calculated transfer matrix method using Schrödinger equation \( H\psi = E\psi \). In 1-dimensi, the equation can be written as:

\[
-t_{i-1,i}\psi_{i-1} + \left(\epsilon_i - E\right)\psi_i - t_{i,i+1}\psi_{i+1} = 0
\]

Equation (4) can be transform into matrix equation

\[
\begin{pmatrix}
\psi_{i+1} \\
\psi_i
\end{pmatrix} = T(i)
\begin{pmatrix}
\psi_i \\
\psi_{i-1}
\end{pmatrix},
\]

where \( T(i) \) is transfer matrix [9] and in 2x2 matrix can be written as

\[
T(i) = \begin{pmatrix}
\epsilon_i - E & -t_{i-1,i} \\
t_{i,i+1} & 1 - t_{i,i+1}
\end{pmatrix}
\]

Equation (5) can be used to calculate wave function amplitude at one sites as long as the wave functions at two previous sites are known. Even more, through multiplication of consecutive transfer matrices ones obtain the relation of wave function amplitude at both ends of a molecule. To reduce error due to many multiplicative operation, in the calculation to types of multiplication are employed which are forward transfer matrix multiplication and, then, backward transfer matrix multiplication, gram-schmidt orthonormalization method are employed after certain number of matrix multiplication.

Following reference [9], after several times of matrix multiplication, the Lyapunov exponents \( \gamma_{cl} \) is calculated using

\[
\gamma_{cl} = \frac{\ln \left( \prod_r a_r^{\alpha_{cl} - 1} \right)}{2K(L - 1)}
\]

where \( cl \) is order of matrix columns, \( \alpha \) is normalization coefficient obtained from orthonormalization process, \( K \) is repetition of multiplication, \( L \) is DNA length, and \( r \) is number of orthonormalization. The inverse of smallest \( \gamma_{cl} \) gives the localization length \( (\lambda) \)

\[
\lambda = \frac{1}{\gamma}
\]

3. Results and discussion

Electron localization lengths of G4-DNA molecule under the influence of electric field and temperature have been calculated at twisting oscillations frequency of 0.51 meV. The localization length in 102 base pair long DNA as function of electron energy has been calculated for voltages of 0, 1 mV, 3 mV, and 7 mV at temperature of 4.2 K and 30 K, respectively.

Electron localization length of G4 DNA molecule at temperature 4.2 K and various voltages are shown in figure 2. Spectrum of localization length shows the existence of extended states and localized states, which form bands. Extended state has localization length longer than 102 base pair, while states with electron localization length smaller than 102 base pair are called localized state.

Figure 2a shows localization length when the electric field is absent. It shows two bands of states with localization length greater than zero separated by one gap which is in the energy range of 8.9 eV to 9.4 eV. In the energy range of 7.35 eV to 8.9 eV and 9.5 eV to 9.7 eV many states are extended states. However, there are no extended states in the energy below 7.35 eV. The localization lengths in the presence of electric field are shown in Fig 2(b-c). It is shown that the electric field decreases the localization length at certain energy. With the increment of electric field, more states changes from extended to be localized states. It can be seen clearly at energy greater than 8.4 eV. However, at energy below 7.35 eV some states experience an increment of localization length and become extended states. In addition to that, energy gap is slightly getting wider as voltage increases. This trend
of localization length changes may be the result of the decrement of electron hopping constant in the direction of electric field. Sergiy nokhrin et al. find threshold voltage of 1 volt at a distance of 5 nm leads to decrease conductivity of M-DNA by at least 10-fold [10].

In figure 3 shows localization length calculated at temperature 30 K for several values of voltage. The increase in temperature leads to localization length decreases such that at this temperature all states become localized. Thermal fluctuations can affect the twist angle of DNA molecule so that the distribution of the twist angle of bases becomes wider. It causes the DNA structure becomes more irregular as temperature increases, thus disrupting electrons to jump. The result shows that temperature increases disorder in system so that inhibit charge transport in G4-DNA molecule. This result of calculation are in agreement to Suhendro et al. [5] research, which showed that localization length of double strand DNA molecule decreases due the increase in temperature, especially at low frequencies because of the distribution of DNA rotating angle widen. All states are localized is observed at all voltages used in the calculation. The effect of electric field is not as dramatic as at temperature 4.2 K in the sense of the decrease in localization length is much smaller. There is competing effect of twisting motion and electric field in the localization length.

4. Conclusions
Electron localization length in G4-DNA molecule under the influence of external electric field and at temperature 4.2 K and 30 K has been studied. The increment of electric field leads to lesser number of extended states. The electric field affects the electronic state more at higher energy where electron states become localized. This results shows that, in the scheme of electric field dependent hopping constant model we used, the electric field decreasing electron localization length and it leads to the deterioration of G4-DNA transport property. This trend is observed at both temperature used in the study. However, electric field influence on electron localization length becomes weaker as the temperature increases since the temperature effect is dominant.

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