Current Applied Physics 14 (2014) 1116–1139

Contents lists available at ScienceDirect

Current Applied Physics

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

Nonlocal discrete and continuous modeling of free vibration of stocky ensembles of vertically aligned single-walled carbon nanotubes

Keivan Kiani*

Department of Civil Engineering, K.N. Toosi University of Technology, P.O. Box 15875-4416, Tehran, Iran

ARTICLE INFO

Article history:
Received 12 October 2013
Received in revised form
4 May 2014
Accepted 7 May 2014
Available online 11 June 2014

Keywords:
Ensemble of SWCNTs
Frequency analysis
Nonlocal discrete models
Nonlocal continuous models
Galerkin approach

ABSTRACT

Free dynamic analysis of transverse motion of vertically aligned stocky ensembles of single-walled carbon nanotubes is of particular interest. A linear model is developed to take into account the van der Waals forces between adjacent SWCNTs because of their bidirectional transverse displacements. Using Hamilton's principle, the discrete equations of motion of free vibration of the nanostructure are obtained based on the nonlocal Rayleigh, Timoshenko, and higher-order beam theories. The application of such discrete models for frequency analysis of highly populated ensembles would be associated with so much computational effort. To overcome such a problem, some useful nonlocal continuous models are established. The obtained results reveal that the newly developed models can successfully capture the predicted fundamental frequencies of the discrete models. Through various numerical studies, the roles of slenderness ratio, radius of the SWCNT, small-scale parameter, population of the ensemble, and intertube distance on the fundamental flexural frequency of the nanostructure are examined and discussed. The capabilities of the proposed nonlocal continuous models in predicting flexural frequencies of the nanostructure are also addressed.

1. Introduction

A forest or an ensemble of single-walled carbon nanotubes (ESWCNTs) consists of multiple SWCNTs at the vicinity of each other in which interact with each other by the van der Waals (vdW) forces. Using chemical vapor deposition in a suitably controlled environment, growth of randomly oriented ESWCNTs [1,2] or even vertically aligned ESWCNTs [3–6] on an appropriate substrate would be possible. The orientation of the SWCNTs within the layered ensemble should be chosen such that the nanosystem could perform more appropriately and efficiently for the assigned jobs. For instance, from applied mechanics standpoint, the arrangement and directions of the SWCNTs within an ensemble network should be taken into account such that the exerted electro-mechanical forces cause lower stresses and displacements within the nanostructure. Herein, without dealing about the engineering design of such nanosystems, we are interested in examining free dynamic analysis of vertically aligned ESWCNTs.

Carbon nanotubes (CNTs) have been under great investigation because of their brilliant physical and chemical properties [7,8]. Such excellent properties have been provided them for a broad range of applications such as drug delivery systems [9–12], nanosensors [13–16], nanocomposites [17–19], and nano-electromechanical systems [20–24]. For these potential applications, determination of the dynamic behavior of ESWCNTs is a basic step toward their optimal design.

To date, various aspects of vibrations of individual CNTs have been studied and a sufficient knowledge regarding the roles of the influential parameters on their vibration behavior have been accumulated. Most of the undertaken works before 2008 had been performed in the context of the classical theory of elasticity. Several examples of such an evidence are the free transverse vibration of CNTs [25,26], their transverse vibrations and instabilities due to moving inside fluids flow [27–29], and their nonlinear frequency analysis [30,31]. Further experimental and theoretical studies [32–34] show that the common continuum mechanics cannot accurately capture the mechanical and vibration behavior of nanostructures. This fact becomes highlighted when the wavelength of the propagated wave would be comparable with the interatomic bonds. Under such a circumstance, irrespective of the influence of the propagated wave on the vibration of each point of the continuum, the state of stress at each point is also affected by those of its neighboring points. Such an important phenomenon cannot be interpreted by the models which are inherently established

* Tel.: +98 21 88779473; fax: +98 21 88779476.
E-mail addresses: k_kiani@kntu.ac.ir, keivankiani@yahoo.com.

http://dx.doi.org/10.1016/j.cap.2014.05.018
1567-1739/

based on the classical continuum mechanics. To remove such a deficiency, some advanced continuum mechanics have been developed during the past century including micropolar of Cosserat and Cosserat [35], couple stress of Toupin and Mindlin [36,37], gradient elasticity of Aifantis [38–40], and nonlocal continuum mechanics of Eringen [41–45]. The latter theory has been paid attention to by many researchers who study dynamic behavior of nanostructures. The main reason of this fact maybe its simplicity in application to the classical governing equations. Based on the nonlocal continuum theory, the stress of each point (i.e., nonlocal stress) does not rely on the state of stress at that point, but also is affected by the stress of its neighboring points. Such a dependency is formulated by using appropriate kernel functions for the under study spatial domains. The influence domain of the kernel functions is commonly specified by a so-called small-scale parameter. In limit, when the small-scale parameter vanishes, the nonlocal stress approaches the local stress (i.e., classical stress). Through choosing an appropriate value for the small-scale parameter, a reasonably good agreement between the predicted results by this theory and those of atomic models has been reported for various problems [46–51]. So far, the nonlocal continuum theory of Eringen has been employed for dynamic analysis of individual CNTs including free vibrations [52–57], dynamic instability [58,59], their interactions with inside fluid flow [60–64] and moving nanoparticles [65–71]. However, free vibrations of ensemble networks of vertically aligned SWCNTs and their related dynamical problems have not been addressed.

