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VARIATIONAL PRINCIPLES FOR STABILITY ANALYSIS OF MULTI-WALLED CARBON NANOTUBES BASED ON A NONLOCAL ELASTIC SHELL MODEL

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ABSTRACT

The nonlocal continuum theories are capable to reflect the small length characteristic of nanostructures. In this work, variational principles are presented for the stability analysis of multi-walled carbon nanotubes under various mechanical loadings based on the nonlocal elastic Donnell's shell by the semi-inverse method. In this manner, a set of proper essential and natural boundary conditions for each layer of the multi-walled nanotube is derived.

KEYWORDS:

Variational principles, Carbon nanotubes, Small length scale, shell, stability analysis

INTRODUCTION

Since the discovery of carbon nanotubes (CNT) in 1991 [1], great interests between researchers have been inspired to study the response of nanotubes in different physical and mechanical problems. There are several ways for the investigation of nanostructures' behavior which includes: I) experimental observations, II) molecular dynamics (MD) simulations, III) quantum-based methods, IV) density function based tight binding (DFTB) method and V) continuum-based methods.

The nano-sized experimental setups are quite difficult and expensive. Also, quantum-based methods and atomistic models like MD or DFTB are relatively time-consuming and they are associated with high computational cost for large-sized systems. Meanwhile, continuum-based modeling is relatively faster and much less expensive. Specially, when nanostructure is considered as parts of an assembled nano-device, where the atomistic behaviors are not the object of the analysis, continuum-based modelings give much more satisfying results. For these reasons, modeling nanostructures such as CNTs, graphene sheets, fullerenes and hybrid nano-structures based on the continuum theories has attracted the growing interests of researchers during the past decade in this field of science and engineering. As an example, the stability analysis of nanotubes has been studied using classical beam and shell theories under various mechanical loading [2-5].

At small sizes in nano meter range (10^{-9} m), the atomistic structure such as lattice spacing between individual atoms is important, so that small scale effects can not be ignored. Eringen initiated the idea of non-classic theories in which the small scale effects is added into the classical continuum constitutive equations for the study of structures with atomic scales [6-9]. The non-local continuum theory is one of these non-classic theories, which considers the small scale effects in its formulation, however in a macroscopic manner.

In nanostructures, range of the internal characteristic length (e.g. lattice parameters and bond lengths) is relatively close to the range of external characteristic lengths (e.g. wave length and crack length). The small length scales of nano-structures may call the reasonability of application of classical continuum theories, which neglect the small scale effects, into uncertainty. Hence, non-classic continuum theories such as the nonlocal elasticity theory have advantages to consider the small length scales. Peddieson et al. used the nonlocal elasticity in modeling of nanotubes for the first time in 2003 [10]. During recent years, much attention has been directed in modeling the nanostructures specially the multi-walled carbon nanotubes (MWCNT) by using the nonlocal continuum-based theories, in buckling (structural instability), vibration and wave propagation analyses [11-17].

The differential equations governed for the stability MWCNT are somewhat complicated, such that approximate and numerical methods are usually used for obtaining the critical loads at the onset of instability. Also, deriving the associated boundary conditions directly from the governing PDEs are quite difficult. Hence, deriving the variational functional seems to be very advantageous as a part of the solution procedures for the stability analysis in some numerical methods (e.g. Finite Element, Galerkin and Ritz methods). Moreover, the variational approach smoothes the derivation of the boundary conditions.

Recently, Adali presented the variational principles for MWCNT resting on an elastic foundation undergoing buckling under axial loading based on the nonlocal Euler-Bernoulli beam theory [18]. Modeling MWCNT as a set of concentric shells instead of beams provides more accurate results and makes the stability analysis possible under various mechanical loadings (including external pressure and torsional moment). To this goal, in this paper the variational equations have been derived for the multi-walled carbon nanotubes embedded in an elastic foundation based on the Donnell's nonlocal elastic shell. The van der Waals interaction between the adjacent layers of MWCNT is modeled by an equivalent pressure distribution. The semi-inverse method proposed by He [19,20] has been used to derive the functional for the Donnell's nonlocal elastic coupled PDEs. Also, all essential and natural coupled boundary conditions are derived using the obtained variational functional.

