I-V characteristics on G4 DNA molecule: Electric field and current dependent hopping amplitude model

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Abstract. We study the charge transport property of G4 DNA molecule by calculating the I-V characteristics at several temperatures. The G4 DNA we used consists of 32 G-tetrads built from four guanine bases and is contacted to metallic electrodes at both ends. The molecule is represented mathematically by using tight binding Hamiltonian model. Miller-abrahams scheme is used in calculating electron hopping constant under electric field which is applied along the molecular axis of DNA. Temperature is considered in the model by assuming twisting angles are distributed following Gaussian distribution. The current as voltage function is calculated using Landauer-Buttiker formalism from transmission probabilities. The result show that twisting motion due thermal agitation weakens the effect of electric field.

1. Introduction
The measurement of charge transport in DNA molecules [1] gave controversial results, DNA molecule has various conductivity properties ranging from insulators to proximity-induced superconductor [2]. Many factors can be the cause of these various results such as the influence of environment and molecule itself. Environmental effects may come from factors such as DNA-electrode contact, electric field, magnetic field [3], temperature [4], etc. The physical nature molecule itself may come to play in the form of DNA base sequence, DNA molecular length, internal DNA movement, etc. [5].

Recently the charge transport on G4 DNA has attracted the attention of researchers to study it. These attentions stems from its unique properties [6] and its long size so that more overlapping orbital which makes better conductivity [7]. In many charge transport experiments, a DNA molecule is directly connected to metallic electrode at both ends in order to obtain characteristics of electric current as voltage function [8]. In this study, we take into consideration the environmental influence on the G4 DNA molecules. The environmental influences brought into equation are electric field and temperature. The electric field effect of DNA molecule, which in turn affecting the transport process, in our knowledge is absent in the theoretical study of I-V characteristics of DNA molecule. In the model, the electric field causes significant change in electron hopping constant from a site to other site. The temperature causes structural fluctuations, such as vibration of DNA chain so that there is a change in the rotating angle between the nearest base pair and distance between one base to another base [9]. The structural vibration, in this study model with the twisting motion of G-quarted, can be seen as phonon excitation in DNA. The I-V characteristic of G4 DNA were studied using tight binding Hamiltonian model [5]. The electron transmission probability on the DNA molecule calculated using Green’s function method was used in calculating I-V characteristics by using the Landauer-Buttiker formula.
2. Experimental

2.1. Theoretical model
In this study, we use tight binding approach in modelling single electron system in G4 DNA molecule. In this model, we assume that electrons can move from one base to neighboring base, both on the same strand (intrastrand hopping) and different strands (interstrand hopping diagonally and interstrand hopping vertically) but electrons cannot move from one backbone to backbone other [10].

G4-DNA is a structure constructed from square planar structures called G-quadruplex or G-quartet which consists of four guanine bases structure that are piled on top of each other and connected via Hoogsteen hydrogen bond. In G-quadruplex there is a cation between each pair of tetrad making G4 DNA structure more stable. Two adjacent G-quartets in the stack is separated by a distance of 3.4 Å makes a twisting angle of 30° [11]. In this study, the length of DNA molecule is 32 G-quartets.

The single electron tight binding Hamiltonian model of G4 DNA molecule maybe written mathematically as follows.

\[
H = \sum_{n=1}^{N} \sum_{\tau=1}^{4} \left\{ \left( e_n + Q_n \right) |n, \tau\rangle \langle n, \tau| + t_{n,n+1}^{n+1,\tau} |n, \tau\rangle \langle n+1, \tau| \right\} \\
+ \sum_{\tau'=1}^{4} \left\{ t_{n,n+1}^{n+1,\tau'} |n, \tau+1\rangle \langle n, \tau| + t_{n,\tau+1}^{n+1,\tau} |n, \tau\rangle \langle n+1, \tau+1| \right\} \\
+ \sum_{\tau'=1}^{4} \left\{ B_{n,n+1}^{\tau,\tau'} |n, \tau\rangle \langle n, \tau| + t_{n,\tau+1}^{\tau,\tau'} |n, \tau\rangle \langle n, \tau+1| \right\} + h.c
\] (1)

The parameters in equation (1) have been explained in other report [12]. Based on Miller-Abrahams formula, effect of electric field which is applied parallel to the symmetrical axis of DNA on the electron hopping constant is modelled as follows [13]:

\[
t_{i,i+1} = t_0 \exp \left\{ -\frac{eE}{K_B T} \right\} \left( \frac{Z(i+1) - Z(i)}{Z(i+1) + Z(i)} \right)
\] (2)

In equation (2), \( t_{i,i+1} \) is electric field affected electron hopping constant from initial site \((i+1)\) to final site \((i)\). \( t_0 \) is electron hopping constant in the absence of electric field, \( K_B \) is Boltzmann constant and \( T \) is temperature, \( e \) is electron charge, \( Z(i) \) is site-\( i \) position in the \( z \) axis of DNA. The effect of temperature in the form of G-quarted twisting motion is considered in this study following the model discussed in ref [9].

2.2. Electric current calculation
Transmission probability as explained in ref [14] is used to calculate electric current as voltage function using Landauer-Buttiker formula [11]:

\[
I = \frac{2e}{h} \left[ T(E) [f_L(E) - f_R(E)] dE \right]
\] (3)

where is \( f_L(R)(E) \) is Fermi-Dirac distribution function
Under bias voltage $V$, the chemical potential $\mu_{L(R)}$ of left (right) electrode can be written as

$$f_{L(R)}(E) = \{1 + \exp\left(\frac{E - \mu_{L(R)}}{k_B T}\right)\}^{-1}$$

(4)

In this study, Fermi energy $E_f$ and electron hopping constant on metallic electrode respectively are set to 8.45 eV and 0.75 eV following ref. [4].

