Twisting Motion Frequency Dependent I-V Characteristics of 102 Base Pairs Poly(dG)-Poly(dC) DNA Molecule

Efta Yudiarsah1*
1Departemen Fisika, FMIPA, Universitas Indonesia, Depok 16424
* E-mail: e.yudiarsah@sci.ui.ac.id

Abstract. The I-V characteristic of 102 base pair Poly(dG)-Poly(dC) DNA molecule have been calculated for several base pairs twisting motion frequencies. The calculation is carried out on doubled-stranded DNA model sandwiched in between two metallic electrodes. The effect is studied by taking into account twisting angle dependent on-site energy and hopping constant in the tight binding Hamiltonian of double-strand DNA model. We use semi-empirical Slater-Koster theory in the twisting angle dependent intra- and inter-strand hopping constant. We consider the temperature dependent sugar-phosphate backbone on-site energy by employing random energy disorder using uniform distribution function. The standard deviation of twisting angle is obtained by assuming that the average kinetic energy of twisting motions is proportional to system temperature. The transfer and scattering matrix methods are used simultaneously in calculating the transmission probability of charge on the molecule. We choose the contacts between molecule and both electrodes such that the main features of transport properties of the molecule do not change much by the presence of metallic electrodes. By assuming the voltage drops symmetrically at the contacts, Landauer-Buttiker Formalism is used in calculating the I-V characteristic of the molecule from transmission probability. The results show that the magnitude of current increases by twisting motion frequency increment. Larger current magnitude increment is observed at higher voltage. The influence of twisting motion frequency on the I-V characteristic is stronger at higher temperature, in the range of considered temperature.

1. Introduction

In the last decades, DNA molecules have attracted much attention of physicists. This interest stems from the hope of using DNA molecules as an active element in electronic devices, such as biosensor [1] and molecular transistor [2]. Research done by Eley and Spivey in 1962 [3] shows that DNA can conduct current. It opens an opportunity of using DNA molecule in electronic devises. DNA molecule also has a potential to be used as a template in fabricating nanoscale wire [4] for its long nature. Experimental results that show electrical conduction through DNA may involve in several biological processes, such as DNA mutation [5], damage detection and self-repairing [6, 7], as well as sensor and signaling system [8, 9], also increases the interest of physicist.

Unfortunately, different groups measuring conductivity of DNA molecule using different types of DNA reports different results. The transport property of DNA can span from insulator to proximity-induced superconductor [10]. Its results in a controversy about the transport property of DNA molecules. Beside due to the different in DNA sequence [11, 12] used, other factors such as medium or substrate [13, 14], base pairing mismatch [15], and internal motion of DNA [16, 11] may lead to this controversy.

Since DNA is a long and flexible molecule, this report will be focused on the effects of base pair twisting motion on the I-V characteristic of 102 base pairs Poly(dG)-Poly(dC) DNA molecule. Semi-empirical theory of Slater-Koster [10] has been used in representing twisting motion dependent electron
hopping constant. Landau-Büttiker formalism [17] has been used in calculating current from transmission probability which is calculated using transfer matrix technique and scattering matrix method, simultaneously [18]. The calculation is done by assuming potential drops at contact symmetrically. The results show the twisting motion influences the current such that the magnitude of current increases with twisting motion frequency increment.

The organization of this report is as follow. In the next section, DNA molecule model and calculation method will be explained. Then, calculation results will be discussed. In the last section, a conclusion will be stated.

2. Material and Method

In the model we used, we consider that electron can hop from one base to other base and to sugar-phosphate back bone side versa. However, the model exclude hopping from one sugar-phosphate back bone to the other. Inter-base hopping can occur from one base to other base in the same strand (intra-strand hopping), to its pair in Watson-Crick base pair (Watson-Crick pair hopping), and to other base in other strand (inter-strand hopping). Tight binding Hamiltonian of the model can be written as follow.

\[ H_{\text{DNA}} = \sum_{i,j} \sum_{\alpha=\pm} \left[ \epsilon_i' \phi_i' + t_{i,j}^{\pm} \left( \cos \Delta i,j^\alpha - \cos \phi \right) + b_{i,j}^\alpha \left( \cos \Delta i,j^\alpha - \cos \phi \right) \right] \]

In Eq. (1), \( \epsilon \), \( B \), and \( t \), consecutively, represent base on-site energy, sugar-phosphate backbone on-site energy, and electron hopping constant from one base to the other or to sugar-phosphate backbone. \( N \) is the length of DNA molecule, in this case \( N = 102 \) base pairs.