In this paper, free transverse vibrations of ESWCNTs are of concern. For this purpose, the interactional vdW forces between two adjacent SWCNTs due to their transverse displacements are evaluated via Lennard-Jones potential function. Using Hamilton's principle, the discrete and continuous equations of motion of the nanostructure based on the nonlocal Rayleigh, Timoshenko, and higher-order beam theories are established. Using modal analysis as well as Galerkin approach, the frequencies of the nanostructure are extracted via proposed nonlocal discrete and continuous models. In a particular case, the predicted results by the nonlocal discrete models are compared with those of another work, and a reasonably good agreement is achieved. The efficiency of the proposed continuous models is successfully checked. The roles of influential factors on the fundamental frequencies of the ESWCNTs are then addressed in some details.

2. Description of the nanomechanical problem

Consider an ensemble of vertically aligned SWCNTs whose intertube distances in both y and z directions are equal to d as demonstrated in Fig. 1(a). The ensemble consists of N_y and N_z tubes along the y and z axes, respectively. For nonlocal continuum-based modeling of the problem, each SWCNT is substituted by an equivalent continuum structure (ECS) whose most of dominant frequencies are identical to those of the SWCNT evaluated by an appropriate atomistic approach. The research works of Gupta and Batra [72] and Batra and Gupta [73] showed that such an ECS is a hollow cylindrical shell of length, l_b, and mean radius, r_m, similar to those of the SWCNT. The density, elastic moduli, shear elastic modulus, Poisson's ratio, cross-sectional area, moment of inertia of the ECS's cross-section in order are denoted by ρ_b, E_b, G_b, ν_b, A_b, and I_b. The dynamic transverse displacement components of the (m,n) th SWCNT along the y and z axes are represented by $V_{mn} = V_{mn}(x,t)$ and $W_{mn} = W_{mn}(x,t)$, respectively (see Fig. 1(b)). Every SWCNT interacts with its neighboring tubes because of the existing vdW forces between their atoms.

In the upcoming part, a linear model is developed to take into account the interactional vdW forces between each tube with its adjacent ones. Based on the developed spring-tube model for such forces (see Fig. 1(b)), the discrete equations of motion of ESWCNTs are then established via nonlocal Rayleigh, Timoshenko, and higher-order beam theories.

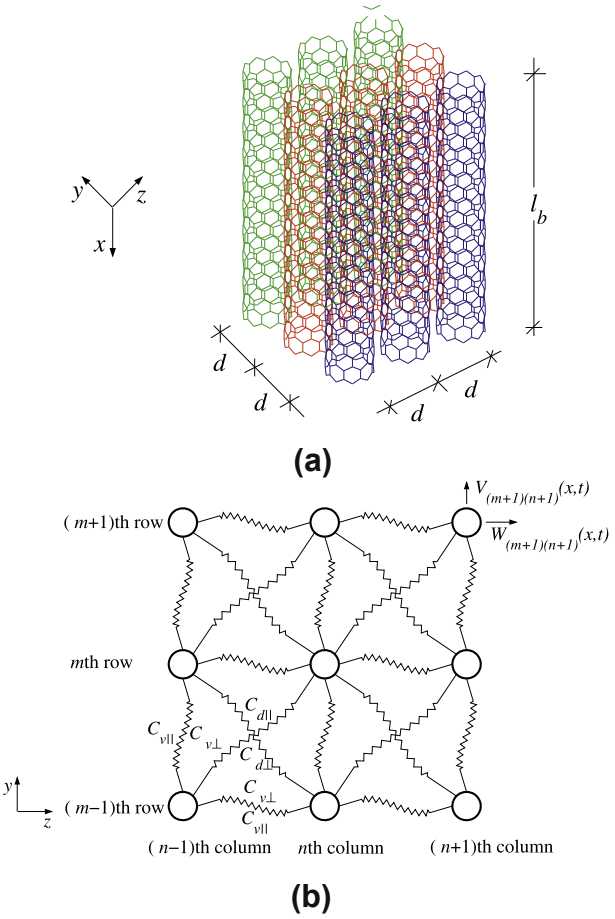

Fig. 1. (a) A schematic representation of an ensemble of vertically aligned SWCNTs with uniform distribution; (b) an elastic linear model to the considered ESWCNTs accounting for intertube vdW forces.

3. Assessing vdW forces between two adjacent-deformed SWCNTs

In this part, a simple model for evaluation of the interactional vdW forces between two adjacent tubes due to their transverse motions is proposed. This model explains that not only transverse displacements of the tubes along the plane passes their center-lines but also those displacements which are perpendicular to this plane would contribute to the vdW forces. Such forces are applied in the parallel and perpendicular directions to the plane's surface, respectively.

According to the Lennard-Jones's potential function [74,75] for two atoms:

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

where λ is the distance between the ith and jth atoms, $\sigma = r_a/\sqrt[6]{2}$, ε denotes the well depth, and r_a represents the distance between two atoms at the equilibrium state. The vdW force between two atoms i and j, $\mathbf{f}_{ij}$, is evaluated as: