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Free vibrations of single-walled carbon nanotubes in the vicinity of a fully constrained graphene sheet

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ABSTRACT

Carbon nanotubes (CNTs) have been recently taken into consideration as mechanical resonators of distinguished capabilities. This study aims at investigating the free vibration characteristics of a single-walled CNT in the vicinity of a fully constrained graphene sheet. Using a molecular structural mechanics model and considering nonlinear van-der-Waals interactions, the static deformation of the nanotube is obtained using an iterative procedure. Then, the governing equations of motion are linearized about the static equilibrium state and the natural frequencies are obtained. The molecular structural mechanics model is verified using established results in literature and then a survey is performed on the natural frequencies of the CNT's beam-like modes in various distances from the graphene sheet.

1. Introduction

Since carbon nanotubes (CNTs) were discovered in 1991 [1], their outstanding features such as extraordinary mechanical, electrical and thermal properties have been the motivation of many earlier studies in this field of research. Single- and multi-walled carbon nanotubes (SWCNT and MWCNT) are recently considered as nanoscale components for the development and design of many Nano-Electro-Mechanical-Systems (NEMS) [2–5]. There is a growing interest in investigation of the mechanical behavior of CNTs, due to their extensive applicability, and thus numerous studies are devoted to develop analysis method for this purpose [6–9]. Owing to the huge cost and difficulty of nanoscale experimental analysis, scientists turned to device computational methods for analysis and prediction of nanostructures properties [10]. Molecular Dynamics (MD) is a high-accuracy tool that enables to simulate the dynamics of a system of particles based on numerical solution of Newton's equations of motion. Besides the advantages of MD for the exact simulation of the nanostructures, the high computational cost and expensive operations of such methods, especially for large-scales systems, have been the major motivation for developing alternate fast methods even with less accuracy for the primary studies. For this purpose, continuum mechanics based models have been used to analyze the mechanical properties of nanoscale structures [8,11,12]; however, there are still some uncertainties in such models. Another proposed method is Molecular Mechanics (MM) which is used to simulate the mechanical behavior of nanostructures by simulating the atomic interactions as by linear springs. A similar approach is based on using an equivalent finite element model instead of the nanostructure which is named molecular structural mechanics [13–18]. There is no remarkable deference in results of finite element model compared to the MM method [19]. These methods are often utilized for the design and development of nanodevices like various nanoscale sensors and resonators [20–22].

Mechanical resonators are known as key components in signal processing systems [23]. Reducing the size of a resonator increases its resonant frequency and decreases its energy consumption [7]. In fact, obtaining a higher resonant frequency is of interest since it causes to enhance the sensor's sensitivity [24]. Also higher resonant frequency of a resonator, facilitates the construction of higher frequency filters, oscillators, and mixers for wireless communications [7]. High-frequency NEMS are demanded in new applications ranging from mechanical mass or charge detectors [25,26] and nanodevices for high-frequency signal processing of biological imaging [27,28]. Recently, some researchers have studied CNTs as resonators [29] and oscillators [30]. The great properties and perfect atomic structure, combined with nanoscale size of CNTs, imply that they have extensive potential applications in various NEMS [24,25]. Zhao and Cummings [31] investigated free vibrations of double walled carbon nanotube of different chiralities and various lengths under constant energy and constant temperatures using MD simulations. They observed that at a constant energy level, the oscillation frequency is independent of the initial temperature; however, it slightly varies with temperature at

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constant temperatures. Using a new combination of drive and detection methods, Peng et al. [32] measured both oscillation amplitude and phase and illustrated the relative mobility of static charges near the nanotube. They showed that, a CNT-based electromechanical resonators with the fundamental frequency over than 1.3 GHz, can be used as a sensitive mass detector with resolution of 10^{-18} grams. Sawano et al. [33] investigated the vibration of CNT cantilevers in water using the optical detection technique. They found that due to the viscosity resistance in water, the cantilever loses its fundamental oscillation as compared with the vacuum condition. Based on this result, they concluded that since the temperature variation affects the liquid viscosity, the resonant frequency of the immersed CNT changes with the temperature. Kang et al. [5] investigated oscillators based on a single-walled CNT bundle using classical MD simulations. This CNT bundle oscillator was initiated by an electrostatic capacitive force that extruded it and then, van-der-Waals (vdW) energy sucked it into the bundle. Therefore, the CNT oscillator could be oscillated by both Coulomb and the vdW interactions. They controlled the operation frequency of a CNT bundle oscillator by varying both the size and the length of the bundle. Also they investigated the effect of the number of CNTs in the bundle on oscillator's chaotic signature. The transverse elasticity and vibration behavior of the bilayer graphene sheets are respectively investigated by Scarpa et al. [34] and Chandra et al. [35]. vdW interactions have been treated as spring-like elements using linearized Lennard–Jones potential formulation. He et al. [36] considered the effect of vdW interaction between different layers of a CNT and investigated the size effect on the vdW interactions using a more refined vdW model. Also He et al. [37] investigated the effect of vdW interaction on the natural frequencies of the multi-layered graphene sheets (MLGSs). They showed that mode shapes which are associated with the classical frequencies for each sheet of an MLGS are identical. In contrast, the vibration modes that are associated with the resonant frequencies are non-identical and give various vibration patterns, which indicate that MLGSs are highly suited to use as high frequency resonators.

