Physics Letters A 376 (2012) 3267–3271

Contents lists available at SciVerse ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

A study on interaction of DNA molecules and carbon nanotubes for an effective ejection of the molecules

N. Wu, Q. Wang *

Department of Mechanical and Manufacturing Engineering, University of Manitoba, Winnipeg, MB, R3T 5V6, Canada

ARTICLE INFO

Article history:
Received 18 August 2012
Accepted 19 September 2012
Available online 24 September 2012
Communicated by R. Wu

Keywords:
Single-walled carbon nanotubes
DNA ejection
Interaction energy
Friction
Template effect

ABSTRACT

The ejection of DNA molecules from carbon nanotubes is reported from interaction energy perspectives by molecular dynamics simulations. The critical ejection energy, which is to be applied to a DNA molecule for a successful ejection from a carbon nanotube, is investigated based on a study on the friction and binding energy between the DNA molecule and the tube. An effective ejection is realized by subjecting a kinetic energy on the DNA molecule that is larger than the solved critical ejection energy. In addition, the relationship between ejection energies and sizes of DNA molecules and carbon nanotubes is investigated.

1. Introduction

Carbon nanotubes (CNTs) attract much attention from researchers owing to their remarkable physical properties such as high mechanical strengths, coherent electron transportability, and excellent thermal properties [1]. Because of the unique properties, CNTs are being explored for development of devices for micro-electro mechanical and nano-electro mechanical system applications. In addition, the morphology of their hollow tubes, specific large surface areas, small diameters, smooth walls and elongated geometries enables CNTs an excellent ability to encapsulate and transport molecules and the great potential in areas of medicine delivery, spot-welding and nanopumping devices [2–8]. Mechanical properties of CNTs containing different molecules have been well studied by researchers. The instabilities of CNTs containing C60 fullerenes and polyethylene molecules were investigated by Wang [9,10] using molecular dynamics. The deformation of CNT oscillators encapsulating copper nanowires was studied by Kang et al. [11].

In addition to studies on mechanical properties of CNTs containing different molecules, the molecule transportation in CNTs is another important research topic. The migration of carbon interstitials in CNTs under electron irradiation was observed [12]. A nanopipette action for metals using multi-walled CNTs (MWCNTs) was demonstrated experimentally [13]. The electromigration forces, created at high electron current densities, were found to enable transportation of materials inside the hollow core of a CNT. In addition to the electric field, mechanical driving force has also been used to realize the delivery or transportation of atoms and molecules in CNTs. The ejection of helium and hydrogen atoms and water molecules from single-walled CNTs (SWCNTs) subjected to torsion were reported by Wang et al. [8,14,15] with molecular dynamics simulations. The separation of different species of atoms using CNTs in torsion was also discussed and realized [16]. A domino wave process was developed by Chang [17] in single-walled CNTs (SWCNTs) to show a possible collapse of a section of an SWCNT with an appropriate diameter (>3.5 nm) by applying a radial compressive loading on the SWCNT wall. These works show that the van der Waals (vdW) force between the encapsulated atoms or molecules and the collapsed wall of CNTs plays a role of a driving force to push the atoms or molecules out of the tubes. In biomedical applications, CNTs were proven to be non-toxic and safe for the delivery and transportation of biological cargos, such as deoxyribonucleic acids (DNAs), proteins, and drug molecules using CNTs [18,19]. A DNA molecule was reported to be spontaneously inserted into a $(10, 10)$ CNT in a water solute environment by Gao et al. [20]. The ejection of a single strain DNA (ssDNA) chain from SWCNTs subjected to torsion loadings was simulated by Wu et al. [21]. The detailed driving process of the ssDNA molecule in SWCNTs subjected to torsion was presented and discussed.

From the previous studies, it is seen that the interaction between encapsulated molecules and CNTs affects the transportation, ejection and separation process significantly, especially for some large molecules, for example polymers, protein and DNA molecules. Studies on interactions between different molecules

* Corresponding author. Tel.: +1 204 474 6443.
E-mail address: q_wang@umanitoba.ca (Q. Wang).

0375-9601/$ – see front matter
http://dx.doi.org/10.1016/j.physleta.2012.09.020

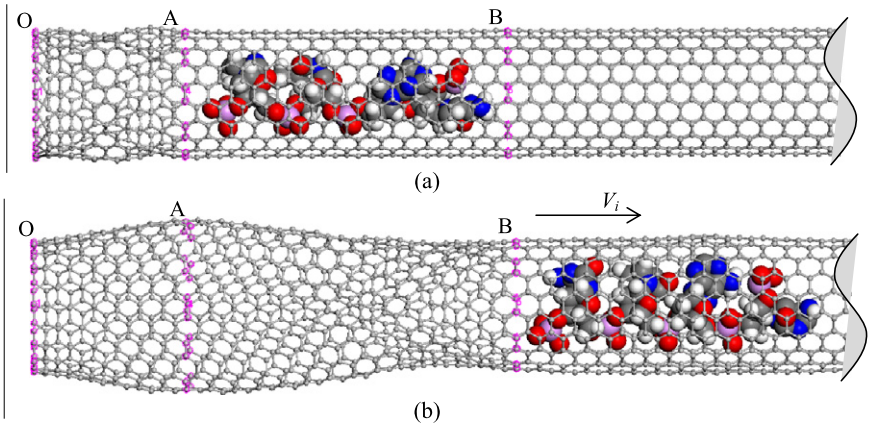

Fig. 1. The motion of an ssDNA molecule encapsulated in an SWCNT subjected to a torsion: (a) the initial position of the ssDNA molecule in the SWCNT; (b) the ssDNA molecule at the entrance of the transportation channel with an initial velocity excited by the torsion.

