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بررسی اثر میدان الکتریکی استاتیک در صفحه گرافن بر عبور DNA از نانوروزنه گرافنی

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چکیده: به دلیل ضخامت کم و خواص مکانیکی و الکتریکی مناسب، نانوروزنه گرافنی یک ابزار قوی در زمینه توالی یابی *DNA* است. استفاده از جریان یونی ایده‌ی اولیه‌ی نسل سوم توالی یاب‌های *DNA* بود. همچنین خواندن اطلاعات جریان الکتریکی در صفحه گرافن از تحولات مهم این زمینه بوده است. برای دست یابی به دقت کافی در تشخیص نوکلئوتیدها، سرعت عبور *DNA* از نانوروزنه باید کاهش یابد. در این مقاله رفتار پویای یک *DNA* دو رشته‌ای در هنگام عبور از نانوروزنه گرافنی و در حضور میدان‌های الکتریکی عمودی و افقی بوسیله شبیه‌سازی کلاسیک دینامیک ملکولی بررسی می‌شود. سرعت عبور *DNA* در شرایط گوناگون محاسبه شده و نتایج آن نشان می‌دهد که در آینده‌ای نزدیک می‌توان سرعت عبور *DNA* را به کمک انتشار امواج پلاسمونی در گرافن کاهش داد.

کلید واژه- گرافن، نانوروزنه، *DNA*، دینامیک ملکولی

Effect of Static Electric Field Parallel to the Graphene Plate on DNA Translocation through Graphene Nanopore

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Abstract- *Graphene nanopore is a promising device in the field of nanopore DNA sequencing due to its sub-1-nm thickness and good mechanical/electrical properties. Using ionic current in this device was the main driving force for the third generation DNA sequencing devices. Reading the DNA's transverse conductance was another innovative idea in these devices. To achieve single-base resolution these devices need low translocation speed. In this paper, we investigate dynamic properties of a double-stranded DNA (dsDNA), 5'CGCGAATTCGCG3', molecule with an external voltage drop in graphene nanopore with effect of static electric field parallel to the graphene nano ribbon using molecular dynamics simulation. DNA translocation speed calculated under different conditions and the results show the potential of the method to control the translocation speed experimentally in near future with surface plasmons propagating in the graphene.*

Keywords: Graphene, Nanopore, DNA, Molecular Dynamics

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1 Introduction

Graphene is a single-atom thick material which with nanometer sized pores has the potential to act as a single-molecule detector and single-base resolution DNA sequencing device [1, 2]. Graphene is a two dimensional carbon layer packed onto a honeycomb lattice with remarkable conducting and mechanical properties. Drilling a nanopore into the graphene layer can be made by the highly focused electron beam of a transmission electron microscopy (TEM) [3]. DNA translocation under an applied vertical electric field to the graphene nanopore has been considered both experimentally and theoretically by the classical molecular dynamics simulation [1, 3]. Temporary changes in the ionic current through the nanopore was the first driving force for the third generation DNA sequencing devices [4]. The main challenges of these sequencing devices are fast DNA translocation, high membrane thickness and also how to achieve single-base resolution. In the conventional solid-state membranes the thickness is significantly higher than the height of DNA's base-pair. So the current blockade resulting from DNA translocation is due to a large number of bases (~100). Miraculously, graphene thickness is almost equal to the base-pair's height [3]. Recently, DNA translocation through MoS2 nanopore investigated which shows good potential to be used instead of graphene [5]. DNA and ion transport into a nanometer-sized graphene pore considered theoretically [1, 6], but only with the consideration of an applied vertical electric field, pore charge and temperature. The translocation speed of the DNA is a function of its mass, charge, vertical electric field and non-bonded forces applied to the atoms. Thus, any electric field parallel and closed to the graphene membrane may reduce translocation speed and be useful in the mentioned DNA sequencing devices. In this paper, we model the translocation of a double-stranded DNA (dsDNA) through a graphene nanopore while there are two different electric field applied to them. First one is normal to the graphene plate and second one is parallel to it. This transverse electric field is a simplified and non-accurate model for surface plasmon waves. Molecular dynamics simulation of the proposed system performed in the LAMMPS package [7].

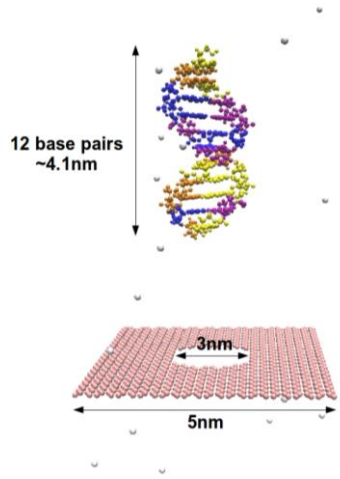


Figure 1. The proposed structure contains a graphene nano ribbon membrane with a nanopore, a DNA molecule and some Sodium ions.

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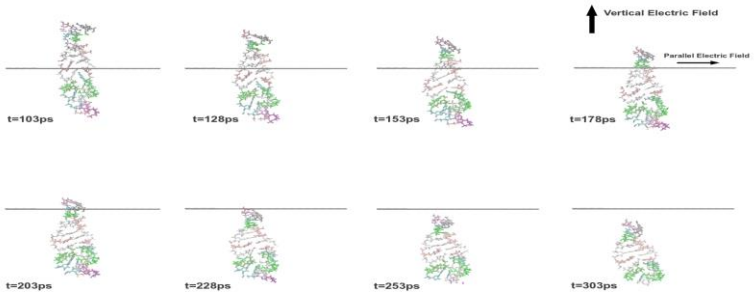


Figure 2. Snapshots of the dsDNA translocation procedure.

