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Abstract

Advances in technology have led to the creation of many nano-scale devices and carbon nanotubes are representative materials to construct these devices. Double-walled carbon nanotubes with the inner tube oscillating can be used as gigahertz oscillators and form the basis of possible nano-electronic devices. Such gigahertz oscillating devices made from carbon nanotubes might be instrumental in the micro-computer industry, which is predominantly based on electron transport phenomena. There are many experiments and molecular dynamics simulations which show that a wave is generated on the outer cylinder by the oscillation of the carbon nanotubes and that the frequency of this wave is also in the gigahertz range. However, conventional applied mathematical modelling techniques are generally lacking. In order to analyse and model such devices, it is necessary to estimate accurately the resultant force distribution due to the inter-atomic interactions. Here, we find the van der Waals force using the Lennard-Jones potential to calculate the oscillation frequency using Newton's second law for double-walled carbon nanotubes of any length of the inner and the outer tubes, $2L_1$ and $2L_2$, respectively. These results are based on work by the present authors derived in (Baowan and Hill).

Keywords

Force, distribution, for, double, walled, carbon, nanotubes

Disciplines

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Force Distribution for Double-Walled Carbon Nanotubes

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Abstract — Advances in technology have led to the creation of many nano-scale devices and carbon nanotubes are representative materials to construct these devices. Double-walled carbon nanotubes with the inner tube oscillating can be used as gigahertz oscillators and form the basis of possible nano-electronic devices. Such gigahertz oscillating devices made from carbon nanotubes might be instrumental in the micro-computer industry, which is predominantly based on electron transport phenomena. There are many experiments and molecular dynamics simulations which show that a wave is generated on the outer cylinder by the oscillation of the carbon nanotubes and that the frequency of this wave is also in the gigahertz range. However, conventional applied mathematical modelling techniques are generally lacking. In order to analyse and model such devices, it is necessary to estimate accurately the resultant force distribution due to the inter-atomic interactions. Here, we find the van der Waals force using the Lennard-Jones potential to calculate the oscillation frequency using Newton's second law for double-walled carbon nanotubes of any length of the inner and the outer tubes, $2L_1$ and $2L_2$, respectively. These results are based on work by the present authors derived in [1].

Keywords - Lennard-Jones potential, van der Waals, double-walled carbon nanotubes

I. INTRODUCTION

The discovery of carbon nanotubes (CNTs) by Iijima [2] has given rise to speculation on many new potential nanodevices. Due to their unique mechanical and electrical properties, such as flexibility, high strength and low weight, both multi-walled and single-walled carbon nanotubes (MWNTs, SWNTs, respectively) promise many new applications in nanomechanical systems. Double-walled carbon nanotubes (DWNTs), with the inner tube oscillating, can be used as gigahertz oscillators and form the basis of a possible nano-electronic device. There are many experiments and molecular dynamics simulations that have studied CNT oscillators. Cumings and Zettl [3] use experiments to show MWNTs oscillating by pulling the inner tube out and releasing it. They find that the inner tube can oscillate inside the outer tube with a very high frequency, because of the ultra-low frictional force. Following their study, Zheng and Jiang [4] consider MWNTs by using the Lennard-Jones potential and Newton's second law to calculate the frequency of the oscillation. They find that the oscillation frequency is in the gigahertz range and also conclude that the frictional force

between the inner and outer tubes can be neglected. A theoretical study of their findings can be found in [5]. Moreover, this phenomenon is confirmed by Legoas *et al.* [6], who use molecular dynamics simulations to study the oscillation behaviour. Rivera *et al.* [7, 8] show that the frictional force is very low when compared with the van der Waals force, which is in agreement with Zheng and Jiang [4].

In this paper, our approach is to use simple mechanical principles and classical applied mathematical modelling techniques to formulate explicit analytical criteria and ideal model behaviour in a scientific context. We investigate the force distribution for DWNTs with general half-lengths L_1 and L_2 ($L_1 < L_2$) by using the Lennard-Jones potential and neglecting the frictional force. In the following section, we introduce the Lennard-Jones potential energy and the van der Waals force. The calculation for the potential energy of DWNTs is in section III. The oscillatory behaviour for DWNTs is in section IV. Sections V and VI give the numerical results and conclusions, respectively. The results presented in this paper constitute a summary of results derived in [1].

II. LENNARD-JONES POTENTIAL FUNCTION

The van der Waals force between DWNTs is found by differentiating the standard Lennard-Jones [4, 5, 9, 10]. In this paper, we assume that the frictional force is negligible [3-5, 7-8], so that only the van der Waals force needs to be considered in the direction of the oscillation.