In this paper, the molecular structural mechanics is used to obtain the natural frequencies and corresponding mode shapes of a clamped–clamped SWCNT in vicinity of a fully constrained graphene sheet. For this purpose, the static deformation of the SWCNT under the influence of nonlinear vdW interactions with the graphene sheet is calculated. Then, the governing equations of motion are linearized about the static deformation of the SWCNT and the natural frequencies are calculated.

2. Nanostructures and molecular structural mechanics approach

The carbon atoms in a graphene sheet are arranged in a hexagonal array so that each atom has three nearest neighbors which are joined together by strong covalent bonds. The length of a covalent bond almost is about $r_0 = 0.142$ nm. CNT structures are similar to those of graphene sheets and a CNT is made by rolling a graphene sheet about a vector perpendicular to the chiral vector. The geometric properties of CNTs are completely described by translational indices (n, m) and their length (L), thus the diameter of a CNT is calculated as follows [38]:

$$d = \frac{\sqrt{3}r_0(m^2 + mn + n^2)}{\pi} \tag{1}$$

Fig. 1 shows a SWCNT of length L and diameter of D near a fully constrained graphene sheet in the global coordinate system xyz. The SWCNT is clamped at both ends in a distance of W from the graphene sheet and its axis coincides with the x axis. The SWCNT and graphene sheet are modeled using the molecular structural mechanics following Odegard's method [39]. The covalent bonds are modeled by equivalent beam elements with circular cross-section (A) which can simulate the pair potentials between the carbon atoms. The mechanical properties of the beam are obtained according to the equivalency of the bond stretching, bending, and dihedral angle and out of plan torsion with the strain energy stored in the beam as following

$$\frac{EA}{L} = k_r, \quad \frac{EI}{L} = k_\theta, \quad \frac{GJ}{L} = k_\tau$$

where EI, GJ and EA are respectively the bending, torsional and stretching stiffness of the beam element and the k_r, k_θ and k_τ are the bond stretching force constant, bond angle bending force constant and torsional resistance respectively [6]. Using this approach, the SWCNT is modeled as a frame structure which can simulate its mechanical properties. The element stiffness matrix is given as

$$\mathbf{K}_n^c = \begin{bmatrix} \mathbf{k}_{ii} & \mathbf{k}_{ij} \\ \mathbf{k}_{ij}^T & \mathbf{k}_{jj} \end{bmatrix} \tag{2}$$

where the superscript 'c' denotes the covalent bond stiffness matrix and n is the bond number. The submatrices of $\mathbf{K}_n$ are

$$\mathbf{k}_{ii} = \begin{bmatrix} EA/L & 0 & 0 & 0 & 0 & 0 \\ 0 & 12EI_x/L^3 & 0 & 0 & 0 & 6EI_x/L^2 \\ 0 & 0 & 12EI_y/L^3 & 0 & -6EI_y/L^2 & 0 \\ 0 & 0 & 0 & GJ/L & 0 & 0 \\ 0 & 0 & -6EI_y/L^2 & 0 & 4EI_y/L & 0 \\ 0 & 6EI_x/L^2 & 0 & 0 & 0 & 4EI_x/L \end{bmatrix}$$

$$\mathbf{k}_{ij} = \begin{bmatrix} -EA/L & 0 & 0 & 0 & 0 & 0 \\ 0 & -12EI_x/L^3 & 0 & 0 & 0 & 6EI_x/L^2 \\ 0 & 0 & -12EI_y/L^3 & 0 & -6EI_y/L^2 & 0 \\ 0 & 0 & 0 & -GJ/L & 0 & 0 \\ 0 & 0 & 6EI_y/L^2 & 0 & 2EI_y/L & 0 \\ 0 & -6EI_x/L^2 & 0 & 0 & 0 & 2EI_x/L \end{bmatrix}$$

$$\mathbf{k}_{jj} = \begin{bmatrix} EA/L & 0 & 0 & 0 & 0 & 0 \\ 0 & 12EI_x/L^3 & 0 & 0 & 0 & -6EI_x/L^2 \\ 0 & 0 & 12EI_y/L^3 & 0 & 6EI_y/L^2 & 0 \\ 0 & 0 & 0 & GJ/L & 0 & 0 \\ 0 & 0 & 6EI_y/L^2 & 0 & 4EI_y/L & 0 \\ 0 & -6EI_x/L^2 & 0 & 0 & 0 & 4EI_x/L \end{bmatrix}$$

Considering the mass of carbon atoms ($m_c = 1.9943^{-23}$ g) as lumped mass elements at the nodes of the frame, gives a mechanical model which governs small motions of SWCNT in the vicinity of the graphene sheet. The mass matrix of the lumped masses can be written as

$$\mathbf{M} = m_c \begin{bmatrix} \mathbf{I} & 0 \\ 0 & 0 \end{bmatrix}_{6\times 6} \tag{3}$$

where $\mathbf{I}_{3\times 3}$ is the identity matrix.

By transforming the stiffness and mass matrices of the elements from the local coordinate system to the global frame and assembling them, the global mass ($\overline{\mathbf{M}}$) and stiffness ($\overline{\mathbf{K}}^{\mathbf{c}}$) matrices of the molecular structural mechanics model is obtained. Thus, the governing equation of motion is read

$$\overline{\mathbf{M}}\ddot{\mathbf{u}} + \overline{\mathbf{K}}^{\mathbf{c}}\mathbf{u} = \mathbf{f} \tag{4}$$

where $\mathbf{u}$ is a vector containing the translations and rotations of all nodes of the frame structure. Furthermore, $\mathbf{f}$ is the vector of