In this paper the Rayleigh's principle [21] is applied to obtain those functions which by minimizing them, one can obtain the critical axial load and critical torsional moment.

NONLOCAL VARIATIONAL PRINCIPLES FOR MULTI-WALLED CARBON NANOTUBES

In the classical theories of elasticity, the stress tensor $\boldsymbol{\sigma}$ at the reference point $\mathbf{x}$ of continua, is a function of the local point strain $\boldsymbol{\varepsilon}$ tensor at $\mathbf{x}$. Eringen proposed the idea that for taking into account the small scale effects, the constitutive equations should be modified and presented the nonlocal elasticity theory [6,7]. The nonlocal elasticity theory is based on the assumption that the stress tensor $\boldsymbol{\sigma}$ at the local point $\mathbf{x}$ is a function of strain tensor $\boldsymbol{\varepsilon}$ at all points of a continuum Ω, both local and nonlocal points. The constitutive equation in the nonlocal elasticity theory is displayed in the integral form as [6-10, 16]:

$$\sigma(\mathbf{x}) = \iiint_{\Omega} \psi\left(\left|\mathbf{x}'-\mathbf{x}\right|,\tau\right)\mathbf{C}:\boldsymbol{\varepsilon}(\mathbf{x}')\,dV(\mathbf{x}'), \qquad (1)$$

where, the function $\psi(|\mathbf{x}'-\mathbf{x}|,\tau)$ is called the nonlocal modulus [9], $|\mathbf{x}'-\mathbf{x}|$ is the distance between the local point $\mathbf{x}$ and nonlocal point $\mathbf{x}'$, $\mathbf{C}$ denotes the forth order elasticity tensor, and $\tau = e_0 a/l$, with a as the internal characteristic length (e.g. C-C bond length or granular size), l as the external characteristic length (e.g. crack length or wave length) and e_0 as a material parameter determined for nanostructure to coincide their experimental and continuum models results [16]. [16]. Eringen developed the differential form of constitutive equation of the nonlocal elasticity theory from the integral form Eq. (1) which is given as [9]

$$\left(1-\eta^2\nabla^2\right)\boldsymbol{\sigma} = \mathbf{C}:\boldsymbol{\varepsilon}, \qquad (2)$$

stating that $\eta = e_0 a$ is called the small scale parameter [14,16]. Eq. (2) can be written in the component form as

$$\left(1-\eta^2\nabla^2\right)\sigma_{ij} = C_{ijkl}\,\varepsilon_{kl}\,, \qquad (3)$$

It is noted that in the special cases with $e_0 a \to 0$, i.e. when the internal characteristic length is negligible, the nonlocal elasticity constitutive equation (Eq. (3)) approaches the classical elasticity constitutive equation $\sigma_{ij} = C_{ijkl}\varepsilon_{kl}$.

Now, let us consider a multi-walled carbon nanotube composed of n concentric cylindrical nanotubes with length L which is embedded in a Winkler elastic foundation. We consider each layer as a Donnell's shell. Also, we consider x, y and z as the longitudinal, circumferential and radial coordinates of the nanotube, respectively (see Fig. 1).

