



# Dynamic interactions of doubly orthogonal stocky single-walled carbon nanotubes



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## ABSTRACT

Nonlocal continuum-based modeling of free transverse vibration of doubly orthogonal stocky single-walled carbon nanotubes (DOSWCNTs) which are embedded in an elastic matrix is of particular interest. A basic step towards such a crucial goal is to establish a rational model for evaluating the van der Waals interactional force between two tubes. By employing Hamilton's principle, the nonlocal governing equations associated with the free vibration of the nanosystem are obtained using Timoshenko and higher-order beam theories. Inherently, these are sets of four coupled integro-partial differential equations which are very difficult to be solved analytically. To bridge such a dilemma, reproducing kernel particle method is exploited and the essential boundary conditions of each shear-deformable beam model are exactly satisfied by implementing the corrected collocation method. In a special case, the predicted natural frequencies by the proposed models are checked with those of other models analyzed via mode summation method, and a reasonably good agreement is achieved. Subsequently, the effects of the slenderness ratio, small-scale parameter, aspect ratio, nanotubes' radii, intertube distance, transverse and rotational stiffness of the surrounding elastic medium on free vibration of the nanosystem are comprehensively addressed for various boundary conditions.

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## 1. Introduction

Carbon nanotubes (CNTs) have extensively attracted a lot of interest in the past two decades. It is chiefly related to their extraordinary physical, chemical, and mechanical properties. Nowadays potential applications of such unique materials in a vast range of engineering branches, medical purposes, and military aids have been explored. For engineering applications, CNTs have been proposed to be used as nanosensors [1,2], nanoelectromechanical systems (NEMS) [3,4], tissue engineering [5,6], and structural health monitoring [7–9]. From medical point of view, the recent researches show that CNTs can be effectively exploited in the fields of drug delivery [10,11], biosensing approaches for disease treatment [12–14], and noninvasive monitoring of blood levels and other chemical properties of the human body [15–17]. For military purposes, CNTs can be exploited as the basic elements of nanocomposite matters to reduce the effects of the impact [18] as well as nerve agents detection [19]. In most of these applications, ensembles or forests of CNTs are utilized for the considered jobs.

Even though vertically synthesized as well as horizontally growth of CNTs have been widely investigated, the growth and

mechanical modeling of ensembles consist of both horizontal and vertical CNTs have not been fairly well explored. In an attempt for growth a more complex nanostructure, Zhou et al. [20] reported an efficient approach for constructing forests of CNTs made of vertical nanotubes plus to horizontally aligned arrays on a single substrate. Perhaps the simplest forms of the family of orthogonal three-dimensional CNTs are orthogonally oriented membranes made of parallel single-walled carbon nanotubes (SWCNTs) which are located in a flat plane. To study vibrations of such nanostructures, a basic step is to realize the vibrations of two perpendicular nanotubes which are placed at the vicinity of each other. To this end, newly developed models are established to study transverse vibrations of doubly orthogonal SWCNTs (DOSWCNTs) which are embedded in an elastic matrix. Subsequently, the influential parameters of such a nanosystem on its free vibration will be comprehensively addressed.

At the nanoscale, inter-atomic bonds play a crucial role in vibration behavior of the nanostructure. When the ratio of bonds' lengths to the wavelength (in wave propagation problems) or length of the nanostructure (in transverse vibrations of beam-like structures) magnifies, the obtained results by the classical continuum mechanics (CCM) would be questionable. It is mainly because of this fact that this theory does not consider the effect of the inter-atomic bonds in its formulations. To conquer such a deficiency of the

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CCM, some advanced continuum mechanics have been developed in the last century such as micro-polar theory of Cosserat–Cosserat [21], couple-stress theory of Mindlin and Toupin [22,23], strain gradient theory of Aifantis [24,25], and the nonlocal continuum theory of Eringen [26–28]. A simple form of the latter theory has been widely employed for vibration problems of SWCNTs. Possibly it may be related to its simplicity in application to the classical version of the equations of motion. To date, many dynamical problems associated with CNTs including free transverse vibration of straight and wavy CNTs [29–38], linear and nonlinear forced vibrations [39–42], their interactions with moving inside fluid flow [43–45], vibrations in the presence of magnetic fields [46–48], free and forced vibrations of vertically aligned forests of SWCNTs [49–51] have been examined. In the present work, transverse vibrations of a nanosystem of stocky DOSWCNTs are of interest. For this purpose, shear deformable beam models in conjunction with the nonlocal continuum theory of Eringen are implemented.

