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Potential energy, force distribution and oscillatory motion of chloride ion inside electrically charged carbon nanotubes

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HIGHLIGHTS

- Mechanics of chloride ion inside functionalized CNTs is examined using a continuum method.
- Potential energy, force distribution and the resulting oscillatory motion are studied.
- Incorporating electrostatic interactions leads to enhancing the operating frequency.
- Escape velocity increases in the case of positively charged CNTs.
- Strong dependence of oscillation frequency to the system parameters is shown.

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ABSTRACT

In this research, a continuum-based model is presented to explore potential energy, force distribution and oscillatory motion of ions, and in particular chloride ion, inside carbon nanotubes (CNTs) decorated by functional groups at two ends. To perform this, van der Waals (vdW) interactions between ion and nanotube are modeled by the 6-12 Lennard-Jones (LJ) potential, whereas the electrostatic interactions between ion and functional groups are modeled by the Coulomb potential and the total interactions are analytically derived by summing the vdW and electrostatic interactions. Making the assumption that carbon atoms and charge of functional groups are all uniformly distributed over the nanotube surface and the two ends of nanotube, respectively, a continuum approach is utilized to evaluate the related interactions. Based on the actual force distribution, the equation of motion is also solved numerically to arrive at the time history of displacement and velocity of inner core. With respect to the proposed formulations, comprehensive studies on the variations of potential energy and force distribution are carried out by varying functional group charge and nanotube length. Moreover, the effects of these parameters together with initial conditions on the oscillatory behavior of system are studied and discussed in detail. It is found out that chloride ion escapes more easily from negatively charged CNTs which is followed by uncharged and positively charged ones. It is further shown that the presence of functional groups leads to enhancing the operating frequency of such oscillatory systems especially when the electric charges of ion and functional groups have different signs.

1. Introduction

Recent advances in nanotechnology have led to the fabrication of numerous nanoscale devices [1] among those ultra-high frequency nanoscale oscillators have drawn considerable attention from the scientific community. This is mainly attributed to the difficulties encountered for micromechanical oscillators to achieve frequencies in the gigahertz (GHz) range. Potential applications of GHz oscillators might include ultra-fast optical filters for fiber optic systems and nanoantennae sensitive to high-frequency electromagnetic signals [2,3]. Up to now, different types of nano-oscillators [4–6] have been proposed since Cumings and Zettl [7] reported an ideal low-frictional telescopic oscillation between two nested multi-walled carbon nanotubes (MWCNTs). In their experiment, by extruding the inner tube and then releasing it, they observed that the inner core quickly retracts inside the host nanotube owing to the restoring force resulting from the van der Waals (vdW) interatomic interaction acting on the core.

A great number of studies have been conducted on the oscillatory behavior of such devices by employing the molecular dynamics (MD) simulations [8,9]. Using this method, Legoas et al. [10,11] approved the GHz frequency of nested CNTs and

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demonstrated that there is a sustained oscillation when the difference between the radii of outer and inner walls is almost equal to 0.34 nm. Liu et al. [12] pointed out that the oscillation behavior of MWCNTs is dependent on the choice of geometrical parameters and the number of outer shells. Rivera et al. [13,14] presented a MD-based model to study the damping effects of oscillatory motions in double-walled carbon nanotubes (DWCNTs). Liu et al. [15] performed the MD simulations to study the behavior of a C_{60} fullerene oscillating through a single-walled carbon nanotube (SWCNT) and reported that such behavior is sensitive to both the diameter and degree of helicity of nanotube.

It is generally accepted that the MD simulations are very time-consuming so that their computational time increases exponentially with increasing the number of atoms required for simulation. Another approach available for modeling nanostructured materials is continuum approximation of discrete atoms arising from the assumption that discrete distribution of atoms on the surface or volume of molecules can be replaced by a constant atomic density on the surface or volume of each of them [16,17]. Unlike MD-based models whose computations are entirely done in a numerical way, continuum-based methods are capable of giving analytical and semi-analytical expressions for evaluation of vdW interactions. Generally, so as to estimate vdW interactions between two nanostructures based on the continuum approximation, one must perform surface or volume integrals over both smeared surfaces or volumes leading to a multiple integral [18,19].