A. Lennard-Jones potential energy

The classical Lennard-Jones potential between two atoms at a distance ρ apart is given by

$$V(\rho) = -\frac{A}{\rho^6} + \frac{B}{\rho^{12}}, \quad (1)$$

where A and B are the attractive and repulsive constants, respectively. The equilibrium distance ρ_0 is given by

$$\rho_0 = 2^{1/6} \sigma = \left(\frac{2B}{A} \right)^{1/6}. \quad (2)$$

B. The van der Waals force

The van der Waals interaction force between all the atoms of the inner tube and all the atoms of the outer tube can be written as

$$F_{\text{vdW}} = -\nabla V^{\text{tot}}, \quad (3)$$

where V^{tot} is the total potential energy obtained by integration of the Lennard-Jones potential over each of the inner and outer tube surfaces.

Due to the symmetry of the problem, we are only concerned with the force in the axial direction. We obtain the resultant axial force (Z-direction) by differentiating (1) with respect to Z, which is defined as the distance between the centres of the inner and the outer tubes.

III. MATHEMATICAL DERIVATION FOR TWO CONCENTRIC TUBES OF LENGTH L_1 AND L_2

Using a continuum approximation, which assumes that the inter-atomic interactions can be modelled by smearing the atoms uniformly across the surfaces, the potential energy between the inner and the outer tubes is determined. With reference to the rectangular Cartesian coordinate system, the inner and the outer tubes are in the same co-axial, Z-direction, with radii a and b , respectively, as shown in Fig. 1. The parametric equations for the any arbitrary point on the inner and the outer tube is in the form $(a\cos\theta_1, a\sin\theta_1, z_1)$ and $(b\cos\theta_2, b\sin\theta_2, z_2)$, respectively, then the distance ρ is given by

$$\rho^2 = (b\cos\theta_2 - a\cos\theta_1)^2 + (b\sin\theta_2 - a\sin\theta_1)^2 + (z_2 - z_1)^2. \quad (4)$$

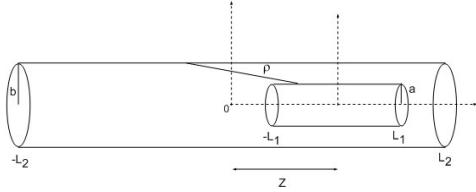


Figure 1. Double-walled carbon nanotubes with lengths $2L_1$ and $2L_2$

Thus the total potential energy is

$$v^{\text{tot}}(\rho) = n_{\sigma}^2 ab \int_0^{2\pi} \int_0^{2\pi} \left[\int_{-L_2}^{L_2} \int_{-L_1}^{L_1} \left(-\frac{A}{\rho^6} + \frac{B}{\rho^{12}} \right) dz_1 dz_2 \right] d\theta_1 d\theta_2, \quad (5)$$

where n_{σ} denotes the mean surface density of a carbon nanotube.

We observe that there are four critical positions (see Fig. 2) for these two carbon nanotubes, $\beta_1 = -L_1 - L_2$, $\beta_2 = L_1 - L_2$, $\beta_3 = L_1 + L_2$, and $\beta_4 = -L_1 + L_2$, which give interesting behaviour for the potential energy and force distribution, as shown in the section V. By using appropriate substitutions, series expansion and integration, we obtain the full expression for $V^{\text{tot}}(\rho)$ which is in terms of Appell's hypergeometric functions of two variables for any lengths of the inner and outer tubes, $2L_1$ and $2L_2$, respectively. More details are given in work recently presented by the authors [1].

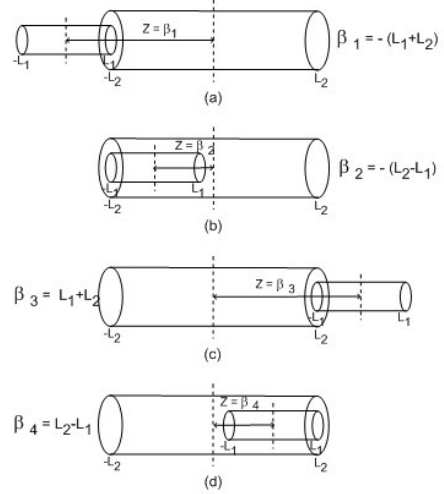


Figure 2. Four critical positions for two concentric carbon nanotubes

IV. OSCILLATORY BEHAVIOUR FOR DWNTS

In order to study the oscillatory behaviour of DWNTs, we use Newton's second law with friction neglected, to obtain

$$M \frac{d^2 Z}{dt^2} = -\frac{\partial V^{\text{tot}}}{\partial Z}, \quad (6)$$

where M is the mass of the inner tube. Following Cumings and Zettl [2], we pull the inner tube out a distance d and then release it, and the distance between centres becomes $Z_0 = L_2 - L_1 + d$, which leads to the geometric constraint $d \leq 2L_1$. By using the equations of motion and for the particular case when the initial velocity is zero, the oscillation frequency can be written as

$$f = \frac{\alpha^2 \sqrt{d}}{4[\sqrt{d} + \alpha(2d + \beta_4)]}, \quad (7)$$

where α is the initial condition parameter given by $\alpha^2 = |V^{\text{tot}}(0)|/ML_1$ and $V^{\text{tot}}(0)$ is the total potential energy at $Z = 0$.

