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Controlling DNA translocation speed through graphene nanopores via plasmonic fields

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Abstract. This study proposes a novel plasmonic-based method for controlling translocation speed of DNA molecule through a graphene nanopore. Dynamic properties of a double-stranded DNA molecule passage through a graphene nanopore are investigated by employing molecular dynamics simulation. In addition, the effect of plasmonic fields parallel to the graphene plane on the translocation speed of the DNA molecule is studied. The DNA translocation speed is calculated for different values of confinement, spectral width, and power of the plasmonic field. Results show the potential of the method to control translocation speed of DNA via surface plasmons in a graphene nanopore. The plasmonic field power, confinement depth, and spectral width can increase translocation time of DNA up to 107, 62, and 15%. Moreover, a strong plasmonic field can trap the DNA molecule in the nanopore. The suggested method can be utilized to solve the fast-translocation challenge of the nanopore DNA sequencers.

1. Introduction

Graphene with a nanometer-sized pore (nanopore) has the potential to act as a single-molecule detector and a single-base-resolution sequencer in the interesting field of the nanopore-based DNA sequencing [1,2]. Recent researches in the field of nanopore-DNA sequencing have shown that any changes in the ionic and tunneling-electron currents, or plasmonic resonance frequency, can be utilized to determine the unknown type of the DNA nucleotide presented in sequence to the graphene nanopore [3-7]. Due to the single-atom thickness of the single-layer graphene membrane, single-base resolution DNA sequencing in a graphene nanopore is achievable, at least theoretically [2,3]. Fast DNA translocation speed and slow sensing mechanisms are the main challenges of the graphene nanopore DNA sequencing [3,6,7]. Recent studies have shown that plasmonic signals in graphene-based nanopores and bowtie structures are fast and accurate sensing mechanisms, which may slow the sensing mechanism challenges, experimentally [6,7]. Moreover, the self-integrated optical antenna in graphene [8] and surface-enhanced Raman spectroscopy in gold-based bowtie nanostructures [9] are new suggested mechanisms for DNA nucleotide detection in which the latter can reduce translocation speed of the DNA molecule, simultaneously. Making a nanometer-sized hole into mono- and multi-layer graphenes is achievable now by a highly focused electron beam [2]. The DNA molecule passage through the graphene nanopore under an applied vertical voltage has been studied by the Molecular Dynamics (MD) simulation [4-8]. Moreover, the MD-based investigation of the single-stranded DNA molecule passage through a nanometer-sized pore in

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a mono-layer graphene demonstrated that one nucleobase identification and classification is achievable by analyzing the DNA pulling force profile [10]. As an important challenge of the nanopore DNA sequencing, the translocation speed of the DNA molecule through it is a function of the molecule mass, dimension, charge value and sign, vertical voltage and forces, and non-bonded forces applied to the DNA, water, ions, and graphene atoms. Recent studies have introduced applicable methods to control the DNA translocation speed based on optical tweezers, carbon nanotubes, and modification of the nanopore size and shape [11]. Moreover, one recent study has utilized the graphene plasmonic force in particle sorting, counting, and manipulating [12]. Thus, any plasmonic field close to the graphene membrane may control the translocation speed of the DNA molecule through the graphene nanopore, which would be useful in solving the fast translocation-speed challenge of the nanopore-based DNA sequencing; this is the main goal of the present study.

This paper proposes and analyses a new plasmonic-based method for controlling translocation speed of the DNA molecules through the graphene nanopore. By employing molecular dynamic simulations, our study shows great control of the plasmonic field on the DNA passage through the graphene nanopore.

