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Mechanics of nested spherical fullerenes inside multi-walled carbon nanotubes

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ABSTRACT

Based on the continuum approximation and Lennard-Jones (LJ) potential, mechanics of nested spherical fullerenes, known as carbon onions, inside multi-walled carbon nanotubes (MWCNTs) is investigated in this study. To this end, direct method is first utilized to determine van der Waals (vdW) interaction force and potential energy between a carbon onion molecule and a semi-infinite MWCNT. According to this method, the interactions between each pair of shells from carbon onion and CNT are summed up over all of the pairs. Thereafter, the suction and acceptance energies for carbon onions entering semi-infinite MWCNTs are evaluated. On the basis of Newton's second law, an analytical expression is then presented to predict the oscillation frequency of a carbon onion molecule inside a MWCNT of finite length. The effect of geometrical parameters on the nature of suction and acceptance energies, vdW interactions and oscillatory characteristics of carbon onion-MWCNT oscillators is thoroughly examined. For a given carbon onion structure, it is found that there exists an optimal value for the number of nanotube shells beyond which the maximum oscillation frequency does not increase considerably. Furthermore, the maximum oscillation frequency decreases as the carbon onion gets larger.

1. Introduction

Nanostructured materials such as carbon nanotubes (CNTs) (Iijima, 1991) and fullerenes (Kroto et al., 1985) have found a wide variety of applications in many nanoelectromechanical systems (NEMS) in recent years (Kim and Lieber, 1999; Postma et al., 2001; Fennimore et al., 2003; Liu et al., 2005). This is mainly due to their exceptional properties such as low weight, high strength and flexibility making them promising candidates for such purposes (Saito et al., 1992; Yeung et al., 2009; Wong et al., 1997). High-frequency nanoscale oscillators, known as gigahertz (GHz) oscillators, are one of the proposed devices which have captured tremendous attention worldwide. Potential applications of these oscillators might include nanoantennae sensitive to high-frequency electromagnetic signals and optical filters for fiber optic systems (Tuzun et al., 1995; Damnjanović et al., 1999).

In the year 2000, Cumings and Zettl (2000) reported an ideal low frictional effect for a sliding inner tube inside multi-walled carbon nanotubes (MWCNTs). They demonstrated that if the inner core pulls out and set free, it spontaneously retracts inside the outer shells due to the van der Waals (vdW) interatomic interaction acting on the core. Subsequently, by using a static mechanical model, Zheng and Jiang (Zheng and Jiang, 2002) exposed that CNT-based oscillators are capable of reaching frequencies up to several GHz. Also, Zheng et al. (2002) incorporated the frictional forces into their model and reported that these forces have almost insignificant effect on the oscillation frequency. Up to now, several types of nano-oscillators have been proposed in the published literature (Hilder and Hill, 2007a; Cox et al., 2008; Alisafaei et al., 2011; Ansari et al., 2013a). A great number of researchers employed molecular dynamics (MD) simulations to predict the behavior of such oscillatory systems (Rivera et al., 2003; Legoas et al., 2004; Kang et al., 2006; Ansari et al., 2013b). On the basis of these simulations, Legoas et al. (2003) confirmed that CNT oscillators can generate frequencies in the GHz range.

They also reported that these nano-oscillators are dynamically stable when the interwall spacing is about 0.34 nm. Rivera et al. (Rivera et al., 2005) adopted MD-based models to examine the damping effects of these oscillatory motions. Some other investigations have been also conducted on the issues of energy dissipations and frictional forces through MD simulations (Guo et al., 2003; Zhao et al., 2003; Servantie and Gaspard, 2006).

In spite of the fact that MD models may be the most reliable approaches for analysis of nano-oscillators, their main drawback is that they are not computationally efficient, especially in the

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case of large number of atoms for simulation. Furthermore, as a result of numerical evaluations of MD-based models, it is impossible to derive analytical expressions for evaluation of vdW interactions while applying these kinds of models. Another approach for modeling vdW interactions between two nanostructures is the continuum approximation of discrete atoms where a constant atomic surface density is used on the surface of each molecule instead of the discrete distribution of carbon atoms. Generally, in order to evaluate vdW interactions between two nanostructures through continuum approach, surface integrals must be performed over both smeared surfaces which leads to a quadruple integral (Ansari et al., 2012). Girifalco and his elaborates (Girifalco et al., 2000; Hodak and Girifalco, 2001; Kniaz et al., 1995) demonstrated successful application of this continuum model to several types of molecular systems. They also asserted that these models are preferable to the discrete model of atoms in some cases. Hilder and Hill (2007b) reported that interactions of CNT–CNT, C_{60}–CNT, C_{70}–CNT and C_{80}–CNT modeled through continuum approach are in reasonable agreement with those modeled through discrete model. Using the continuum model together with elementary mechanical principles, Hill and his colleagues (Cox et al., 2007a) presented an analytical formula for the oscillation frequency of C_{60} fullerene-CNT oscillator. In their model, for the case of long nanotubes, they estimated the vdW interaction force with an impulse-like function acting near the ends of nanotube. This model was then extended to examine the oscillatory behavior of nested spherical fullerenes inside single-walled carbon nanotubes (SWCNTs) (Thamwattana and Hill, 2008). Besides, Ansari and his colleagues employed continuum model to present new semi-analytical expressions to determine vdW interactions as well as oscillation frequency of different types of nano-oscillators such as nested CNT (Ansari and Motevalli, 2009, 2011), spherical fullerene-CNT (Ansari et al., 2013c) and ellipsoidal fullerene-CNT (Ansari and Sadeghi, 2012) systems. Their studies revealed some distinctive features of such oscillatory systems for the first time in the literature. Applying the continuum approach, acceptance condition and suction energy of different nanoparticles, which are going to be encapsulated into a nanotube, have been also studied in the open literature (Cox et al., 2007b; Alisafaei and Ansari, 2011; Sadeghi and Ansari, 2012; Ansari and Kazemi, 2012; Ansari et al., 2013d).