3. Results and Discussion

In this study, the properties of charge transport on G4 DNA molecule, the I-V characteristics of this molecule has been calculated on 32-stack of guanine tetrad at G-quarted twisting motion frequency of 2.0 meV, temperatures of 77.2 K, 150 K, and 300 K. I-V Characteristics is calculated using Landauer-Buttiker formula from transmission probability. The transmission probability at temperature of 77.2 K shows that the increase of electric field causes transmission probability spectrum change in the form the energy gap becomes wider and energy bands become narrower. However, the maximum

![Figure 1. Electron transmission probability on 32 G-quarted stack of G4 DNA molecule calculated at temperature of 77.2 K and G-quarted twisting motion frequency of 2.00 meV for several voltages.](image-url)
transmission probability at first increases with the electric field, and after reaching a particular value its start decreasing. Figure 1 shows transmission probability calculated at temperature of 77.2 K and oscillation frequency of 2.0 meV for several voltages. The red vertical line is for showing the change in transmission probability spectrum around the Fermi energy. The states involved in the transport process are the states around Fermi energy of 8.45 eV in the range $E_f \pm 1/2 \text{eV}$ (chemical potential of left/right electrode). Since the transmission probability is used in calculating the I-V characteristics, the change in its spectrum with the electric field manifest in the I-V characteristics curve.

At temperature 77.2 K and low voltage of 2.0 mV, the charge transport process occurs in energy range of $8.45 \text{eV} \pm 1/2 \ (0.002)$, which is around $8.449 \text{eV} - 8.451 \text{eV}$. Even though the transmission probabilities are quite high, see Figure 1, since the number of state involved in the process is small, the current obtained is very small as can seen in Figure 2. As the voltages increases, the number of states involved in the transport process in increases since the Fermi energy still inside the band of states with high transmission probability. Therefore current increases considerably with voltages. At voltage of 0.8 V the charge transport process occurs in energy range of $8.45 \text{eV} \pm 1/2 \ (0.8)$ which is around $8.05 \text{eV} - 8.85 \text{eV}$. In this range a large number of states involved in the process and have high transmission probabilities. Despite of Fermi energy is located near band edge in energy band, the current through the molecule is very large. In contrast, at voltage of 1.5 V the charge transport process occurs in energy range of $8.45 \text{eV} \pm 1/2 \ (1.5)$ which is around $7.7 \text{eV} - 9.2 \text{eV}$ below the Fermi energy. Other than low transmission probability, at this voltage less states involve in the transport process since the Fermi energy is located in energy gap, so the current flow smaller than the one at 0.8 V. As we increase the voltage even more, the current keep decreases, since the transmission probability becomes small and the energy band becomes farther away from Fermi energy. Similar trend is observe at current calculated for temperatures of 150 K and 300 K. The current to the voltage function tends to decrease when temperature is increased, this is because the structural irregularity in DNA molecule increases thus disrupting the electron transport process [4]. As the temperature increases, the voltage at which the current starts to decreases becomes higher, and at 300 K the current keep increasing with voltage up to voltage around 2.5 V, and then it decreases. This model shows that the change in the internal of G4 DNA molecule which affected the electron hopping constant may change the I-V characteristics curve of the molecule.
Figure 2. I-V characteristics calculated on 32 G-quarted stack of G4 DNA molecule for G-quarted twisting motion frequency of 2.00 meV and temperature of 77.2 K, 150 K, and 300 K

4. Conclusion
The I-V characteristics of 32 G-quarted stacked G4 DNA molecule have been studied under the influence of temperatures of 77.2 K, 150 K and 300 K. The I-V characteristic are calculated by taking into consideration the effect of electric field on the molecule in the form of electric field dependent electron hopping constant at G-quarted twisting frequency of 2.0 meV. The results show that the current increases with the electric field up to a certain value and then start to decreases. This trend is observed at all frequency used in this report. The increase of temperature causes electric current decreases because thermal fluctuations makes the structure of DNA molecule becomes irregular so that it hinder the transport process. In addition to that, the increase in temperature also results in the voltage where the current start to decreases becomes higher.

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References
[1] Slinker J D, Muren N B, Renfrew S E and Barton J K 2011 Nat. Chem. 3 230-235
[2] Simchi H, Esmaeilzadeh M and Mazidabadi H 2013 J. Appl. Phys. 113 074701
[3] Endres R G, Cox D L and Sing R R P 2004 Rev. Mod. Phys. 76 195-214
[4] Suhendro D K, Yudiarisah E and Saleh R 2010 Phys. B Phys. Condens. Matter 405 4806–4811
[5] Schmidt B B, Hettler M H and Schönh G 2007 Phys. Rev. B 75 115125
[6] Guo A and Xiong S 2009 Phys. Rev. B - Condens. Matter 80 035115
[7] Woiczikowski P B, Kuba T, Gutierrez R, Cuniberti G and Elstner M 2010 J. Chem. Phys. 133 035103

[8] Kang D, Sun M, Zuo Z, Wang H, Lv S, Li X and Li L 2016 Phys. Lett. A 380 977–982

[9] Yudiarsah E, Suhendro D K and Saleh R 2014 AIP Conf. Proc. 1617 35

[10] Sinurat E N and Yudiarsah E 2017 AIP Conf. Proc. 1862 020033

[11] Kang D, Jiang H, Sun Z, Qu Z and Xie S 2011 J. Phys. Condens. Matter 23 55302

[12] Wiliyanti V and Yudiarsah E 2016 AIP Conf. Proc. 1729 020033

[13] Ling L, Meller G, and Kosina H 2007 Microelectronics J. 38 47-51

[14] Qi J, Edirisinghe N, Rabbani M G, and Anantram M P 2013 Phys. Rev. B 87 85404