Based on a continuum approximation of discrete atoms, Zheng and Jiang [20] theoretically calculated the frequency of MWCNTs and reported that the frequency is in the GHz range. Zheng et al. [21] also demonstrated the negligible effect of frictional forces on the oscillatory behavior of such systems. The successful application of continuum approximation to several forms of molecular systems is also reported in [22–24]. For a number of particular systems including the interactions of CNT-CNT, C_{60}-CNT, C_{70}-CNT and C_{80}-CNT, Hilder and Hill [25] demonstrated that the results obtained from continuum approach are in reasonable agreement with those predicted through the discrete model. Ansari et al. adopted continuum approach to investigate the oscillatory characteristics of different nanoscale oscillators such as nested CNTs [26], spherical fullerenes-CNTs [27], ellipsoidal fullerenes-CNTs [28], C_{60} fullerene-CNT bundle [29] and CNT-CNT bundle [30] oscillators. Their results revealed the strong dependence of oscillation frequency on the geometrical parameters and initial conditions. Employing the continuum approximation, several studies have been also performed on the suction energy and acceptance condition which are considered as two significant issues for medical applications such as drug delivery [31–34].

Enhancing the operating frequency of nanoscale oscillators is of vital importance in the design and fabrication of nano-oscillators. In all continuum-based studies performed so far, considerable effort has been made to achieve this goal through using either different types of nanostructures or different system parameters. This study, however, proposes that one initiative to considerably enhance the operating frequency of such devices is to use electrically charged particles instead of uncharged ones. To accomplish this, applied mathematical modeling is used herein to investigate the mechanics of ions, and in particular chloride ion, inside CNTs decorated by functional groups (for instance carboxylic groups –COOH) at both ends. This paper is organized as follows: In Section 2, utilizing a continuum approach, analytical expressions are derived for evaluation of vdW interactions between ion and CNT and electrostatic interactions between ion and functional groups. The vdW and electrostatic interactions are modeled by the 6-12 Lennard-Jones (LJ) and Coulomb potentials, respectively. Knowing about the behavior of potential energy and interaction force is of high importance for the perception of oscillatory motion. For this reason, a comprehensive study is conducted in this section to get an insight into the effects of functional group charge and nanotube length on the potential energy and interaction force distribution. In Section 3, escape velocity is introduced and calculated for different values of functional group charge and nanotube length. In Section 4, based on the actual force distribution, the equation of motion is solved numerically to arrive at the displacement and velocity of inner core. Numerical results of this section are devoted to examine the effects of functional groups charge, nanotube length and initial conditions on the oscillatory characteristics of chloride ion tunneling through an electrically charged CNT.

2. Interactions between a chloride ion and an electrically charged CNT

This section describes mathematical modeling of interactions between a chloride ion and a CNT decorated by functional groups at both ends. The ion is modeled by a point charge and the functional groups are assumed to have identical sign and quantity of electric charge. Fig. 1 depicts a chloride ion located co-axially near the open end of a positively charged CNT. The electric charge of ion is symbolized by q, while the total electric charge distributed over each end of nanotube is represented by Q. As shown in this figure, the origin of the Cartesian coordinate system (x, y, z) is assumed to be located at the center of nanotube of radius R_c and length $2L$. Moreover, the ion traveling along the nanotube axis is supposed to be lie at a distance Z from the origin. Assuming that the carbon atoms and the electric charges are all uniformly distributed over the surface and both ends of nanotube, respectively, one can utilize a continuum approach to evaluate the total interactions of system which consist of two terms, namely vdW and electrostatic

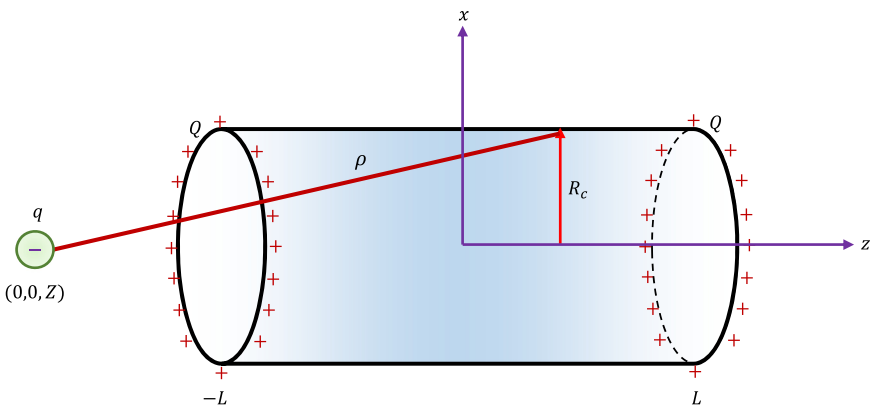

Fig. 1. Geometry of a chloride ion penetrating into a CNT decorated by positively charged functional groups at both ends.