V. NUMERICAL RESULTS

In this section, the numerical values for the potential energy and force distribution are evaluated. Following the work of Girifalco *et al.* [9, 10] and Ma *et al.* [11], we obtain the parameter values for DWNTs, shown in Table 1. Using the algebraic package MAPLE, we plot the potential energy and van der Waals force versus the difference between the centres of the tubes Z , for variations of the inner tube length, as shown in Figures 3, 4 and 5.

In the case that the length of the inner and the outer tubes are equal, the minimum potential energy occurs at $Z = 0$, which is the position that the tubes overlap. Moreover, the forces at this point balance each other and therefore represent an equilibrium position. Considering the case where the inner tube is laid inside the outer tube at $Z = 0$ and perturbing the inner tube in the axial direction, it will oscillate and quickly return to this equilibrium position. On the other hand, if the inner tube is outside the outer tube, it cannot come inside by itself because there are repulsive forces at the ends of the outer tube. As such,

we have to initiate the force to overcome these repulsive forces as shown in Fig. 3.

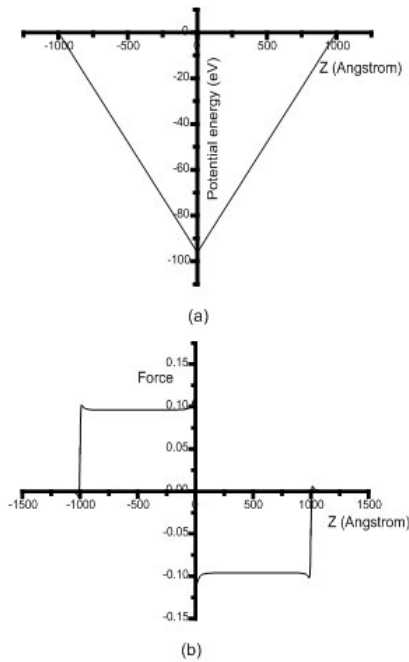


Figure 3. Force distribution for $L_1 = 500 \text{ \AA}$ and $L_2 = 500 \text{ \AA}$ where the Z-axis is the distance between centers (a) potential and (b) van der Waals force.

The potential energy and the force distribution for $L_1 = 250 \text{ \AA}$ and $L_2 = 500 \text{ \AA}$ are shown in Fig. 4. The minimum potential energy is also in the position $Z = 0$, and maintains this constant value in the range between β_2 to β_4 which are the two critical positions. In terms of the van der Waals force, there are two attractive forces at both ends of the outer tube to keep the inner tube moving inside with the oscillatory behaviour. We note that the ends of each phase for the attractive forces are also the critical positions, β_1 and β_3 . Again, the repulsive forces at the ends will not allow the inner tube to go inside. An initial force is necessary to push the inner tube and induce the oscillation.

We further reduce the length of the inner tube in such a way that the ratio L_1/L_2 tends to zero. In this case, the inner tube behaves like a buckyball. The minimum energy is everywhere along the outer tube and there are two strong attractive forces at the ends to keep the inner tube oscillating. As shown in Fig. 5, we observe that the forces are very close to zero everywhere except at both ends of the tube. Accordingly, the forces can be estimated by delta functions, similar to the observation made by Cox, *et al.* [12].

Using Newton's second law, we calculate the oscillation frequency of the DWNTs with the inner tube oscillating, shown in Fig. 6. When we pull the inner tube out a distance d and release it, the inner tube will move back into the outer tube with the potential energy of the tubes and kinetic energy from the initial velocity. Moreover, there are repulsive and attractive forces at the ends of the outer tube to keep the inner tube in and maintain the oscillation behaviour. Of particular practical interest is the case where the initial velocity is zero, where we

find that the maximum frequency occurs when the inner tube is pulled out a distance $d = (L_2 - L_1)/2$.

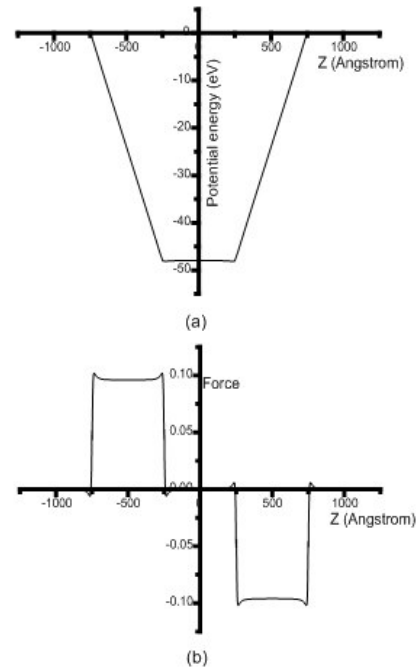


Figure 4. Force distribution for $L_1 = 250 \text{ \AA}$ and $L_2 = 500 \text{ \AA}$ where the Z-axis is the distance between centers (a) potential and (b) van der Waals force.