and CNTs become a popular research topic. Zhong et al. [22] studied the interfacial interaction between SWNTs and various gas molecules (H_2, He, and N_2) at different pressures by in situ X-ray absorption near-edge structure (XANES) spectroscopy. It was reported by Xue and Chen [23] that in the absence of water solvation, the vdW interaction between different molecules and CNTs can induce a rapid spontaneous encapsulation of molecules inside nanotube channels. The intermolecular interactions of different encapsulated molecules and CNTs were studied by Khlobystov et al. [24]. The impact of the confinement on the molecular packing, orientation, translation, rotation, and reactivity was demonstrated for a range of fullerene and non-fullerene molecules. Saito et al. [25] studied the temporally dynamic photopolymerization of C60 fullerenes encapsulated in CNTs. They declared that the 'frictional heat' was generated by the interaction between C60 molecules with the inner wall of the nanotube. The friction between an encapsulated ssDNA molecule and an SWCNT due to the vdW force was found to affect the ejection velocity of the ssDNA significantly by Wu et al. [21]. In the research, the driving process of the ssDNA molecule was particularly presented by investigating the propagation of the collapsed tube wall owing to a torsion applied to the tube, the effects of the atmosphere temperature, the applied torsion angle and the size of the CNT. The effect of the friction between the transported molecule and the tube wall on an effective ejection was not comprehensively established. In addition, exact critical energies, that are sufficient for an effective ejection or departure of encapsulated molecules from CNTs, have not been well acknowledged.

This Letter presents a general guidance on ejection or departure of encapsulated DNA molecules from CNTs by molecular dynamics simulations from the interaction energy perspectives. The critical ejection energy, which is to be applied to a DNA molecule for a successful ejection from a CNT, is investigated based on a study on the friction and the binding energy between the DNA molecule and the tube wall.

2. Critical driving energy for an effective ejection of a DNA molecule from an SWCNT

Molecular dynamics simulations are used to study the ejection process. In simulations, the Nose feedback thermostat is used in the thermostat to control temperature and generate the canonical ensemble. The atomic interactions are described by the universal force field (UFF) [26], which is a purely diagonal, harmonic force field. In the UFF, the potential energy of an arbitrary geometry of a molecule is provided as a superposition of various two-body, three-body, and four-body interactions. The total potential energy E is expressed as follows [26]:

$$E = E_R + E_\theta + E_\phi + E_\omega + E_{vdW} + E_{el}, \tag{1}$$

where E_R, E_θ, E_ϕ and E_ω are valence terms of bond stretching, bond angle bending, dihedral angle torsion, and inversion energies, respectively. E_{vdW} and E_{el} are nonbonding terms of vdW and electrostatic (ES) energies. The full expressions for these energy items are given in [26]. The default dielectric constant is 1 for UFF and no distance cutoff is used. Partial charges are obtained using the published charge equilibration (QEq) scheme [27].

The excitation of an initial velocity of an ssDNA molecule encapsulated in an SWCNT is realized by applying a torsion angle at the end of the SWCNT. The detailed design and driving process of an ssDNA molecule encapsulated in an SWCNT by torsion was described by Wu et al. [21]. The schematic diagram of driving a DNA molecule in an SWCNT is given in Fig. 1. The two ends of the SWCNT are fixed to restrain the motion of atoms. A torsion angle is applied to the restrained area around the left side of the SWCNT from position O to A as shown in Fig. 1(a). A stopper, a small fixed portion on the CNT to prevent the collapsed wall from propagating in front of the DNA molecule, is located at position B. Once the restraint at position A is removed to allow the propagation of the local torsion buckling, a resultant driving force by the vdW interacted between the SWCNT wall and the ssDNA molecule will excite an initiate velocity of the ssDNA molecule, V_i, for a possible ejection from the SWCNT, when the left end of the ssDNA chain passes the position B as shown in Fig. 1(b). The portion from the position B to the outlet of the SWCNT serves as a transportation channel for the ssDNA molecule.

2.1. Energy dissipation during the transpiration of the DNA molecule in the SWCNT

With the initial velocity, V_i, the ssDNA chain moves toward the right end of the tube as shown in Fig. 1, the transportation is not frictionless. The friction due to the vdW interaction between the encapsulated ssDNA molecule and the tube wall retards the movement of the ssDNA molecule and reduces its velocity. As shown in the schematic diagram of Fig. 2, the velocity of the ssDNA molecule at position 1 is V_1 while the velocity is reduced to be V_2 at the position 2 after a period of t ($V_2 < V_1$). It is observed that the acceleration of the movement of ssDNA molecules in a long SWCNT is a constant and hence the friction between ssDNA chains and long SWCNTs is virtually a constant as well. The acceleration of the movement of the ssDNA molecule in the SWCNT as shown in Fig. 2 due to the friction, a, is $(V_2 - V_1)/t$. Based on the second