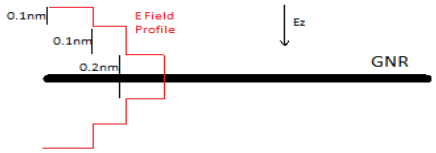


Figure 3. Static electric field profile parallel to the graphene nano ribbon (GNR).

2 Material and Methods

Graphene layer size is 5nm both in width and length and its thickness is almost 0.3nm, the pore radius is about 1.5nm, Figure 1. The proposed DNA molecule is a double-stranded DNA and it is a sequence of 12 base pairs, 5'CGCGAATTCGCG3'. All molecular dynamics simulations are performed in the LAMMPS package, employing periodic boundary conditions, CHARRM27 force field parameters are used for DNA, TIP3 water molecules and ions. The parameters for carbon atoms are those of type CA in CHARRM27 force field parameters, known as the type of benzene carbons. Simulation time step is 0.5fs and a Nose-Hoover thermostat is used to maintain the temperature at 300K with a time constant of 10ps. To prevent drift of the graphene membrane, induced force to the carbon atoms at the boundary set to zero. Constant number of atoms, volume of simulation and temperature ensemble (NVT) are used. After achieving 300K, by applying a uniform electric field directed normal to the graphene membrane and an electric field parallel and closed to it, simulations are done for 300ps. Figure.3 shows the profile and directions for these two electric fields. The red profile shows the parallel field's profile which exists almost 0.4nm top and bottom of the graphene membrane. Also the field decreases with increasing distance from the membrane. The snapshots of the molecular structure from the molecular dynamics simulations are depicted with VMD [8].

3 Results To obtain the desired parameters we need to first calculate the DNA's center of mass (COM). In our simulations, z-coordinate zero point is where the graphene plate exists. DNA translocation is happened when the DNA's COM arrives to the graphene's z-coordinate. Our DNA molecule consists of 696 atoms of several types with several masses. So we need to calculate this molecule's COM. In Fig.2, some snapshots of the DNA molecules demonstrated and it is obvious that DNA's center of mass is exactly in the graphene plate coordinate in the z-direction when almost 103 ps elapsed. First, we simulate the translocation while there is no parallel electric field, and as shown in Fig. 4, it has the minimum translocation speed and its COM arrives to the graphene plate after 102 ps. Then the above-mentioned parallel electric field (E_x) to the graphene plate added to the system and simulation are repeated again. In Fig. 4, z-coordinate of the DNA's center of mass shown for four cases, changing E_x from zero to 0.015 (Volt/Angstrom). Obviously, increasing this electric field results in longer translocation time. In all the simulations, vertical electric field is 0.05 (Volt/Angstrom) and in Table. 1, we show that how increasing the parallel electric field from zero to 0.015 (Volt/Angstrom) can increase translocation time over 80 ps. Also Fig. 5 proves that our system temperature arrives to the 300K after 0.5 ps and both vertical and electrical fields applied to the system after 3 ps. However the temperature remains constant. The second electric field added to the system, has an important effect on DNA translocation speed. The proposed DNA has 12 base-pairs and each of them translocates the nanopore in 8.5 ps, while no parallel field exists. But with the parallel field, the translocation time

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increases to 16 ps, which is almost two times slower than the previous amount. It means that with this new parallel field, the ionic or tunnelling currents have much more time to be affected by the nucleotide presented to the nanopore. Localized or propagating electromagnetic waves with high intensities, known as surface plasmons, exist in-

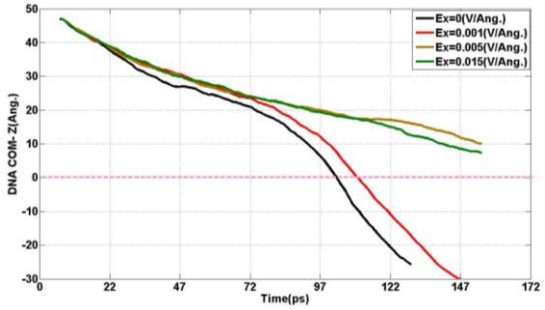


Figure 4. Z-coordinate of the DNA's center of mass

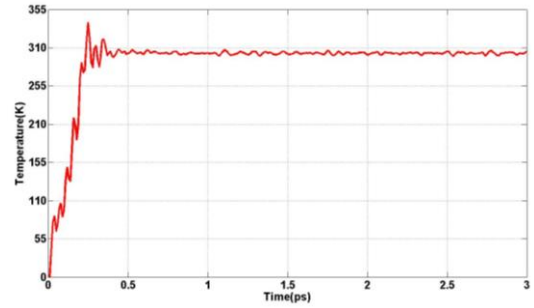


Figure 5. Temperature of the system

Table 1: DNA translocation time

Ez (V/Ang.)	Ex (V/Ang.)	Translocation time (ps)
0.05	0.015	>180
0.05	0.005	>160
0.05	0.001	110
0.05	0.0001	106
0.05	0	102

plane to the graphene and closed to it. Also, they are practically excitable by metallic nano-antenna, prisms and metallic tips. So, surface plasmon is a good choice to play the role of the above-mentioned parallel electric field and consequently, decreasing DNA translocation speed.

4 Conclusion

In this study, DNA translocation in graphene nanopore was studied with the application of two electric field vertical and parallel to the graphene plate. The graphene nano ribbon size is 5nm-5nm and the nanopore diameter is 3nm. Increasing the parallel electric field results in lower translocation speed and above a specific level, DNA cannot transport in the pore. This parallel electric field is a non-accurate classical model for the electric part of a surface plasmon wave and the results show the potential of this electromagnetic wave to practically reduce DNA translocation speed.

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