2. Materials and methods

In our proposed model, the graphene sheet size is $5 \times 5 \times 0.34$ nm^3, whose sheet thickness is 0.34 nm. A nanopore is created at the center of the sheet, whose pore radius is about 1.25 nm. The surrounding medium of the presented structure in Figure 1(a) is assumed to be water, and dimensions of the simulation box are $50 \times 50 \times 120$ Å^3 in x, y, and z directions, respectively. The intended DNA molecule is double-stranded (dsDNA) and consists of a sequence of 12 base pairs (nucleotide), CGCGAATTCGCG, where A is the adenine, C is the cytosine, G is the guanine, and T is thymine, the nucleotides of the DNA molecule. In Figure 1(b), the electrode separation is 120 Å; thus, the electric field value corresponds to 0.5 V, and vertical power supply is about 4 mV/Å. All the classical MD-based calculations are performed in the LAMMPS package [13], while the periodic boundary conditions are employed for the all six boundaries in all three directions. For proper modelling of atom interactions and based on previous studies, the force field parameters [14,15] for the DNA and water molecules, and also ions (Na^+ and Cl^-) are chosen by the CHARRM force field parameters [14]. For modelling carbon atoms (for example, in graphene), the type of benzene carbons known as the type CA in CHARRM force field parameters is selected [14]. An algorithm for constant-temperature molecular dynamics simulation, named Nose-Hoover thermostat, is used to maintain the temperature at 295 K with a time constant of 10 ps. The long-range electrostatic interactions are important in MD simulations, and the Ewald summation method is applied to evaluate these interactions [16]. Induced forces to the carbon atoms at the boundaries of the graphene membrane are set to zero, according to the experimental condition of the graphene membrane in nanopore DNA sequencers, hence preventing drift of the graphene membrane. During the MD simulation of biomolecules, proper ensemble selection is important; moreover, in this study, a constant number of atoms, volume of simulation, and temperature, sometimes called NVT ensemble, are used. Ions are placed randomly in the simulation box at the beginning of the simulations; after energy minimization, the system is equilibrated. Then, the DNA molecule is forced to pass the graphene nanopore by applying a uniform electric field directed normally to the graphene plane and a plasmonic field parallel and close to the graphene plane for DNA translocation control; simulations are done for 1000 ps (time step is 1 fs) in this condition. The proposed plasmonic field is time varying and its frequency is set to 1000 THz, equivalent to $\lambda_{\text{vacuum}} \cong 300$ nm related to interband π plasmons of graphene [6]. It should be noted here that the selected frequency is exactly at the range where we proved in our previous studies that plasmon could detect DNA nucleotides [6,7]. Thus, this type of plasmon can be used simultaneously to sense DNA and reduce translocation speed. Modelling of the proposed structure, including the nanopore, DNA, water and ions, and snapshots of

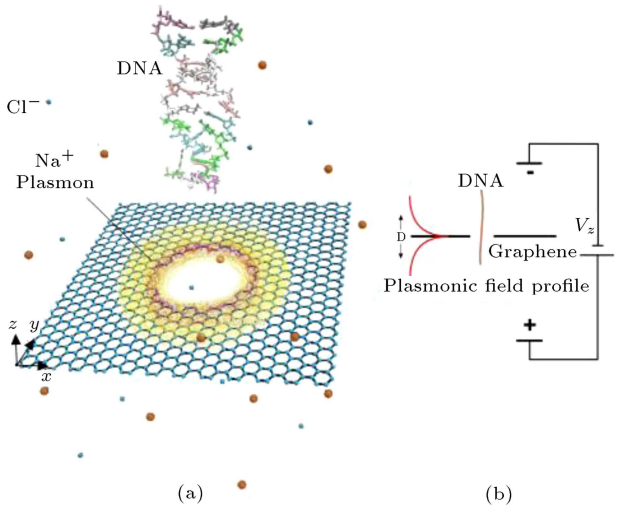

Figure 1. Three-dimensional (a) and two-dimensional (b) views of the proposed structure. The graphene plane, DNA molecule, water, ions, the vertical voltage source (electrode separation is 120 Å) for DNA translocation and plasmonic field profile are shown.

the molecular structures, is done in VMD [17]. The proposed plasmonic field is modelled by an electric field parallel to the graphene plane, as shown in Figure 1(b). The plasmonic profile is designed so that the maximum field intensity is placed on the graphene surface in Figure 1(b). The plasmonic electric field is directed along the parallel to the graphene plane, and this is the key driving force for controlling DNA passage through the graphene nanopore. Parameter D is the total confinement depth of the plasmonic field in the surrounding medium (Figure 1(b)). The proposed plasmon profile is symmetric along z-axis, and it is assumed to be uniform in $x-y$ plane. The plasmonic power is defined as $P = \pi R^2 c\varepsilon_0 \bar{n}|E|^2/2$, where R is the laser spot radius, $(\bar{n})$ is the surrounding medium refractive index, c is the speed of light in vacuum, ε_0 is the vacuum permittivity, and E is the electric field related to plasmon. The electric field enhancement of the graphene plasmons near 1000 THz is calculated based on our previous study, which is about 20 [6]. Finally, the plasmonic field power is defined as the power related to a laser source in water, with 400 nm spot radius, and is assumed to be totally coupled to the graphene plasmons. It should be noted that the assumption of which the laser output is totally coupled to the graphene plasmons is not realistic. However, if we do not consider this assumption in our results, the plasmonic power is only reduced by a constant factor. Therefore, the assumption does not change the main results. Finally, the proposed results only emphasize the applicability of the plasmonic waves in a graphene nanopore for DNA translocation speed control; however, the experimental plasmonic power and DNA translocation speed are highly different.

