International Journal of Mechanical Sciences 122 (2017) 156–166

Contents lists available at ScienceDirect

International Journal of Mechanical Sciences

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

Vibration of single-walled carbon nanotubes with elastic boundary conditions

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A R T I C L E I N F O

Keywords:
Single-walled carbon nanotubes
Vibration
Molecular dynamics
Fourier series method
Elastic boundary conditions

A B S T R A C T

The vibrational behaviours of single-walled carbon nanotubes (SWCNTs) bridged on a silicon channel are investigated using a three-segment Timoshenko beam model and a one-segment Timoshenko beam model with elastic boundaries together with molecular dynamics (MD) simulation. A modified Fourier series method (MFSM) is proposed to analyse the free vibration of the Timoshenko beam models with elastic boundary conditions. Explicit formulas are derived for the van der Waals (vdW) interaction coefficients between the SWCNTs and silicon substrates. The boundary elastic constants of the SWCNTs bridged on the silicon channel are obtained by fitting the bending curve of SWCNTs subjected to a static uniformly distributed lateral load simulated via the MD method. The MD simulations show that both the three-segment Timoshenko beam model and the one-segment Timoshenko beam model with elastic boundaries have a relatively good ability to predict the vibrational behaviours of SWCNTs bridged on a silicon channel.

1. Introduction

As mechanical structures are scaled down to the nanometer range, the van der Waals (vdW) forces play an important role in the interactions between nanostructures. Ru [1] presented an elastic shell model to study the effect of vdW forces on the axial buckling of a double-walled carbon nanotube (DWCNT). Yoon et al. [2] used multiple-Euler beam models, considering the vdW interactions, to study the free vibration of an embedded multi-wall carbon nanotube (MWCNT). Han and Lu [3] constructed a double-shell model to study the torsional buckling of a DWCNT and discussed the effect of the vdW forces between the inner and the outer nanotubes on the critical buckling loads. He et al. [4] derived an explicit formula for the vdW interactions between any two layers of an MWCNT. A continuum cylindrical shell model was presented to investigate the buckling of an MWCNT. Wang et al. [5] used a double Euler beam model with consideration of the intertube vdW interactions to study the resonant frequencies and the associated vibrational modes of an individual DWCNT. Ansari et al. [6] investigated the free vibration of DWCNTs via the nonlocal continuum shell model and molecular dynamics (MD) simulation.

The carbon nanotubes (CNTs) are often embedded in an elastic substrate. The interactions between CNTs and a substrate are mainly vdW forces. The vdW forces play a key role in the mechanical behaviours of CNTs [7–12]. Jiang et al. [7] developed a cohesive law between CNTs and polymers based on the vdW force using interatomic potential. The tensile cohesive strength and the cohesive energy were given in terms of the area density of the CNT and volume density of the polymer, as well as the parameters in the vdW force. Subsequently, the cohesive law between the CNT and the polymer was used to study the mechanical behaviours of the CNT-reinforced composites [8]. Lu et al. [9] established a cohesive law for the vdW force of interfaces between the MWCNTs and the polymer. Zhao et al. [11] developed coarse-grained (CG) potentials of the single-walled carbon nanotubes (SWCNTs) in the CNT bundles and the buckypaper to study their mechanical behaviours. The non-bonded CG potentials between the CG beads using the vdW cohesive energy between the SWCNTs in a bundle were derived via analytical methods.

The boundary conditions of the CNTs embedded in elastic substrates are far different from those of classic cases in nature. In fact, the boundary conditions of CNTs are commonly elastically restrained edges. Thus, it is essential to consider the vdW interactions between CNTs and substrates effect on the vibrational behaviours for their potential applications in nanoelectromechanical systems. CNTs that are bridged on two substrates at both ends due to vdW forces can be considered equivalent to a continuum beam model with elastically restrained edges. It has been widely accepted that it is very difficult to obtain an analytical solution for the beams, except for very few simple boundary cases. Thus, efficient numerical techniques have been employed to solve the vibration problems of the beam with elastic boundary conditions. Kiani [13] used the reproducing kernel particle

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http://dx.doi.org/10.1016/j.ijmecsci.2017.01.012
Received 27 June 2016; Received in revised form 22 December 2016; Accepted 8 January 2017
Available online 10 January 2017
0020-7403/

method to study the free transverse vibrations of embedded SWCNTs with arbitrary boundary conditions using the nonlocal Euler beam, Timoshenko beam, and higher order beam models. Wattanasakulpong and Mao [14] used Timoshenko beam theory to study the dynamic response of beams made of functionally graded materials with various classical and non-classical boundary conditions using the Chebyshev collocation method. Rosa and Lippiello [15] adopted the differential quadrature method to investigate the free vibrations of embedded SWCNTs based on Euler beam theory.

Recently, an analytical modified Fourier series method (MFSM) was proposed for the vibration analysis of elastically supported beams [16]. The flexural displacement of the beam is sought as the linear combination of a Fourier series and an auxiliary polynomial function. This method was subsequently used to analyse the vibrations of elastically supported beams and plates [17–21]. There have also been numerous experimental studies on the vibration of SWCNT bridged on elastic substrates [22–24]. To the best knowledge of the authors, however, no continuum beam model with elastic boundaries has been used to describe the effect of elastic substrates on the vibrations of SWCNTs. Therefore, an analytical MFSM is proposed for the free vibrations of SWCNTs by means of Timoshenko beam models with elastic boundary conditions.

The primary objective of this work is to investigate the vibration of an SWCNT bridged on a silicon channel using two types of Timoshenko beam models via MFSM. The paper is organized as follows. Three- and one-segment Timoshenko beam models with elastic boundary conditions are proposed to model the free vibrations of SWCNTs via an analytical MFSM in Sections 2 and 3, respectively. Then, the MD model for the vibrations of SWCNTs is given in Section 4. Next, vibration analyses of SWCNTs with elastic boundary conditions are presented and discussed in Section 5. Finally, some concluding remarks are made in Section 6.

2. Three-segment Timoshenko beam model

2.1. The governing differential equations and boundary conditions

As mechanical structures are scaled down to the nanometer range, the dominated interactions between CNTs and elastic substrates become vdW forces. Thus, an SWCNT bridged on the elastic substrates at both ends, as shown in Fig. 1(a), can be considered equivalent to an ideal three-segment Timoshenko beam model (TSB), as shown in Fig. 1(b). The governing equations for the classic Timoshenko beam describing the free vibration in each segment are as follows

$$\begin{cases} k_sGA\left(\frac{\partial\phi_1}{\partial x_1}-\frac{\partial^2 w_1}{\partial x_1^2}\right)+C_{vdW}w_1-\omega^2\rho A w_1=0, & x_1\in[0,L_1] \\ k_sGA\left(\phi_1-\frac{\partial w_1}{\partial x_1}\right)-EI\frac{\partial^2\phi_1}{\partial x_1^2}-\omega^2\rho I\phi_1=0, & x_1\in[0,L_1] \end{cases}, \tag{1a}$$

$$\begin{cases} k_sGA\left(\frac{\partial\phi_2}{\partial x_2}-\frac{\partial^2 w_2}{\partial x_2^2}\right)-\omega^2\rho A w_2=0, & x_2\in[0,L_2] \\ k_sGA\left(\phi_2-\frac{\partial w_2}{\partial x_2}\right)-EI\frac{\partial^2\phi_2}{\partial x_2^2}-\omega^2\rho I\phi_2=0 & x_2\in[0,L_2] \end{cases}, \tag{1b}$$

$$\begin{cases} k_sGA\left(\frac{\partial\phi_3}{\partial x_3}-\frac{\partial^2 w_3}{\partial x_3^2}\right)+C_{vdW}w_3-\omega^2\rho A w_3=0, & x_3\in[0,L_3] \\ k_sGA\left(\phi_3-\frac{\partial w_3}{\partial x_3}\right)-EI\frac{\partial^2\phi_3}{\partial x_3^2}-\omega^2\rho I\phi_3=0, & x_3\in[0,L_3] \end{cases}, \tag{1c}$$

where w_j and ϕ_j ($j = 1, 2, 3$) are the transverse displacement and the slope of the beam due to bending deformation, respectively. ρ is the mass density, A is the area of the cross section of the beam, I is the moment of inertia for the cross section, E is the Young's modulus, $G = E/2(1 + \nu)$ is the shear modulus, k_s is the shear correction factor of the beam, ν is Poisson's ratio [25], C_{vdW} is the vdW coefficient between per unit length of the CNT and the substrate.