In the present study, continuum approximation is employed to fully investigate the mechanics of nested spherical fullerenes inside MWCNTs. Nested spherical fullerenes, or the so-called carbon onions, were synthesized in 1992 under electron beam irradiation of CNTs and nanoparticles (Ugarte, 1992). Experimental studies also demonstrated that this shape of carbon onion is more energetically favorable than ellipsoidal and tetrahedral ones (Ugarte, 1992; Banhart and Ajayan, 1996). Besides, Korto and McKay (Korto and McKay, 1988) proposed a plausible structure for carbon onions made up of concentric Goldberg type 1 fullerenes of I_h symmetry. This kind of carbon onion, which is considered in this article, consists of C_{60}@ C_{240}@ C_{540}@C_{960}@ … @C_N spherical fullerenes where N denotes the number of carbon atoms. In addition, the intershell spacing of this structure is very close to the interlayer spacing of graphene which is equal to 0.34 nm (Girifalco et al., 2000).

In the following sections, first of all, the continuum Lennard-Jones (LJ) model is introduced. Afterward, direct method is used to evaluate vdW interaction force and potential energy between nested spherical fullerenes and semi-infinite MWCNTs. Also, suction and acceptance energies for a carbon onion located coaxially near an open end of a semi-infinite MWCNT are evaluated. On the basis of Newton's second law and neglecting the frictional forces, an analytical expression is then given to estimate the oscillation frequency of a carbon onion traveling along the axis of a finite MWCNT. Finally, numerical results are presented to get an insight into the effect of geometrical parameters on the distributions of suction and acceptance energies, vdW interactions and oscillatory behavior of carbon onion-MWCNT oscillators.

2. Continuum approximation

Here, it is assumed that the vdW interaction between two carbon atoms at a distance ρ apart is given by the following 6–12 LJ potential function as

$$\Phi(\rho) = -\frac{A}{\rho^6} + \frac{B}{\rho^{12}} \tag{1}$$

where A and B specify the attractive and repulsive constants, respectively. Eq. (1) can be also rewritten in the following form

$$\Phi(d) = \frac{A}{a^6}\left(\frac{1}{2}\frac{d_0^6}{d^{12}} - \frac{1}{d^6}\right) \tag{2}$$

in which d shows the normalized distance between the atoms, a is the carbon–carbon bond length and d_0 denotes the normalized equilibrium distance expressed as

$$d_0 = \frac{1}{a}\left(\frac{2B}{A}\right)^{1/6} \tag{3}$$

The total potential energy between the two nanostructures can be obtained by summing the potential energy between the pair of atoms from each molecule

$$\Phi^{tot} = \sum_i \sum_j \Phi(\rho_{ij}) \tag{4}$$

where $\Phi(\rho_{ij})$ is the potential energy function for atoms i and j on each molecule at a distance ρ_{ij} apart. Based on the continuum approximation, which assumes that carbon atoms are uniformly distributed over the surfaces of the molecules with a constant atomic surface density, a double surface integral can be used instead of the double summation in Eq. (4) as

$$\Phi^{tot} = \eta_1\eta_2 \int\int \Phi(\rho) d\sum_1 d\sum_2 \tag{5}$$

in which η_1 and η_2 denote the mean atomic surface density of atoms on each molecule and ρ represents the distance between two typical surface elements $d\sum_1$ and $d\sum_2$.

In addition, the corresponding vdW interaction force can be attained through differentiating the total potential energy as follows

$$F_{\mathrm{vdW}} = -\nabla\Phi^{tot} \tag{6}$$

3. VdW interaction force and potential energy between a carbon onion and a semi-infinite MWCT

In this section, direct method is applied as a straight method to evaluate vdW interaction force and potential energy between nested spherical fullerenes and semi-infinite MWCNTs. On the basis of this method, the interaction between each shell of carbon onion molecule with each shell of MWCNT is first determined and then the total interaction is obtained through summing the interactions between each pair of shells.