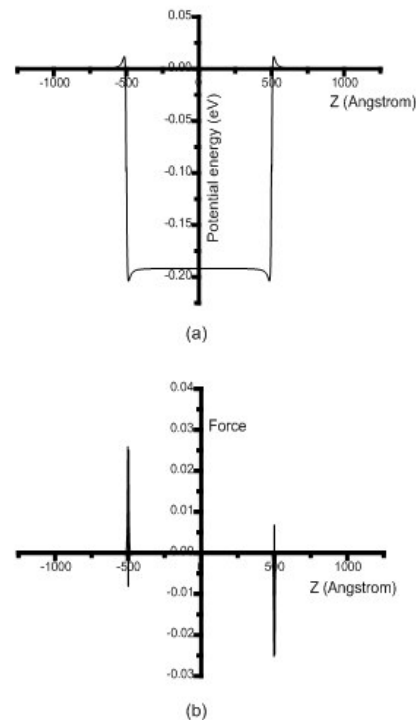


Figure 5. Force distribution for $L_1 = 1 \text{ \AA}$ and $L_2 = 500 \text{ \AA}$ where the Z-axis is the distance between centers (a) potential and (b) van der Waals force.

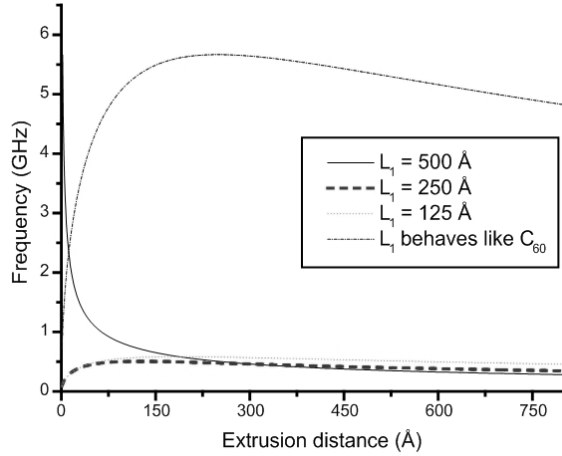


Figure 6. The frequency profile for the several of the inner tube in gigahertz range versus the extrusion distance d in angstrom.

TABLE I. CONSTANTS USED IN THE MODEL

Parameter	Value
Radius of inner tube (a)	1.957 Å
Radius of outer tube (b)	5.423 Å
Half length of outer tube (L_2)	500 Å
Attractive constant (A)	$15.2 \text{ eV} \times \text{Å}^6$
Repulsive constant (B)	$24.1 \times 10^3 \text{ eV} \times \text{Å}^{12}$
Mean surface density of carbon atoms (n_σ)	$4\sqrt{3}/(9\sigma^2)$
Carbon-carbon bond length (σ)	1.42 Å

VI. CONCLUSION

In this paper, we consider the force distribution for two concentric tubes of finite length L_1 and L_2 by using a continuum approximation. The Lennard-Jones potential function is used to evaluate the van der Waals force and the formal mathematical expression, derived in [1], is displayed graphically. Due to the symmetry of the tubes, only the van der Waals force in the axial direction is considered. We obtain a mathematical equation that can be used to describe the force distribution and oscillation behaviour for DWNTs, with arbitrary lengths $2L_1$ and $2L_2$ for the inner and outer tubes, respectively.

There are four critical positions in this model given by $\beta_1 = -L_1 - L_2$, $\beta_2 = L_1 - L_2$, $\beta_3 = L_1 + L_2$, and $\beta_4 = -L_1 + L_2$. The oscillatory behaviour is most likely to occur in the range where the ends of the inner and outer tubes coincide. Subsequently, there will be forces which are acting in the opposite direction to the direction of motion of the inner tube and therefore it will reverse the direction and hence become an oscillator.

Furthermore, we see that if we pull the inner tube out with the extrusion distance d and then release it, the inner tube will

oscillate inside the outer tube without escape. This is because of the strong attractive forces at the ends of the outer tube that maintain the oscillatory behaviour. However, not all inner tubes can be sucked in by the van der Waals force between the two tubes because there are two repulsive forces at the ends. In this situation, we have to give an initial force to push the inner tube in, which can overcome these repulsive forces and gives rise to the oscillatory behaviour. We observe that the longer the extrusion distance and the shorter the inner tube length, the higher the oscillatory frequency.

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