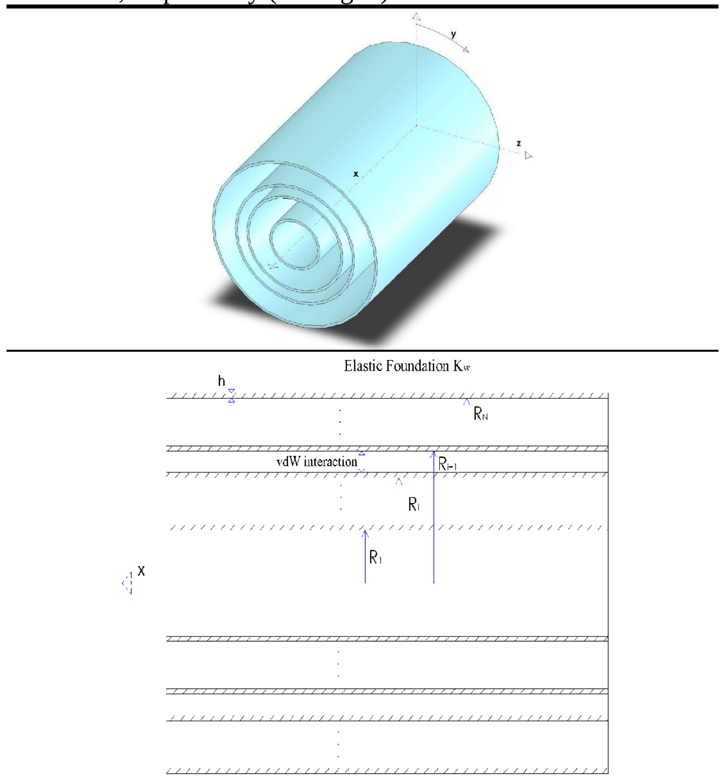

Fig 1: The schematic view of multi walled carbon nanotube, and the configuration of the coordinate system.

The differential equation governing the radial deformation of the i th layer of MWCNT in the axisymmetric conditions based on the nonlocal elastic Donnell's shell has been obtained in the literature as follows [14]

$$D\nabla^8 w_i(x,y) + \frac{Eh}{R_i^2}\frac{\partial^4 w_i(x,y)}{\partial x^4} - (1-\eta^2\nabla^2)\nabla^4 N_i w_i(x,y) = (1-\eta^2\nabla^2)\nabla^4 p_i(x,y); \qquad 1\le i\le n \qquad (4)$$

where $D = Eh^3/12(1-\nu^2)$ denotes the effective bending stiffness of the layer with E, ν and h as the elastic modulus, the Poisson's ratio and the thickness of the nanotube, $w_i(x,y)$ is the displacement of the ith layer of MWCNT in the radial direction, p_i denotes the total pressure exerted on the ith layer of MWCNT. Also, R_i is the radius of the ith layer. The symbol ∇^2 in Eq. (4) denotes the Laplacian differential operator which is defined as

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}; \quad \frac{\partial}{\partial y} = \frac{1}{R_i}\frac{\partial}{\partial \theta} \tag{5}$$

where θ denotes the polar circumferential coordinate. The Differential operator N_i in Eq. (4) can be written as [14]

$$N_i = N_{xi}\frac{\partial^2}{\partial x^2} + 2N_{xyi}\frac{\partial^2}{\partial x \partial y} + N_{yi}\frac{\partial^2}{\partial y^2} \tag{6}$$

where N_{xi}, N_{yi} and N_{xyi} denote the resultant forces on the ith layer due to the axial, circumferential and shearing stresses $(\sigma_{xi}, \sigma_{yi}, \sigma_{xyi})$, respectively. It is noted that they are calculated in the mid-plane of the cylindrical shell. The resultant forces are written in terms of the stress components as

$$N_{xi} = \sigma_{xi} h, \quad N_{yi} = \sigma_{yi} h, \quad N_{xyi} = \sigma_{xyi} h. \tag{7}$$

In continuum based models, the van der Waals (vdW) interactions exerted on the ith nanotube atoms form the jth nanotube atoms can be modeled as an equivalent pressure distribution p_{ij}, which is given in the linear form as [4,14,16,18]

$$p_{ij} = c_{ij}(w_i - w_j) \tag{8}$$

where c_{ij} is the vdW interaction coefficient between the ith and jth layers. Since the vdW is a weak atomic interaction, one can neglect the effects of non-adjacent layers. So, we consider the effects of only adjacent layers interactions in determining the total pressure exerted on each nanotube. By this assumption, the total pressure on layers can be written as

