Composites: Part B 73 (2015) 72–81

Contents lists available at ScienceDirect

Composites: Part B

journal homepage: www.elsevier.com/locate/compositesb

Vibration analysis of two orthogonal slender single-walled carbon nanotubes with a new insight into continuum-based modeling of van der Waals forces

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ARTICLE INFO

Article history:
Received 23 September 2014
Received in revised form 11 December 2014
Accepted 15 December 2014
Available online 24 December 2014

Keywords:
A. Nano-structures
B. Vibration
C. Computational modeling
Doubly orthogonal single-walled carbon nanotubes

ABSTRACT

Transverse vibrations of doubly orthogonal slender single-walled carbon nanotubes (SWCNTs) at the vicinity of each other are of interest. The van der Waals (vdW) forces play an important role in dynamic interactions between two adjacent nanotubes. Using Lennard-Jones potential function, such a phenomenon is appropriately modeled by a newly introduced vdW force density function. By employing Hamilton's principle, the equations of motion are obtained based on the nonlocal Rayleigh beam theory. In fact, these are integro-partial differential equations and seeking an exact or even analytical solution to them is a very difficult job. Therefore, an efficient numerical solution is proposed. The effects of the inter-tube distance, slenderness ratio, small-scale parameter, aspect ratio, and elastic properties of the surrounding medium on the free vibration of the nanosystem are addressed. The obtained results could be regarded as a pivotal step for better realizing of dynamic behaviors of more complex systems consist of multiple orthogonal networks of nanotubes.

1. Introduction

Since the past decade, vibrations of carbon nanotubes (CNTs) have been of focus of attention of the communities of material, structural, and mechanical engineering [1–9]. It is mainly related to the excellent physical, chemical, and mechanical properties of such newly synthesized materials [10–14] in which provide them for a wide range of applications including sensors (both physical and chemical) [15–17], resonators [18–20], nanofluids conveyors [21–23], drug delivery [24–27], and micro-/nano- electromechanical systems (MEMS/NEMS) [28–31]. In all above-mentioned applications, understanding the true mechanics of dynamical behavior of CNTs will surely lead to a more efficient and optimal nanosystem.

To date, vibrations of single-walled carbon nanotubes (SWCNTs) has been broadly examined including free dynamic response [32–34], excitations due to a moving nanoparticle [35–37], wave propagation [38–42], vibrations due to inside fluids flow [43–46], and nonlinear free and forced vibrations [47–49]. Additionally, transverse vibrations of a system of doubly parallel nanobeams were investigated [50,51]. In the latter two works, the interactional van der Waals (vdW) forces between atoms of the adjacent nanostructures were simply modeled by a continuous transverse spring without careful evaluating the spring's constant. In a more general framework, vibrations of two- and three-dimensional ensembles of SWCNTs were also carefully addressed [52–54]. In all these studies, the straight individual tubes were placed parallel to each other and at equal distances from each other. The interactions of adjacent tubes were modeled by appropriate springs whose constants were methodically calculated. A brief review of all above-mentioned works reveals that the vdW forces between neighboring tubes have been modeled by elastic layers whose properties were constant and uniform across the tubes' lengths. The unit of the spring constants is $\frac{N}{m^2}$. It means that the interactional vdW forces between two neighboring tubes was considered as a product of the spring constant and the difference of their transverse displacements. In an attempt for factual modeling of such forces, the vibration problem of a system of double-orthogonal-SWCNTs (DOSWCNTs) is visited in this paper. The obtained results will display that the vdW forces between two tubes are incorporated into the model by a so-called vdW force density function of unit $\frac{N}{m^3}$. In contrast to the previous works, the present work suggests that a more pragmatic version of the vdW force between two adjacent tubes is an integral of the product of the vdW force density function and the difference of transverse

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http://dx.doi.org/10.1016/j.compositesb.2014.12.025
1359-8368/

displacements over the tube's length. Due to this fact, the resulting equations of motion are coupled integro-partial differential equations. It is expected that such a newly established model would lead to a more accurate prediction of free vibrations of DOSWCNTs as well as other systems composed of SWCNTs.

