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A nanoscale rolling actuator system driven by strain gradient fields

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ABSTRACT

A new actuator system to drive the rolling motion of a CNT on a graphene is investigated with the molecular dynamics simulation. The strain gradient field induced by the actuator system can be effectively used to realize the continuous and steady rolling of the CNT. Variations of the potential energy, the kinetic one, as well as the motion of the CNT is comprehensively studied for both cases without defects and those with defects. Effects of both the parameters of the CNT and vacancy defects of the graphene are discussed. It is interesting to find that a single defect results in small fluctuation of the CNT's motion. However, multiple defects may lead to a serious deflection of the movement of the CNT, even failure of the actuator system. These results should be useful for the promising design of nanoscale transportation and functional surfaces.

1. Introduction

Carbon nanotubes (CNTs) [1] and graphene [2] have been widely used in various areas including micro- and nano-electromechanical systems (MEMS and NEMS) [3,4], flexible electronics [5], nanocomposites [6], etc., due to their outstanding mechanical and electrical properties [7,8]. Among these present and potential applications of CNTs and graphene, the challenge of exploring nanoscale driving mechanisms is constantly faced to guide the development of advanced science. Nowadays, accurate manipulation of CNTs or graphenes from one location to another has become one of the most inevitable tasks in the manufacture and assembly of MEMS and NEMS such as nano motors [9–11], sensors [12,13], bearings [14]. Thus, great attentions have been paid to the mechanism of realizing nanoscale manipulation and transportation in different environments.

So far, many literatures have been done to analyze various driving mechanism of nanoscale objects. Schoen et al. [15] found that gold nanoparticles inside a carbon nanotube can be driven by the thermal gradient. Barreiro et al. [16] explored the motion of nanoscale cargoes driven by thermal gradients along CNTs. A quantitative analysis of the motion of the nanoflake on a large graphene substrate was carried out by Becton et al. [17]. Chang et al. [18] proposed a nanoscale equipment with temperature-induced reversible dominoes in CNT, where the controllable collapsed zone varies with a changing temperature. Later, a model of a graphene slider on a graphene substrate powered by the stiffness gradient through molecular dynamic simulation was studied by Chang et al. [19]. The mechanism and quantitative control of rotary motors made of double-walled carbon nanotubes driven by thermal fields were effectively studied by Cai et al. [20–22]. In addition to thermal field and graded stiffness, many other means have been adopted to drive a nanoscale object. The electromechanical rotational actuators and the rotary motors driven by electron tunneling were investigated by Wang et al. [23] and Bourlon et al. [24], respectively. It was found that electrical field can be employed efficiently to actuate molecular motors constructed of a double-walled carbon nanotube [25–27]. Motors driven by the Brownian motion were studied by Rousselet et al. [28], Astumian et al. [29], and Hanggi et al. [30]. What's more, a review of biological motors for nanotechnology powered by the F1-adenosine triphosphate synthase (F1-ATPase) and myosin [31], bacteria [32] and motor proteins [33], was given by Martin et al. [34].

Recently, a new mechanism to realize cell motion was found by Chen and his coauthors [35,36], who found that an elastic strain graded field can be employed to drive spherical bubble on a stretchable substrate in the direction of principal strain. If is possible to employ the strain graded field to drive a rolling motion in nanoscale? How can the energy be converted to another form for a rolling motion? What will happen if there are defects in the actuator system?

In order to answer these questions, a molecular dynamics simulation of the rolling of a nanoscale system loaded by a strain graded field is

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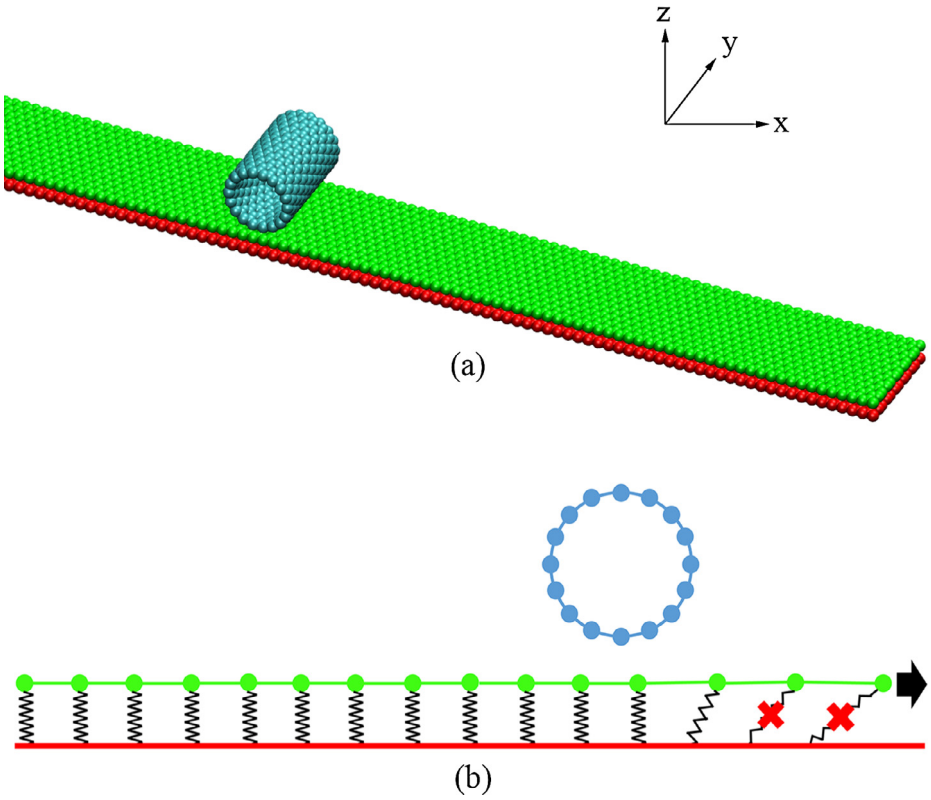