$$p_1 = p_{12} = c_{12}(w_1 - w_2), \tag{9}$$

$$\begin{aligned} p_i &= p_{i(i-1)} + p_{i(i+1)} \\ &= c_{i(i-1)}(w_i - w_{i-1}) + c_{i(i+1)}(w_i - w_{i+1}); \quad i = 2, \ldots, n-1, \end{aligned} \tag{10}$$

$$p_n = p_{n(n-1)} - k_W w_n = c_{n(n-1)}(w_n - w_{n-1}) - k_W w_n \tag{11}$$

where k_W is the Winkler elastic foundation modulus, recalling that the outermost layer rests on a Winkler foundation. It is noted that in the formulation of this work, the innermost tube is subscripted by 1 and the outermost by n. By substituting the total pressure expressions (9)-(11) into the Donnell's nonlocal elastic shell equation (4), the equilibrium differential equations governing the stability of the MWCNT can be derived as [14]

$$\begin{aligned} &D\nabla^8 w_1 + \frac{Eh}{R_1^2}\frac{\partial^4 w_1}{\partial x^4} - (1-\eta^2\nabla^2)\nabla^4 N_1 w_1 \\ &- (1-\eta^2\nabla^2)\nabla^4\left[c_{12}(w_1 - w_2)\right] = 0, \end{aligned} \tag{12}$$

$$\begin{aligned} &D\nabla^8 w_i + \frac{Eh}{R_i^2}\frac{\partial^4 w_i}{\partial x^4} - (1-\eta^2\nabla^2)\nabla^4 N_i w_i - (1-\eta^2\nabla^2) \\ &\nabla^4\left[c_{i(i-1)}(w_i - w_{i-1}) + c_{i(i+1)}(w_i - w_{i+1})\right] = 0; \quad i = 2\ldots n-1, \end{aligned} \tag{13}$$

$$\begin{aligned} &D\nabla^8 w_n + \frac{Eh}{R_n^2}\frac{\partial^4 w_n}{\partial x^4} - (1-\eta^2\nabla^2)\nabla^4 N_n w_n \\ &-(1-\eta^2\nabla^2)\nabla^4\left[c_{n(n-1)}(w_n - w_{n-1}) - k_W w_n\right] = 0 \end{aligned} \tag{14}$$

One can rewrite equations (12)-(14) in the form of differential operators L_i as [18]

$$D_1(w_1, w_2) = L_1(w_1) - (1-\eta^2\nabla^2)\nabla^4\left[c_{12}(w_1 - w_2)\right] = 0, \tag{15}$$

$$\begin{aligned} &D_i(w_{i-1}, w_i, w_{i+1}) = L_i(w_i) - (1-\eta^2\nabla^2)\nabla^4 \\ &\left[c_{i(i-1)}(w_i - w_{i-1}) + c_{i(i+1)}(w_i - w_{i+1})\right] = 0, \end{aligned} \tag{16}$$

$$D_n(w_{n-1}, w_n) = L_n(w_n) - (1-\eta^2\nabla^2)\nabla^4\left[c_{n(n-1)}(w_n - w_{n-1})\right] = 0 \tag{17}$$

where D_i denotes the ith equation. Indeed L_i consists of the uncoupled part of D_i which is given by

$$\begin{aligned} L_i(w_i) = \Bigg[&D\nabla^8 + \frac{Eh}{R_i^2}\frac{\partial^4}{\partial x^4} - (1-\eta^2\nabla^2)\nabla^4 N_i + \\ &+\delta_{in} k_W (1-\eta^2\nabla^2)\nabla^4 \Bigg] w_i; \quad i = 1, 2, \ldots, n \end{aligned} \tag{18}$$

where δ_{in} is the Kronecker's delta with the following definition

$$\delta_{in} = \begin{cases} 1 & i = n \\ 0 & i \neq n \end{cases} \tag{19}$$

In order to obtain the variational functional of the stability equations of the MWCNT, one can assume a trial-functional V based on the semi-inverse method proposed by He [19,20], which can be written as [18]:

$$\begin{aligned} &V(w_1, w_2, \ldots, w_i, \ldots, w_{n-1}, w_n) = V_1(w_1, w_2) + V_2(w_1, w_2, w_3) \\ &+\cdots+V_i(w_{i-1}, w_i, w_{i+1}) + \cdots + V_n(w_{n-1}, w_n) \end{aligned} \tag{20}$$

where one can define $V_i; (0 \le i \le n)$ as

$$V_1(w_1, w_2) = \int_{\Omega_1} U_1(w_1) d\Omega_1 + \int_{\Omega_1} F_1(w_1, w_2) d\Omega_1, \tag{21}$$

$$\begin{aligned} &V_i(w_{i-1}, w_i, w_{i+1}) = \int_{\Omega_i} U_i(w_i) d\Omega_i + \\ &\int_{\Omega_i} F_i(w_{i-1}, w_i, w_{i+1}) d\Omega_i; \quad i = 2\ldots n-1, \end{aligned} \tag{22}$$

$$V_n(w_{n-1}, w_n) = \int_{\Omega_n} U_n(w_n) d\Omega_n + \int_{\Omega_n} F_n(w_{n-1}, w_n) d\Omega_n. \tag{23}$$

Taking the variation of any V_i leads to

$$\delta V_i(w_{i-1}, w_i, w_{i+1}) = \int_{\Omega_i} \delta U_i(w_i) d\Omega_i + \int_{\Omega_i} \delta F_i(w_{i-1}, w_i, w_{i+1}) d\Omega_i, \tag{24}$$

where δ denotes the variational operator and U_i is such that its variation to be:

$$\delta U_i(w_i) = L_i(w_i)\,\delta w_i; \quad i = 1, 2, \ldots, n \tag{25}$$

Also, in Eq. (22), $F_i(w_{i-1}, w_i, w_{i+1})$ denote the unknown functions of w_i to be determined such that the differential equations (15)-(17) correspond to the Euler–Lagrange equations of the trial-functional V given in (20). Indeed, $U_i(w_i)$ stands for the uncoupled term which is related to $L_i(w_i)$, and F_i stands for the coupled term $D_i(w_{i-1}, w_i, w_{i+1}) - L(w_i)$. In view of equations (18) and (25), one can obtain $U_i(w_i)$ as

$$U_i(w_i)=\frac{1}{2}\Big\{D\Big(w_{i,x^{(4)}}^2+4w_{i,x^{(3)}y}^2+6w_{i,x^{(2)}y^{(2)}}^2+4w_{i,xy^{(3)}}^2+w_{i,y^{(4)}}^2\Big)+$$
$$+\frac{Eh}{R_i^2}w_{i,x^{(2)}}^2+N_{xi}\Big[w_{i,x^{(3)}}^2+2w_{i,x^{(2)}y}^2+w_{i,xy^{(2)}}^2+$$
$$+\eta^2\Big(w_{i,x^{(4)}}^2+3w_{i,x^{(3)}y}^2+3w_{i,x^{(2)}y^{(2)}}^2+w_{i,xy^{(3)}}^2\Big)\Big]+$$
$$+N_{yi}\Big[w_{i,y^{(3)}}^2+2w_{i,xy^{(2)}}^2+w_{i,x^{(2)}y}^2+$$
$$+\eta^2\Big(w_{i,y^{(4)}}^2+3w_{i,xy^{(3)}}^2+3w_{i,x^{(2)}y^{(2)}}^2+w_{i,x^{(3)}y}^2\Big)\Big]+ \quad (26)$$
$$-N_{xyi}\frac{\partial^2}{\partial x\partial y}\Big[w_{i,x^{(2)}}^2+2w_{i,xy}^2+w_{i,y^{(2)}}^2+$$
$$+\eta^2\Big(w_{i,x^{(3)}}^2+3w_{i,x^{(2)}y}^2+3w_{i,xy^{(2)}}^2+w_{i,y^{(3)}}^2\Big)\Big]$$
$$+\delta_{in}k_W\Big[w_{n,xx}^2+2w_{n,xy}^2+w_{n,yy}^2+$$
$$+\eta^2\Big(w_{n,x^{(3)}}^2+3w_{n,x^{(2)}y}^2+3w_{n,xy^{(2)}}^2+w_{n,y^{(3)}}^2\Big)\Big]\Big\}$$