The classical continuum theory (CCT) cannot capture the realistic vibrations of nanostructures since the inter-atomic bonds are not introduced to the constitutive relations [55–57]. When the ratio of the bond's length to the nanostructure's length or wavelength of the propagated wave becomes comparable, the effect of the inter-atomic bonds becomes significant (i.e., size-dependency). In such cases, the stress state of each point does not only depend on the stress of that point, but also to the stress states of its neighboring points (i.e., nonlocality). To conquer such a shortage of the CCT, several advanced continuum theories (ACTs) have been established. One of the most well-known theories is the nonlocal continuum field theory of Eringen [68–71]. So far, such a theory has been extensively employed in mechanical modeling of CNTs [37–41,43,46,49,52–54,58,59]. Another popular ACT is the strain gradient theory of Aifantis [60,61] which is also implemented in modeling vibrations of CNTs [62–67].

Since flexural behavior of slender DOSWCNTs is of interest, a nonlocal model based on the Rayleigh beam theory is developed. In such nanosystems, the share of shear strain energy in the total strain energy can be rationally ignored since the ratio of shear strain energy to the flexural strain energy is fairly negligible. For dynamic analysis of stocky CNTs, application of shear deformable beam models would lead to more accurate results [49,53,54,63].

In the present work, using Lennard-Jones potential function, the vdW force density function is introduced. By employing nonlocal Rayleigh beam theory, nonlocal-integro-partial differential equations describe transverse vibrations of the nanosystem are obtained. Seeking an analytical solution to these coupled equations is a very difficult task. By using Galerkin approach in conjunction with assumed mode method, the deflection fields of the nanotubes are discretized in the dimensionless spatial domains of tubes. Subsequently, the natural frequencies of the nanosystem are numerically determined. Through various parametric studies, the influences of the slenderness ratio, intertube distance, aspect ratio, size-dependency, transverse and rotational stiffness of the surrounding elastic medium on the free vibration behavior are studied. The undertaken work can be taken into account as a primary step for better realizing of more complex structures composed of orthogonal membranes of SWCNTs or even multi-walled carbon nanotubes.

2. Assessment of vdW forces between two orthogonal SWCNTs

Based on the Lennard-Jones potential function [72], the interaction between two neutral atoms at distance λ is given by:

$$\Phi(\lambda)=4\epsilon\left[\left(\frac{\sigma}{\lambda}\right)^{12}-\left(\frac{\sigma}{\lambda}\right)^{6}\right], \tag{1}$$

where ϵ is the depth of the potential well, σ denotes the distance at which the potential function becomes zero and is expressed by: $\sigma=\frac{r_a}{\sqrt[6]{2}}$ where r_a is the distance between two atoms at the equilibrium state (i.e., the inter-particle potential reaches its absolute minimum value). The vdW force between a pair of atoms i and j, $\mathbf{f}_{ij}$, is formulated as follows:

$$\mathbf{f}_{ij}=-\frac{\mathrm{d}\Phi}{\mathrm{d}\lambda}\mathbf{e}_{\lambda}=\frac{24\epsilon}{\sigma^2}\left[2\left(\frac{\sigma}{\lambda}\right)^{14}-\left(\frac{\sigma}{\lambda}\right)^{8}\right]\vec{\lambda}, \tag{2}$$

where $\vec{\lambda}$ is the vector position of the atom j with respect to the atom i, and $\mathbf{e}_{\lambda}$ denotes the corresponding unit base vector. According to the Cartesian and cylindrical coordinate systems pertinent to the orthogonal nanotubes (see Fig. 1(a) and (b)), the walls' geometry of these transversely deformed tubes is described by: $(x_1,y_1=r_{m_1}\cos\phi_1,z_1=r_{m_1}\sin\phi_1+w_1(x_1,t))$ and $(x_2,y_2=r_{m_2}\cos\phi_2,z_2=r_{m_2}\sin\phi_2+w_2(x_2,t))$ where d is the intertube distance, $0\leqslant x_i\leqslant l_{b_i}$ and $0\leqslant\varphi_i\leqslant 2\pi$; $i=1,2$. On the basis of the Cartesian coordinate system associated with the first nanotube,

$$\begin{aligned}\vec{\lambda}=&(x_1-l_{11}-r_{m_2}\cos\varphi_2)\mathbf{e}_{x_1}+(r_{m_1}\cos\varphi_1-x_2+l_{21})\mathbf{e}_{y_1}\\&+(r_{m_1}\sin\varphi_1-r_{m_2}\sin\varphi_2+d-\triangle w)\mathbf{e}_{z_1},\end{aligned} \tag{3}$$

where $\mathbf{e}_{x_1}$, $\mathbf{e}_{y_1}$, and $\mathbf{e}_{z_1}$ are the unit base vectors associated with the rectangular coordinate system of the nanotube 1, r_{m_i} is the mean radius of the equivalent continuum structure pertinent to the ith tube, $\triangle w=w_2(x_2,t)-w_1(x_1,t)$, and $w_i(x_i,t)$ represents the transverse displacement field of the ith SWCNT along the z_1 axis. The interactional vdW force per unit square length of tubes due to their relative transverse motions along the z_1 axis is described by:

$$f_z=\frac{24\epsilon\sigma_{CNT}^2}{\sigma^2}\int_0^{2\pi}\int_0^{2\pi}\left[2\left(\frac{\sigma}{\lambda}\right)^{14}-\left(\frac{\sigma}{\lambda}\right)^{8}\right]\begin{pmatrix}r_{m_1}\sin\varphi_1-r_{m_2}\sin\varphi_2+\\ d-\triangle w\end{pmatrix}\mathrm{d}\varphi_1\,\mathrm{d}\varphi_2, \tag{4}$$

where $f_z=f_z(x_1,x_2,t)$, $\sigma_{CNT}=\frac{4\sqrt{3}}{9a^2}$ denotes the surface density of the carbon atoms, and a is the length of the carbon–carbon bond. In order to evaluate the change in vdW force per unit square length due to the small lateral displacements of the nanotubes, it is only suffice to approximate Eq. (4) by the Taylor expansion up to the first-order about the equilibrium state. By doing so, the extra transverse vdW force per unit square length is calculated as:

$$\triangle f_z=C_{vdW}(x_1,x_2)\triangle w, \tag{5}$$

where

$$\begin{aligned}C_{vdW}(x_1,x_2;r_{m_1},r_{m_2},d)=&-\frac{256\epsilon r_{m_1}r_{m_2}}{9a^4}\\&\times\int_0^{2\pi}\int_0^{2\pi}\left\{\begin{matrix}\sigma^{12}\left[\varrho^{-7}-14\varrho^{-8}\left(d+r_{m_1}\sin\varphi_1-r_{m_2}\sin\varphi_2\right)^2\right]\\ -\frac{\sigma^6}{2}\left[\varrho^{-4}-8\varrho^{-5}\left(d+r_{m_1}\sin\varphi_1-r_{m_2}\sin\varphi_2\right)^2\right]\end{matrix}\right\}\mathrm{d}\varphi_1\,\mathrm{d}\varphi_2,\end{aligned} \tag{6a}$$

$$\begin{aligned}\varrho(x_1,x_2,\varphi_1,\varphi_2;r_{m_1},r_{m_2},d)=&\left(x_1-l_{11}-r_{m_2}\cos\varphi_2\right)^2\\&+\left(x_2-l_{21}-r_{m_1}\cos\varphi_1\right)^2+\left(r_{m_1}\sin\varphi_1-r_{m_2}\sin\varphi_2+d\right)^2.\end{aligned} \tag{6b}$$

The parameter C_{vdW} is called the vdW force density function (since its unit is $\frac{\mathrm{N}}{\mathrm{m}^3}$). As it is seen in Eq. (6), radii of the nanotubes, the intertube distance, and the location of the nanotubes' intersection are among the crucial factors that influence on this parameter.

To see the variation of C_{vdW} in the spatial coordinates associated with the nanotubes, let give an example. Consider a system of DOSWCNTs whose tubes cross each other at the midspan point. The geometry of the nanosystem is as: $l_{b_1}=l_{b_2}=30$ nm, $r_{m_1}=r_{m_2}=1.5$ nm, $d=r_{m_1}+r_{m_2}+2t_b$, and $l_{11}=l_{21}=\frac{l_{b_1}}{2}$. In order to evaluate the double integral in Eq. (6a), Gauss quadrature method is exploited. The pyramid of each tube is divided into 10 equal subdomains with 5 Gauss points. The graph of C_{vdW} in terms of dimensionless spatial coordinates of tubes, namely $\xi_1=\frac{x_1}{l_{b_1}}$ and $\xi_2=\frac{x_2}{l_{b_1}}$, has been demonstrated in Fig. 2. As it is seen, shooting of the vdW force density function at the midspan point of both tubes is so obvious. Further studies also reveal that such a fact occurs at the vicinity of the intersection point of the tubes. As a result, a more refined mesh should be considered for evaluating integrals of expressions include C_{vdW} in the regions close to the point of intersection (see Fig. 2). In all carried out calculations in this paper, we subdivide the lengths of tubes into N_p-1 intervals such that about half of them are equally located in a region of length $0.1l_{b_1}$ or $0.1l_{b_2}$ around the intersection point. By choosing N_g Gaussian point in each direction (or $N_g\times N_g$ in each computational cell), a