The boundary conditions at the ends of the beam, as shown in Fig. 1(b), can be expressed as

$$k_sGA\left(\phi_1-\frac{\partial w_1}{\partial x_1}\right)=0,\ EI\frac{\partial\phi_1}{\partial x_1}=0,\ \text{at } x_1=0, \tag{2a}$$

$$k_sGA\left(\phi_3-\frac{\partial w_3}{\partial x_3}\right)=0,\ EI\frac{\partial\phi_3}{\partial x_3}=0,\ \text{at } x_3=L_3. \tag{2b}$$

The continuity conditions at the junctions are

$$w_1|_{x_1=L_1}=w_2|_{x_2=0}, \tag{3a}$$

$$\phi_1|_{x_1=L_1}=\phi_2|_{x_2=0}, \tag{3b}$$

$$EI\frac{\partial\phi_1}{\partial x_1}|_{x_1=L_1}=EI\frac{\partial\phi_2}{\partial x_2}|_{x_2=0}, \tag{3c}$$

$$k_sGA\left(\phi_1-\frac{\partial w_1}{\partial x_1}\right)|_{x_1=L_1}=k_sGA\left(\phi_2-\frac{\partial w_2}{\partial x_2}\right)\Big|_{x_2=0}, \tag{3d}$$

$$w_2|_{x_2=L_2}=w_3|_{x_3=0}, \tag{3e}$$

$$\phi_2|_{x_2=L_2}=\phi_3|_{x_3=0}, \tag{3f}$$

$$EI\frac{\partial\phi_2}{\partial x_2}\Big|_{x_2=L_2}=EI\frac{\partial\phi_3}{\partial x_3}\Big|_{x_3=0}, \tag{3g}$$

$$k_sGA\left(\phi_2-\frac{\partial w_2}{\partial x_2}\right)\Big|_{x_2=L_2}=k_sGA\left(\phi_3-\frac{\partial w_3}{\partial x_3}\right)\Big|_{x_3=0}. \tag{3h}$$

The dimensionless parameters for a TSB with elastic constraints are defined as follows

$$\xi_j=\frac{x_j}{L_j},\ W_j(\xi_j)=\frac{w_j(x_j)}{L_j},\ \Phi_j(\xi_j)=\phi(x_j),\ \beta_j=\frac{I}{AL_j^2},\ \alpha_j=\frac{k_sGAL_j^2}{EI},$$
$$\Omega_j^2=\omega^2\frac{\rho AL_j^4}{EI},\ C_1=\frac{C_{vdW}L_1^4}{EI},\ C_3=\frac{C_{vdW}L_3^4}{EI}. \tag{4}$$

Using the above dimensionless parameters, the dimensionless forms of the governing equations can be expressed as

$$\begin{cases} \alpha_1(\frac{\partial\Phi_1}{\partial\xi_1}-\frac{\partial^2W_1}{\partial\xi_1^2})+C_1W_1-\Omega_1^2W_1=0, & \xi_1\in[0,1] \\ \alpha_1(\Phi_1-\frac{\partial W_1}{\partial\xi_1})-\frac{\partial^2\Phi_1}{\partial\xi_1^2}-\beta_1\Omega_1^2\Phi_1=0, & \xi_1\in[0,1] \end{cases}, \tag{5a}$$

$$\begin{cases} \alpha_2(\frac{\partial\Phi_2}{\partial\xi_2}-\frac{\partial^2W_2}{\partial\xi_2^2})-\Omega_1^2(\frac{L_2}{L_1})^4W_2=0, & \xi_2\in[0,1] \\ \alpha_2(\Phi_2-\frac{\partial W_2}{\partial\xi_2})-\frac{\partial^2\Phi_2}{\partial\xi_2^2}-\beta_2\Omega_1^2(\frac{L_2}{L_1})^4\Phi_2=0, & \xi_2\in[0,1] \end{cases}, \tag{5b}$$

$$\begin{cases} \alpha_3(\frac{\partial\Phi_3}{\partial\xi_3}-\frac{\partial^2W_3}{\partial\xi_3^2})+C_3W_3-\Omega_1^2(\frac{L_3}{L_1})^4W_3=0, & \xi_3\in[0,1] \\ \alpha_3(\Phi_3-\frac{\partial W_3}{\partial\xi_3})-\frac{\partial^2\Phi_3}{\partial\xi_3^2}-\beta_3\Omega_1^2(\frac{L_3}{L_1})^4\Phi_3=0, & \xi_3\in[0,1] \end{cases}. \tag{5c}$$

The dimensionless boundary conditions are written as follows

$$\left(\Phi_1-\frac{\partial W_1}{\partial\xi_1}\right)\Big|_{\xi_1=0}=0,\ \frac{\partial\Phi_1}{\partial\xi_1}\Big|_{\xi_1=0}=0,\ \left(\Phi_3-\frac{\partial W_3}{\partial\xi_3}\right)\Big|_{\xi_3=1}=0,$$
$$\frac{\partial\Phi_3}{\partial\xi_3}\Big|_{\xi_3=1}=0,\ W_1\Big|_{\xi_1=1}=\frac{L_2}{L_1}W_2\Big|_{\xi_2=0},\ \Phi_1\Big|_{\xi_1=1}=\Phi_2\Big|_{\xi_2=0},$$