where comma in $w_{i,x^{(\ell)}y^{(k)}}$ denotes the partial differentiation, ℓ times with respect to x and k times with respect to y. By taking variation of the trial-functional V with respect to the deflection function w_i for each nanotube should give the corresponding Euler-Lagrange equations (here, the governing differential equations (12)-(14)). So that, using the Eq. (25), it can written

$$D_1(w_1,w_2)=L_1(w_i)+\sum_{j=1}^{2}\frac{\delta F_j}{\delta w_1}=0, \quad (27)$$

$$D_i(w_{i-1},w_i,w_{i+1})=L(w_i)+\sum_{j=i-1}^{i+1}\frac{\delta F_j}{\delta w_i}=0;\quad i=2,\ldots,n-1, \quad (28)$$

$$D_n(w_{n-1},w_n)=L_n(w_n)+\sum_{j=n-1}^{n}\frac{\delta F_j}{\delta w_n}=0 \quad (29)$$

where, $\delta F_j/\delta w_i$ is defined as

$$\frac{\delta F_j}{\delta w_i}=\sum_{0\le\ell,k}\frac{(-\partial)^{\ell+K}}{\partial x^\ell\partial y^k}\left(\frac{\partial F_j}{\partial w_{i,x^{(\ell)}y^{(k)}}}\right) \quad (30)$$

where F_j are still unknown functions, which will be determined later. For obtaining $\delta F_j/\delta w_i$ appeared in Eqs. (27)-(29), using Eq. (15)-(17) we arrive at

$$\sum_{j=1}^{2}\frac{\delta F_j}{\delta w_1}=-(1-\eta^2\nabla^2)\nabla^4\left[c_{12}(w_1-w_2)\right], \quad (31)$$

$$\sum_{j=i-1}^{i+1}\frac{\delta F_j}{\delta w_i}=-(1-\eta^2\nabla^2)\nabla^4$$
$$\left[c_{i(i-1)}(w_i-w_{i-1})+c_{i(i+1)}(w_i-w_{i+1})\right];\quad i=2,\ldots,n-1, \quad (32)$$

$$\sum_{j=1}^{2}\frac{\delta F_j}{\delta w_n}=-(1-\eta^2\nabla^2)\nabla^4\left[c_{n(n-1)}(w_n-w_{n-1})\right]. \quad (33)$$

The summations in Eqs. (31)-(33) can be expanded to give

$$\frac{\delta F_1}{\delta w_1}+\frac{\delta F_2}{\delta w_1}=-c_{12}\left(\frac{\partial^4}{\partial x^4}+2\frac{\partial^4}{\partial x^2\partial y^2}+\frac{\partial^4}{\partial y^4}\right)(w_1-w_2)$$
$$+c_{12}\eta^2\left(\frac{\partial^6}{\partial x^6}+3\frac{\partial^6}{\partial x^4\partial y^2}+3\frac{\partial^6}{\partial x^2\partial y^4}+\frac{\partial^6}{\partial y^6}\right)(w_1-w_2), \quad (34)$$

$$\frac{\delta F_{i-1}}{\delta w_i}+\frac{\delta F_i}{\delta w_i}+\frac{\delta F_{i+1}}{\delta w_i}=$$
$$-c_{i(i-1)}\left(\frac{\partial^4}{\partial x^4}+2\frac{\partial^4}{\partial x^2\partial y^2}+\frac{\partial^4}{\partial y^4}\right)(w_i-w_{i-1})$$
$$+c_{i(i-1)}\eta^2\left(\frac{\partial^6}{\partial x^6}+3\frac{\partial^6}{\partial x^4\partial y^2}+3\frac{\partial^6}{\partial x^2\partial y^4}+\frac{\partial^6}{\partial y^6}\right)(w_i-w_{i-1}) \quad (35)$$
$$-c_{i(i+1)}\left(\frac{\partial^4}{\partial x^4}+2\frac{\partial^4}{\partial x^2\partial y^2}+\frac{\partial^4}{\partial y^4}\right)(w_i-w_{i+1})$$
$$+c_{i(i+1)}\eta^2\left(\frac{\partial^6}{\partial x^6}+3\frac{\partial^6}{\partial x^4\partial y^2}+3\frac{\partial^6}{\partial x^2\partial y^4}+\frac{\partial^6}{\partial y^6}\right)(w_i-w_{i+1}),$$