Thermal fluctuation can cause the base pair to twist [13, 19]. The twisting motion influences base on-site energy according to [20]

\[ \epsilon_i' = \phi_i' + b_{i,j}^\alpha \left( \cos \Delta i,j^\alpha - \cos \phi \right) + b_{i,j}^\alpha \left( \cos \Delta i,j^\alpha - \cos \phi \right) \]

In Eq. (2), \( \Delta i,j^\alpha = \phi - \phi_i \) and \( \phi \) is base on-site energy at equilibrium, 7.84 eV for G and 8.85 eV for C. \( b \) is coupling parameter between charge and base pair twisting motion. \( \phi \) is twisting angle of base relative to base position at equilibrium. The twist angle is assumed following Gaussian distribution with zero average and \( \sqrt{k_b T / (I_b \omega^2)} \) deviation standard, where \( T \) is temperature, \( k_b \) is Boltzmann constant, \( I_b \) is base moment of inertia, and \( \omega \) is twisting motion frequency. \( I_b \) is assumed to be in the order of theoretical value, i.e. \( 1.0 \times 10^{-44} \) kgm² [22]. \( \phi_{\text{avg}} \) is angle between two neighboring base pairs at equilibrium and assumed to be 36°.

Angle dependent intra-strand, Watson-Crick pair hopping constant, and inter-strand obtain by expanding semi-empirical theory of Slater-Koster [10]. They are written, consecutively, as

\[ t_{i,j}^{\pm} = t_{i,j}^\pm \left[ 1 - \alpha_{i,j,1}^\alpha \sin^2 \left( \Delta i,j^\alpha / 2 \right) \right] \left[ 1 - \alpha_{i,j,2}^\alpha \sin^2 \left( \phi_{\text{avg}} / 2 \right) \right], \]

where \( \alpha_{i,j,1}^\alpha = 2.00 \), \( \alpha_{i,j,1}^\alpha = 0.42 \), and \( \alpha_{i,j,2}^\alpha = 1.00 \). The values of parameter \( b \) and \( t_{i,j} \) can be seen in table 1.

In this study, the effect of medium and temperature on the back-bone on site energy is involved as back bone energy disorder (\( W \)) and back bone on-site energy \( B \) is assumed to be distributed uniformly in the range \([D-W, D+W]\). \( D \) is chosen to be equal to 9.36 eV, back bone on-site energy without disorder. Other parameters used in this study are metal on-site energy 8.45 eV and electron hopping constant in metal 0.75 eV. Moreover, in calculating current, Fermi energy is set equal to 8.45 eV.

### Table 1. Parameter for electron hopping constants (\( t_{i,j} \)) and coupling constant between charge and base pair twisting motion (\( b_{i,j} \)) for tight binding Hamiltonian. [20, 21].

| Base (X,Y) | \( t_{i,j}^{\text{pp}} \) (eV) | \( t_{i,j}^{\text{sl}} \) (eV) | \( t_{i,j}^{\text{pa}} \) (eV) | \( b_{i,j} \) (eV) |
|------------|-----------------|-----------------|-----------------|-----------------|
| C,G        | 0.30            | 0.14            | -               | 0.0334          |
| C,C        | 0.23            | 0.28            | -               | 0.0341          |
| C,G        | 0.14            | 0.27            | 0.57            | 0.0299          |
FIGURE 1. Transmission probabilities as a function of energy on 102 base pairs long poly(dG)-poly(dC) DNA molecule at 4.2 K and $W = 0.3$ eV for various twisting frequencies ($\omega$), (a) 0.51 meV, (b) 1.02 meV, (c) 2.00 meV and a static DNA.

FIGURE 2. The I-V characteristic of 102 base pairs long poly(dG)-poly(dC) DNA molecule at 4.2 K and $W = 0.3$ eV for various twisting frequencies and a static DNA.

3. Experimental Results and Discussion

Transmission probabilities calculated at $T = 4.2$ K and $W = 0.3$ for static DNA and dynamics DNA with various frequency are shown in figure 1. This result and other calculation results is the average of 1000 twisting angle configurations. The figure shows that there are three bands of energy with transmission greater than zero. For static DNA, there is no energy with transmission maximum one, since the present of back bone disorder, destroying uniform potential profile of periodic poly(dG)-poly(dC) DNA molecule. This result is in agreement with others [23, 24]. The base pair twisting motion does not change transmission probability much, except at band I. At band I, the transmission probability increases with the twisting motion frequency.

I-V characteristic calculated at $T = 4.2$ K and $W = 0.3$ for static DNA and dynamics DNA with various frequency are shown in figure 2. Since the Fermi energy is located in band II, current increase immediately with voltages. The plateau in the figure is due to the present of two gaps, one gap between band I and II and the other gap between band II and III. At low voltage, current increases linearly with voltage and is only minutes affected by twisting motion frequency, as shown in the top left inset.
However, at higher voltage, especially after the plateau, current is influenced much by increases with the twisting frequency, as can be seen in bottom right inset. The inset also shows, after the plateau current increases at higher voltage for lower twisting frequency. This indicates that if Fermi energy is located in the gap, then the potential threshold will change with the twisting motion frequency.

Similar trend of change in I-V characteristic with frequency is also observed in the calculation result at \( T = 30 \) K. However, at \( T = 30 \) K the effect of twisting motion on the I-V characteristic is more prominent. Current magnitude increases as twisting frequency increases is higher than the one at \( T = 4.2 \) K. It seems to occur at all the range of voltages used.