3. Results and discussion

To obtain the desired parameters, the DNA's Center Of Mass (COM) was first calculated. The DNA molecule consists of several types of atoms; therefore, if we seek to analyze the translocation process, the COM of the DNA molecule should be calculated at first. In this study, the DNA translocation event is defined when z coordinate of COM of the DNA molecule is equal to z coordinate of graphene membrane ($z = 0$). The DNA position presented in Figure 2 is also the position of COM of the DNA molecule along the z-axis. Translocation time is the total time that the COM of the DNA takes to reach $z = 0$ (graphene membrane position). At the beginning, the translocation process is studied, while plasmonic field is switched off. Effect of the vertical voltage on the DNA molecule position is shown in Figure 2. The proposed DNA rarely passes through the nanopore for vertical voltages smaller than 1.5 V. For example, for 0.5 V vertical voltage, translocation time is very long and DNA molecule is

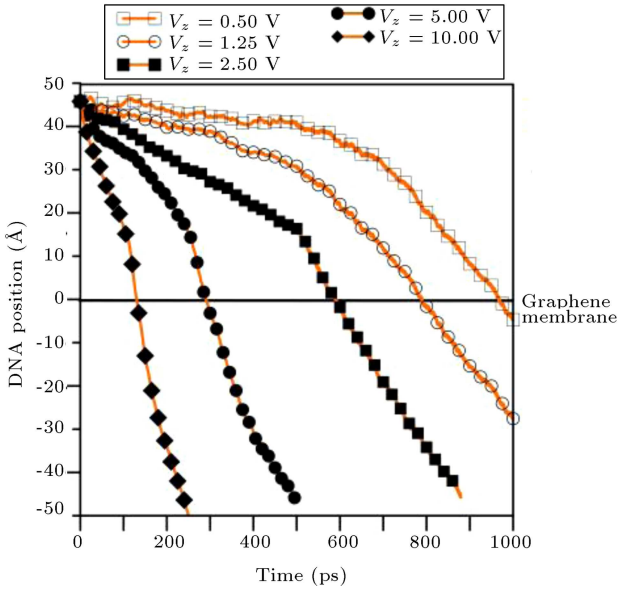

Figure 2. Dynamical process and position of the COM of the DNA molecule are presented as a function of the vertical voltage, while no plasmonic field is applied to the system. Translocation behaviour and translocation time extremely depend on the amount of the vertical voltage.

unlikely to pass through the nanopore before 950 ps. The results show that, for larger vertical voltages, $V_z > 2.5$ V, translocation time is shorter than 500 ps. Generally, increasing the vertical voltage results in a faster translocation process. Then, plasmonic field is switched on and simulations are repeated. As shown in Figure 2, in the plasmonic-off state, the translocation time related to $V_z = 5$ V is equal to about 290 ps. Note that the high voltages are applied to the vertical direction. This is because of the following reasons: The plasmonic signal has minimum effects on the translocation time for higher vertical voltages. Therefore, if the plasmonic signal can control DNA translocation speed for high voltages, it can also control DNA translocation for lower voltages. Indeed, the higher voltage reduces translocation time and, consequently, computational costs. In the previous studies, higher voltages are used [18]; however, we notice that lower voltages should be used which result in higher impact of the plasmonic fields. In Figure 3(a), a comparison of the translocation time between plasmonic-on and plasmonic-off states is shown as a function of the vertical voltage. For large vertical voltages, effect of the plasmonic field on translocation time is decreased, and results show that, for $V_z = 10$ V, the plasmonic field has insignificant effects on the translocation time of the DNA molecule through the graphene nanopore. In the blue region of Figure 3(a), for vertical voltages smaller than 1.5 V, the plasmonic field forces the DNA molecule not to pass through the nanopore. In Figure 3(b), translocation time of the DNA molecule is shown. Changing plasmonic field power from 20 μW to 0.7 W