$$\frac{\delta F_{n-1}}{\delta w_n}+\frac{\delta F_n}{\delta w_n}=-c_{n(n-1)}\left(\frac{\partial^4}{\partial x^4}+2\frac{\partial^4}{\partial x^2\partial y^2}+\frac{\partial^4}{\partial y^4}\right)(w_n-w_{n-1})$$
$$+c_{n(n-1)}\eta^2\left(\frac{\partial^6}{\partial x^6}+3\frac{\partial^6}{\partial x^4\partial y^2}+3\frac{\partial^6}{\partial x^2\partial y^4}+\frac{\partial^6}{\partial y^6}\right)(w_n-w_{n-1}) \quad (36)$$

According to the definition of $\delta F_j/\delta w_i$ in Eq. (30) and the obtained results in (34)-(36), one can derive the unknown functions F_i in the trial-functional V as follows:

$$F_1(w_1,w_2)=-\frac{1}{4}c_{12}\Big[\big(w_{1,xx}-w_{2,xx}\big)^2+\big(w_{1,yy}-w_{2,yy}\big)^2+$$
$$+2\big(w_{1,xy}-w_{2,xy}\big)^2\Big]+\frac{1}{4}c_{12}\eta^2\Big[\big(w_{1,x^{(3)}}-w_{2,x^{(3)}}\big)^2+ \quad (37)$$
$$\big(w_{1,y^{(3)}}-w_{2,y^{(3)}}\big)^2+3\big(w_{1,x^{(2)}y}-w_{2,x^{(2)}y}\big)^2+3\big(w_{1,xy^{(2)}}-w_{2,xy^{(2)}}\big)^2\Big],$$

$$F_i(w_{i-1},w_i,w_{i+1})=-\frac{1}{4}c_{i(i-1)}\Big[\big(w_{i,xx}-w_{i-1,xx}\big)^2+$$
$$\big(w_{i,yy}-w_{i-1,yy}\big)^2+2\big(w_{i,xy}-w_{i-1,xy}\big)^2\Big]+$$
$$+\frac{1}{4}c_{i(i-1)}\eta^2\Big[\big(w_{i,x^{(3)}}-w_{i-1,x^{(3)}}\big)^2+\big(w_{i,y^{(3)}}-w_{i-1,y^{(3)}}\big)^2+$$
$$+3\big(w_{i,x^{(2)}y}-w_{i-1,x^{(2)}y}\big)^2+3\big(w_{i,xy^{(2)}}-w_{i-1,xy^{(2)}}\big)^2\Big]$$
$$-\frac{1}{4}c_{i(i+1)}\Big[\big(w_{i,xx}-w_{i+1,xx}\big)^2+\big(w_{i,yy}-w_{i+1,yy}\big)^2+ \quad (38)$$
$$2\big(w_{i,xy}-w_{i+1,xy}\big)^2\Big]+$$
$$+\frac{1}{4}c_{i(i+1)}\eta^2\Big[\big(w_{i,x^{(3)}}-w_{i+1,x^{(3)}}\big)^2+\big(w_{i,y^{(3)}}-w_{i+1,y^{(3)}}\big)^2+$$
$$+3\big(w_{i,x^{(2)}y}-w_{i+1,x^{(2)}y}\big)^2+3\big(w_{i,xy^{(2)}}-w_{i+1,xy^{(2)}}\big)^2\Big],$$