**FIGURE 3.** The I-V characteristic of 102 base pairs long poly(dG)-poly(dC) DNA molecule at 30 K and \( W = 0.3 \) eV for various twisting frequencies and a static DNA.

4. Conclusion and Future Work

In the region of low voltages, current increases linearly with voltage independent of twisting frequency and temperature. Higher twisting motion frequency results in larger current magnitude. In the range of considered temperature, twisting motion frequency influences the I-V characteristic stronger at higher temperature.

Acknowledgments

The author would like to thank UPP-IPD Universitas Indonesia for laboratory support and Mr. Daniel K. Suhendro for the parameters used in the calculation. This study is funded by Hibah Penelitian Unggulan Perguruan Tinggi (PUPT) Tahun Anggaran 2015 Nomor:0529/UN2.R12/HKP.05.00/2015.

References

1. R. L. Zaffino, M. Mir, and J. Samitier (2014), Label-free detection of DNA hybridization and single point mutations in a nano-gap biosensor, *Nanotechnology* 25, 105501.
2. S. Nokhrin, M. Baru, and J. S. Lee (2007), A field-effect transistor from M-DNA, *Nanotechnology* 18, 095205.
3. D. D. Eley and D. I. Spivey (1962), Semiconductivity of organic substances, *Transaction Faraday Society* 58, 411.
4. E. Braun, Y. Eichen, U. Sivan, and G. Ben-Yoseph (1998), DNA-templated assembly and electrode attachment of a conducting silver wire, *Nature* 391, 775.
5. J. H. Miller Jr, M. Y. S. Villagrán, S. Maric, and S. M. Briggs (2015), Normal and Impaired charge transport in biological system, *Physica B* 460, 119.
6. P. J. Dandliker, R. E. Holmlin, and J. K. Barton (1997), Oxidative Thymine Dimer Repair in the DNA Helix, *Science* 275, 1465.
7. E. M. Boon, A. L. Livingston, N. H. Chmiel, S. S. David, and J. K. Barton (2003), DNA-mediated charge transport for DNA repair, *Proceedings of the National Academy of Sciences of the United States of America* **100**, 12543.

8. P. A. Sontz, N. B. Muren, and J. K. Barton (2012), DNA charge transport for sensing and signaling, *Accounts of chemical research* **45**, 1792.

9. J. C. Genereux, A. K. Boal and J. K. Barton (2010), DNA-mediated charge transport in redox sensing and signaling, *Journal of the American Chemical Society* **132**, 891.

10. R. G. Endress, D. L. Cox, and R. R. P Singh (2004), Colloquium: The quest for high-conductance DNA, *Review of Modern Physics* **76**, 195.

11. Y.-S. Jo, Y. Lee, and Y. Roh (2003), Current–voltage characteristics of λ- and poly-DNA, *Materials Science and Engineering: C* **23**, 841.

12. D. Klotsa, R. A. Römer, and M. S. Turner (2005), Electronic transport in DNA, *Biophysical Journal* **89**, 2187.

13. S. Roche, (2003), Sequence Dependent DNA-Mediated Conduction, *Physical Review Letters* **91**, 1081011.

14. A.-M. Guo, S.-J. Xiong, Z. Yang and H.-J. Zhu (2008), Enhancement of transport in DNA-like systems induced by backbone disorder, *Physical Review E* **78**, 0619221.

15. I. Kratochvílová, et al. (2010), Charge transport in DNA oligonucleotides with various base-pairing patterns, *The journal of physical chemistry. B* **114**, 5196.

16. N. B. Muren, E. D. Olmon, and J. K. Barton (2012), Solution, surface, and single molecule platforms for the study of DNA-mediated charge transport, *Physical chemistry chemical physics* **14**, 13754.

17. E. Maciá, F. Triozon, and S. Roche (2005), Contact-dependent effects and tunneling currents in DNA molecules, *Physical Review B* **71**, 1131062.

18. H. Taniyama and A. Yoshii (1996), Scattering-matrix method for the tight-binding model of heterostructure electronic states, *Physical Review B* **53**, 9993.

19. Z. Yu and X. Song (2001), Variable range hopping and electrical conductivity along the DNA double helix, *Physical Review Letters* **86**, 6018.

20. D. K. Suhendro, E. Yudiarsah, and R. Saleh (2010), Effect of phonons and backbone disorder on electronic transport in DNA, *Physica B: Condensed Matter* **405**, 4806.

21. D. K. Suhendro (2014), private communication.

22. L. V. Yakushevich, (2004), *Nonlinear physics of DNA*. 2nd ed. Weinheim: Wiley-VCH, pp. 174.

23. E. Maciá and S. Roche (2006), Backbone-induced effects in the charge transport efficiency of synthetic DNA molecules, *Nanotechnology* **17**, 3002.

24. A.-M. Guo, Z. Yang, H.-J. Zhu, and S.-J. Xiong (2010), Influence of backbone on the charge transport properties of G4-DNA molecules: a model-based calculation, *Journal of Physics: Condensed Matter* **22**, 20