For two neighboring SWCNTs, van der Waals (vdW) forces between the constitutive atoms of each tube and those of the another one play an important role in the transverse vibrations. To date, in all of the proposed models for continuum-based modeling of two or more adjacent tubes (for example double- or multi-walled CNTs), such forces are incorporated into the governing equations by simple elastic constants. In other words, the intertube interactions due to the vdW forces were modeled by elastic layers whose constants were uniform across the lengths of the tubes (with unit  $\frac{N}{m^2}$ ). As it will be shown, the constants of the elastic layer for a system made of CNTs with finite lengths are not uniform at all. Such a more realistic view to such important forces leads to the definition of the vdW force density function (with unit  $\frac{N}{m^3}$ ). Thereafter, it will be revealed that the resulting governing equations inherently belong to a special class of partial differential equations, called integro-partial differential equations. Finding an exact or even an explicit solution to these equations is not an easy job. Thereby, an efficient meshless technique, namely reproducing kernel particle method (RKPM), is proposed. So far, RKPM has been broadly applied in many vibrational problems of structures in the range of nanoscale [52,53] to macroscale [54–56]. The only concern in application of meshless methods to engineering problems is that an efficient methodology should be implemented for satisfaction of the essential boundary conditions such that does not lead to the irrational response of the internal points. To fulfill such a crucial task, corrected collocation method is exploited in the present study. The application of this method to the dynamical problems of elastic solids will be inclusively explained in the manuscript.

Herein, two novel models are developed to investigate free vibration of elastically embedded DOSWCNTs. The newly developed models are on the basis of the nonlocal Timoshenko beam theory (NTBT) and the nonlocal higher-order beam theory (NHOBT). In moving towards such a crucial issue, the vdW interaction forces between two perpendicular nanotubes are carefully investigated, and a rational model is established. By implementing Hamilton's principle, the strong form of equations of motion describing transverse vibrations of the nanosystem are constructed using nonlocal shear-deformable beam theories. Finding an explicit solution to them is a very problematic task. As a result, an efficient meshless methodology is proposed and the essential boundary conditions of the proposed models are exactly enforced by using corrected collocation method. In the case of fully-simply supported boundary conditions, the obtained results are also verified with those of mode summation method and a reasonably good agreement is reported. In the continuing, the effects of the radii of the nanotubes, slenderness ratio, small-scale parameter, intertube distance, aspect ratio, transverse and rotational interactions of the DOSWCNTs with its surrounding elastic medium are examined in

some detail. The obtained results in the present work would be very useful in rational mechanical modeling of multiple orthogonal membranes of SWCNTs.

## 2. Continuum-based modeling of vdW forces

The interaction between two neutral atoms can be explained by the Lennard-Jones potential function [57,58], namely  $\Phi(\lambda) = 4\epsilon \left[ \left(\frac{\sigma}{\lambda}\right)^{12} - \left(\frac{\sigma}{\lambda}\right)^6 \right]$  where  $\lambda$  is the distance between two atoms,  $\epsilon$  is the potential well's depth,  $\sigma$  is the distance at which the potential function becomes zero, and  $\sigma = \frac{r_a}{\sqrt{2}}$  where  $r_a$  is the distance between two atoms at the equilibrium state. The vdW force between atoms  $i$  and  $j$ ,  $\mathbf{f}_{ij}$ , is evaluated by:

$$\mathbf{f}_{ij} = -\frac{d\Phi}{d\lambda} \mathbf{e}_\lambda = \frac{24\epsilon}{\sigma^2} \left[ 2\left(\frac{\sigma}{\lambda}\right)^{14} - \left(\frac{\sigma}{\lambda}\right)^8 \right] \vec{\lambda}, \quad (1)$$

where  $\vec{\lambda}$  is the position vector of the atom  $j$  with respect to the atom  $i$  and its unit base vector is denoted by  $\mathbf{e}_\lambda$ . The walls' coordinates of the transversely deformed nanotubes are expressed by:  $(x_1, y_1 = r_{m_1} \cos \varphi_1, z_1 = r_{m_1} \sin \varphi_1 + w_1(x_1, t))$  and  $(x_2, y_2 = r_{m_2} \cos \varphi_2, z_2 = r_{m_2} \sin \varphi_2 + w_2(x_2, t))$  where  $d$  is the intertube distance,  $0 \leq x_i \leq l_{b_i}$  and  $0 \leq \varphi_i \leq 2\pi$ ;  $i = 1, 2$  (see Fig. 1). Therefore,

$$\vec{\lambda} = (x_1 - l_{11} - r_{m_2} \cos \varphi_2) \mathbf{e}_{x_1} + (r_{m_1} \cos \varphi_1 - x_2 + l_{21}) \mathbf{e}_{y_1} + (r_{m_1} \sin \varphi_1 - r_{m_2} \sin \varphi_2 + d - \Delta w) \mathbf{e}_{z_1}, \quad (2)$$

where  $\mathbf{e}_{x_1}$ ,  $\mathbf{e}_{y_1}$ , and  $\mathbf{e}_{z_1}$  are the unit base vectors associated with the Cartesian coordinate system attached to the nanotube 1,  $r_{m_i}$  is the mean radius of the equivalent continuum structure (ECS) pertinent to the  $i$ th tube,  $\Delta w = w_2(x_2, t) - w_1(x_1, t)$ , and  $w_i(x_i, t)$  represents the transverse displacement of the  $i$ th tube along the  $z_i$  axis. The ECS is a hollow circular cylindrical structure whose dominant longitudinal, torsional, and breathing frequencies are fairly close to those of the parent nanotube. For an ECS whose length and mean radius are equal to the length and radius of the SWCNT, the effective wall thickness is approximately equal to 0.34 nm [59–62]. However, this value does not satisfy the Vodenitcharova–Zhang criterion [63] that the effective wall thickness of SWCNTs must be smaller than the atomic diameter of carbon atoms. There are also several works that suggest axial and bending stiffness or effective Young's modulus based on the evaluated elastic strain energy from atomistic-based approaches [64–67]. According to the literature, the value of effective wall thickness of SWCNTs for their continuum-based modeling is an open problem. Further research works and advanced theoretical concepts are still needed to explain its exact value and its possible dependencies to the chiral, length to diameter ratio, and so on. Herein, the elastic moduli and effective thickness of SWCNTs are assumed to be 1 TPa and 0.34 nm.

The interactional vdW force per unit square length of the ECSs due to their relative transverse motions along the  $z_1$  axis is calculated as follows:

$$f_z = \frac{24\epsilon\sigma_{CNT}^2}{\sigma^2} \int_0^{2\pi} \int_0^{2\pi} \left[ 2\left(\frac{\sigma}{\lambda}\right)^{14} - \left(\frac{\sigma}{\lambda}\right)^8 \right] \left( \begin{array}{c} r_{m_1} \sin \varphi_1 - r_{m_2} \sin \varphi_2 \\ + d - \Delta w \end{array} \right) d\varphi_1 d\varphi_2, \quad (3)$$

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. Since linear vibration of the nanosystem is of concern, we approximate Eq. (3) by expressing its Taylor expansion up to the first-order about the equilibrium state. Hence, the variation of the transverse vdW forces per square lengths of the tubes due to their relative transverse motions is displayed by:

$$\Delta f_z = C_{vdW} \Delta w, \quad (4)$$

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