Fig. 1. The MD model of the CNT/graphene/rigid base system. (a) Configuration of the rolling actuator system. (b) Schematic of strain gradient field in the graphene strip which is linked to the rigid base with lots of identical springs.

carried out in the present paper. The model composed of a single-walled carbon nanotube and a graphene strip is introduced firstly. The elongation and break of the linear springs beneath the graphene strip was used to generate a strain graded field. Detailed discussion and conclusion of the responses of CNT will be presented subsequently. These results should be useful for the promising design of nanoscale transportation and functional surfaces.

2. Models and methods

As shown in Fig. 1, the model is composed of a (18, 0) single-walled carbon nanotube and a graphene strip with an armchair edge along x axis. The length of the SWCNT is 2.5 nm, and it is placed parallel to the y axis. The vertical distance between the lowest point of the CNT and graphene strip equals to 0.34 nm, which is the equilibrium separation. Beneath the graphene strip, there is a rigid base which is linked to the graphene strip with plenty of identical linear springs. Both of the graphene strip and the rigid base are 50 nm long and 2.5 nm wide (unless stated otherwise), and the distance between the two is also 0.34 nm. In this work, we focus our study in generating a strain gradient field, and explore the possibility to use the strain gradient field to drive nanoscale objects. Similar to the treatment of Wang and Chen [36], the strain gradient in x direction is mainly focused, while the effect of deformation of the graphene strip in y direction of the graphene strip is neglected for simplicity by setting an open boundary condition. When a horizontal tensile force is exerted on the right end of the graphene strip, the springs will be elongated and break as its length exceeds a critical value, thus resulting in a region of strain graded near the debonded region, as illustrated in Fig. 1(b). Note that the aim of the present paper is to generate a strain gradient field using the debonding in the film/substrate system, like the experiment in Chen and Chen [35]. We do not pay much attention on the detail of the interaction at the film/substrate interface. Thus, similar to the treatment of Wang and Chen [36], linear springs are used to generate the gradient field in our simulation. Actually, several methods can be used to introduce bond cross-links between a graphene film and its substrate, including moderate electron-beam irradiation [37] or adding chemical group [38]. Due to the debonding of the springs, a gradient field will be induced.

The simulation is carried out with LAMMPS package [39] and the AIREBO potential [40] is adopted for the C-C bond interaction of the CNT, graphene strip and rigid base. The van der Waals interaction between atoms of the CNT, graphene strip and rigid base is characterized by the lj/cut potential [41] with a potential well $\varepsilon = 0.00284$ eV and an equilibrium distance $\sigma = 3.4$ angstroms. The system contains 10,224 atoms, and is relaxed first at 5 K in a NVT ensemble [42] for energy minimization. After a 30 picoseconds' relaxation, the initial model will be reshaped and the CNT will find its equilibrium position, which removes the effect of other factors in the subsequent motion. The strip is then stretched to induce a strain graded field, and the stretch process will last for 1200 picoseconds. The whole simulation is under the canonical NVT ensemble with $T = 5$ K, which is expected to avoid the effect of thermal vibrations of atoms [43].

In the present simulation, the maximum strength of each spring is $K\delta^2/2$, in which δ is the critical length, K denotes the stiffness of the spring and $K = 2$ eV/angstrom^2 is chosen. Viscous forces proportional to the speed are reasonably imposed on the atoms of the CNT to consume the kinetic energy and to observe a periodic movement on a graphene strip with a finite distance.

3. Results and discussion

In the present analysis, the chiral parameter of the CNT is set as (18, 0), unless otherwise stated. The variation of the kinetic energy and the potential energy of the actuator system as well as the motion of the CNT are mainly focused on in the present simulation. The effects of geometry parameters of the CNT and the defects of the graphene layer in the actuator system is discussed in the section.