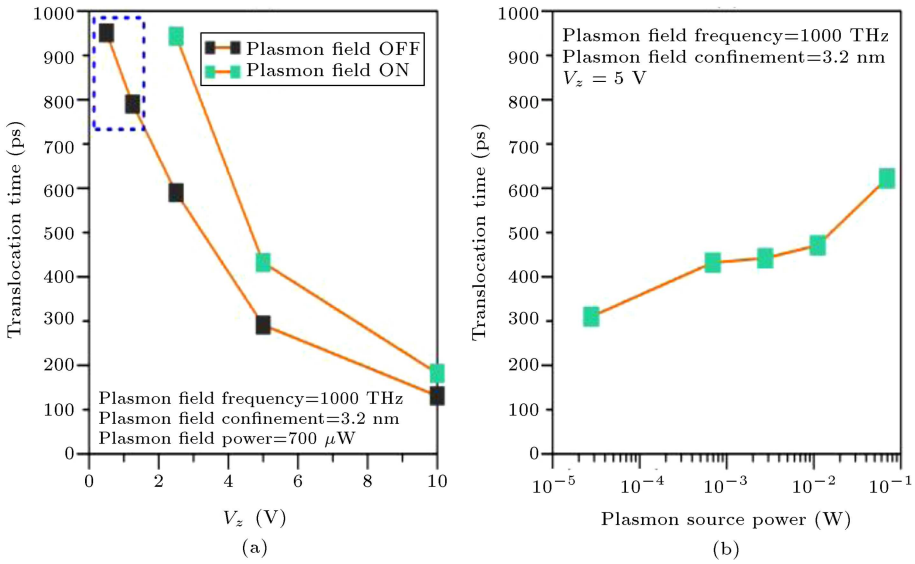

Figure 3. Translocation time of the DNA molecule through the graphene nanopore as (a) a function of the vertical voltage with and without plasmonic field and (b) a function of the plasmonic field power. In these cases, plasmonic field frequency and confinement are 1000 THz and 3.2 nm, respectively.

increases translocation time from 310 to 622 ps: about 107% increment relative to plasmonic-off state. In this case, the vertical voltage is 5 V and plasmonic field frequency is 1000 THz; in addition, depth parameter D is designed, as shown in Figure 1(b), such that plasmonic confinement depth is 3.2 nm. Obviously, increasing the plasmonic field power results in longer translocation time. It should be noted that, despite dependency of the calculated time on the proposed setup, our molecular dynamic results are in good agreement with the previous theoretical and experimental studies on DNA passage in the graphene nanopore [2,18]. However, translocation time extremely depends on the length and sequence of the DNA molecule, nanopore diameter, type of the ions, and number of graphene layers [5,18]. Increasing the vertical voltage and pore diameter results in shorter translocation time. In addition, larger length of the DNA molecule increases translocation time due to larger mass of the DNA molecule and stronger interactions with the water, ion, and graphene atoms. Moreover, an experimental setup for DNA passage through the graphene nanopore proved that translocation time for a dsDNA molecule of 47,000 base pairs through a 5-nm graphene pore is about 2 ms, while vertical voltage is about 0.2 V [2]. In addition, in our study, with the applied vertical voltage of 0.5 V and DNA length of 12 base pairs, translocation time is about 950 ps which corresponds to 0.4 ms for 47,000 base pairs if we consider translocation time as a linear function of DNA length. Moreover, note that considering differences between the practical setup [2] and our proposed condition, including applied voltages, length of DNA molecules, and diameter of the pores, our results are in good agreement with the practical ones [2]. This study does not consider temperature variations and different geometries of the nanopore. This is because of the fact that recent molecular dynamics studies have considered DNA translocation process under heated solid-state and different geometries of graphene nanopores [19,20].

In Figure 4(a), the effect of the spectral width of the plasmonic field is depicted. Our results show that increasing the spectral width from 0 to 100 THz raises the translocation time from 432 to 49 ps, i.e. about 15% increment relative to the plasmonic-off state. In this case, plasmonic field frequency, power, vertical voltage, and confinement depth values are 1000 THz, 700 μW, 5 V, and 3.2 nm, respectively. According to Figures 1-3, it should be noted that the spectral width of the plasmonic field is assumed zero. In Figure 4(b), the effect of plasmonic confinement depth variation is shown on the translocation time of the DNA molecule. Increasing plasmonic confinement depth from 0 to 7 nm raises translocation time from 291 to 473 ps, i.e. about 62% increment relative to the plasmonic-off state. In this case, plasmonic field frequency, power, and vertical voltage values are 1000 THz, 700 μW, and 5 V, respectively. For plasmonic field frequency of 1000 THz, corresponding to about 300 nm wavelength, it is proved experimentally that plasmonic confinement can be down to several nano-meters [21]. As shown in Figure 4, DNA translocation time is highly affected by the plasmonic confinement depth, rather than the spectral width, for the same conditions. To discuss confinement effects of the plasmonic field, two regimes are considered which show different behaviors of the translocation time. For plasmon confinement depths of about 1 nm, translocation time of the DNA molecule

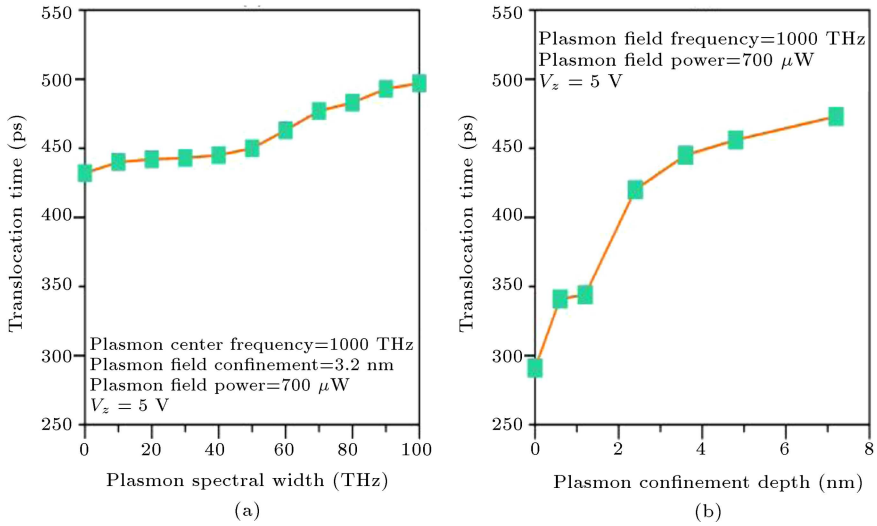

Figure 4. Translocation time of the DNA molecule through the graphene nanopore as (a) a function of the spectral width of the plasmonic field and (b) a function of the confinement of the plasmonic field. In these cases, plasmonic field frequency, power, vertical voltage, and corresponding electric field are 1000 THz, 700 μW, 5 V, and 40 mV/Å, respectively.

through the graphene nanopore is about 340 ps (Figure 4(b)). However, for larger values of plasmon confinement depth, $D > 2$ nm, translocation time is increased rapidly to around 450 ps, i.e. about 62% increment relative to the plasmonic-off state. This happens because smaller confinement depths result in a lower amount of force applied to the DNA molecule to be controlled. In addition, in this case, values of plasmonic field frequency, power, and vertical voltage are 1000 THz, 700 μW, and 5 V, respectively. Generally, the plasmonic field power, spectral width, confinement and vertical voltage are degrees of freedom in our suggested method, while, in the conventional methods [5,18], the vertical supply voltage is the only degree of freedom.

As demonstrated in Figure 5(a), translocation speed of the DNA molecule through the graphene nanopore is presented as a function of the plasmonic field power where DNA molecule is far from the graphene membrane. Increasing plasmonic field power from 20 μW to 1 W causes lower translocation speed by about 0.02 Å/ps (about 20% decrement). In Figure 5(b), translocation speed of the DNA molecule through the graphene nanopore is presented as a function of the plasmonic field power where DNA molecule is close to the graphene membrane. Increasing plasmonic field power from 20 μW to 1 W decreases translocation speed by about 0.21 Å/ps (about 100% decrement). In these two cases, plasmon center frequency, confinement depth, and vertical voltage are 1000 THz, 3.2 nm, and 5 V, respectively. However, this is important to understand that the DNA translocation process is divided into two parts: First, the process of which DNA approaches the pore, and second is the process of which DNA passes through the nanopore. Figure 5(a) and (b) show that the second process is highly affected by the plasmonic field due to strong confinement of the plasmonic field. The plasmonic force can be used to switch the propagating plasmonic field On or Off in graphene [22]. This concept has been developed based on the electrochemical-potential changing of graphene that results in a strong On/Off ratio in the plasmonic force [22]. Using the ionic current changes, the translocation event of the DNA molecule can be monitored [2] and plasmonic field is switched On just at the moment when DNA enters the pore. For a specific intensity of the plasmonic field, the total applied forces counteract each other and DNA molecule is trapped at the pore. Trapping the DNA molecule in the nanopore can be used to overcome the fast translocation limitation of the nanopore DNA sequencers. In Figure 6(a), while the plasmonic field is Off, DNA molecule tries to pass through the pore. At a time DNA molecule arrives at the graphene nanopore, the plasmonic field is switched On. If the plasmonic field power is strong enough, DNA molecule would be trapped at the nanopore. The trapped DNA molecule can be released by switching plasmonic field Off. Figure 6(b) shows the schematic representation of the trapped DNA in the pore depicted by Visual Molecular Dynamics (VMD) [17]; while the DNA molecule arrives at the nanopore, plasmonic field is switched On; after switching the plasmonic field Off, DNA molecule passes through the nanopore. In this case, plasmonic field frequency, confinement depth, power and vertical voltages are 1000 THz, 3.2 nm, 1 W, and 5 V, respectively.

From the feasibility point of view, there are some studies on graphene nanopores that constructed nanopores in graphene by local heating of gold

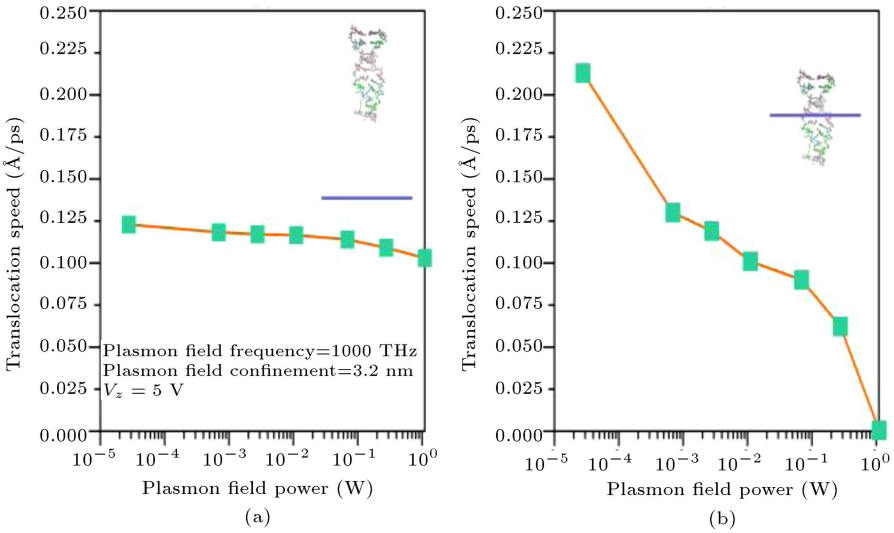

Figure 5. Translocation speed of the DNA molecule through the graphene nanopore in two regimes: (a) DNA molecule far from the nanopore and (b) DNA molecule near the nanopore. For DNA molecule near the nanopore, translocation speed is highly affected by plasmonic field power variations. In these cases, plasmonic field frequency, confinement, vertical voltage, and corresponding electric field are 1000 THz, 3.2 nm, 5 V, and 40 mV/Å, respectively.

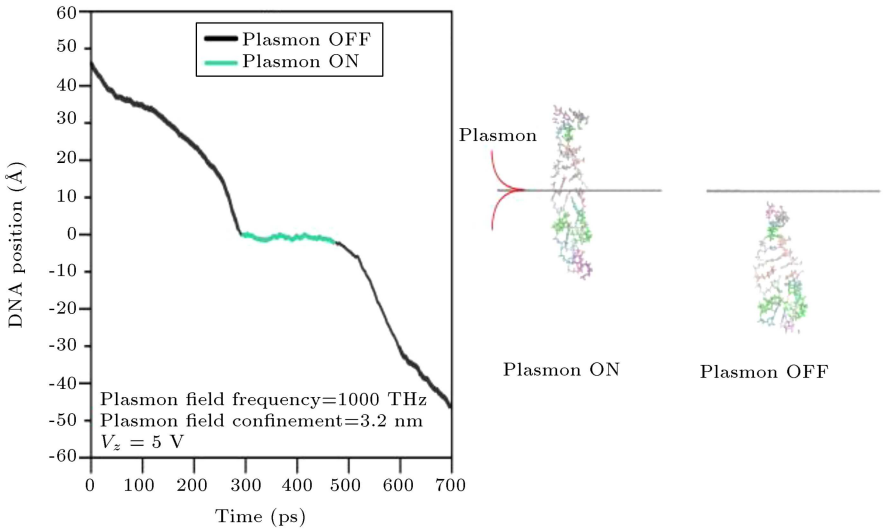

Figure 6. The DNA molecule trapped in the graphene nanopore: (a) DNA position when plasmonic field is switched OFF/ON/OFF and (b) a schematic representation of the trapped DNA in the pore depicted by VMD [17]. In this case, plasmonic field frequency, confinement, power, vertical voltage, and corresponding electric field are 1000 THz, 3.2 nm, 1 W, 5 V, and 40 mV/Å, respectively.

nanoparticles [8] or TEM [2]. Furthermore, the recent studies focused on the practical implementation of the plasmonics in graphene proved that a nanometer-sized confinement depth of plasmonic fields in graphene is achievable [21]. In the most recent studies, novel plasmonic-based mechanisms have been suggested to be used as rapid DNA sequencing methods [6,7]. In the present study, it is proved that surface plasmon resonance, employed previously for DNA sequencing in our group, can control translocation speed of this DNA molecule through the nanopore, simultaneously. Thus, our suggested plasmonic field can be used to overcome the two main challenges of the nanopore DNA sequencers: slow sensing mechanism and fast DNA translocation process. However, the previous studies on plasmonic signals show that the plasmonic signals can increase the number of DNA translocations and enhance the Raman signal [9,19]. In our proposed method, only one plasmonic signal is used for both sequencing [6,7] and translocation-speed control. Using the plasmonic field combined with metallic-bowtie structures needs pre-processes such as DNA amplification [9,19], while graphene thickness and interband-plasmonic-field confinement depth in

graphene are small enough to achieve a single-base resolution, at least theoretically. However, our proposed method for DNA sequencing and DNA translocation speed control meets some challenges. For example, designing a feasible setup for DNA sensing and DNA damages due to UV illuminations is still challenging. The UV light illumination can induce two types of damages to the DNA molecules: First is the dsDNA unzip, and second is the bond between adjacent T nucleotides in the DNA sequence, known as the "direct DNA damage" [23]. However, the dsDNA molecule is considered in this study due to simulation stabilities, and our proposed mechanism for DNA sequencing and DNA translocation speed control is based on the single-stranded DNA molecule [6,7]. Thus, the dsDNA unzipping is not related to our suggested mechanism. However, the direct DNA damages can be induced to the DNA molecules during the DNA translocation and sequencing. Notice that the suggested sequencing method is not in vivo, and utilized DNA molecules are the copies of the original DNA molecule. Thus, the direct DNA damage is not important here and does not result in cell damages. Moreover, the direct DNA damage produces small changes in the structure of the successive T nucleotides by introducing new covalent bands, and one can investigate this type of the damaged T nucleotide for possible sequencing in future studies. Hence, for DNA sequencing by UV plasmons, we should distinguish not only A, C, G, and T nucleotides, but also damaged T nucleotides. Applicability of the proposed method to controlling DNA translocation speed and distinguishing A, C, G and T nucleobases are proved in this study; however, the experimental issues and notes on optofluidic, membranes, and also carbon-based materials such as nanotubes should be considered [6,7, 24-27]. However, to consider the effects of DNA, damages of distinguishing the damaged T nucleotides should also be considered in future studies.

4. Conclusions

In conclusion, a new plasmonic-based method was presented for controlling translocation speed of the DNA molecule through the graphene nanopore. The DNA passage was studied by employing a vertical voltage normal to the graphene plane and a plasmonic field in the graphene membrane. Increasing plasmonic power resulted in lower translocation speed; in addition, above a specific level of power, DNA can be trapped in the nanopore. Our results revealed that plasmon power, confinement depth, and spectral width could increase translocation time up to 107, 62, and 15%, respectively. According to our previous studies, it was shown that plasmonic-based graphene nanopore could be employed not only for DNA sequencing, but also for trapping and controlling passage of DNA molecules. Our suggested method can motivate experimentalists to solve the fast-translocation speed problem of the nanopore-based DNA sequencers. However, effects of direct DNA damage under UV illumination, resulting in a modified type of thymine nucleotides for successive thymine nucleotides in the DNA sequence, should be considered for DNA sequencing in future studies.

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