$$F_n(w_{n-1},w_n)=-\frac{1}{4}c_{n(n-1)}\Big[\left(w_{n,xx}-w_{n-1,xx}\right)^2+$$
$$+\left(w_{n,yy}-w_{n-1,yy}\right)^2+2\left(w_{n,xy}-w_{n-1,xy}\right)^2\Big]+$$
$$+\frac{1}{4}c_{n(n-1)}\eta^2\Big[\left(w_{n,x^{(3)}}-w_{n-1,x^{(3)}}\right)^2+\left(w_{n,y^{(3)}}-w_{n-1,y^{(3)}}\right)^2+ \tag{39}$$
$$+3\left(w_{1x^{(2)}y}-w_{2x^{(2)}y}\right)^2+3\left(w_{n,xy^{(2)}}-w_{n-1,xy^{(2)}}\right)^2\Big]$$

Now with U_i and F_i in hands, the trial functional V which is previously suggested in Eq. (20) can be fully determined.

3. Stability analysis of MWCNT

In this section, the method of determining the critical axial load and torsional moment for the onset of instability of the MWCNT is represented.

3.1 Axial buckling

In axial loading of multi-walled carbon nanotube, only the axial component σ_x of stress tensor is nonzero. Therefore, the corresponding resultant forces in the ith layer can be given as

$$N_{xi}=-\sigma_x h,\quad N_{yi}=0,\quad N_{xyi}=0\,. \tag{40}$$

By applying the Rayleigh's principle [18,21], one can determine the critical axial stress σ_x^{cr} as

$$\sigma_x^{cr}=\min_{w_i}\frac{\sum_{i=1}^{n}\int_{\Omega_i}\left[G_i(w_i)+F_i(w_i)\right]d\Omega_i+\int_{\Omega_n}H(w_n)d\Omega_n}{h\sum_{i=1}^{n}\int_{\Omega_i}J_i^{Axial}(w_i)d\Omega_i} \tag{41}$$

where $G_i(w_i)$, $H(w_n)$ and $J_i^{Axial}(w_i)$ are defined as

$$G_i(w_i)=D\Big(w_{i,x^{(4)}}^2+4w_{i,x^{(3)}y}^2+6w_{i,x^{(2)}y^{(2)}}^2+$$
$$+4w_{i,xy^{(3)}}^2+w_{i,y^{(4)}}^2\Big)+\frac{Eh}{R_i^2}w_{i,x^{(2)}}^2\,, \tag{42}$$

$$H(w_n)=k_W\Big[w_{n,xx}^2+2w_{n,xy}^2+w_{n,yy}^2+$$
$$+\eta^2\left(w_{n,x^{(3)}}^2+3w_{n,x^{(2)}y}^2+3w_{n,xy^{(2)}}^2+w_{n,y^{(3)}}^2\right), \tag{43}$$

$$J_i^{Axial}(w_i)=w_{i,x^{(3)}}^2+2w_{i,x^{(2)}y}^2+w_{i,xy^{(2)}}^2$$
$$+\eta^2\left(w_{i,x^{(4)}}^2+3w_{i,x^{(3)}y}^2+3w_{i,x^{(2)}y^{(2)}}^2+w_{i,xy^{(3)}}^2\right) \tag{44}$$

Thus, the axial buckling load $P_x^{Buckling}$ can be calculated as

$$P_x^{Buckling}=\sigma_x^{Buckling}\left(2\pi h\sum_{i=1}^{n}R_i\right). \tag{45}$$

3.2 Torsional buckling

When the multi-walled carbon nanotube are subjected to the torsional moment T_x, only the shearing component σ_{xy} of the stress tensor is nonzero. Therefore, the corresponding resultant forces in the ith layer (by assuming the equal shearing stress in all layers) can be given as

$$N_{xi}=0,\quad N_{yi}=0,\quad N_{xyi}=h\sigma_{xyi}=h\sigma_{xy}=\frac{T_x}{2\pi\sum_{i=1}^{n}R_i^2}. \tag{46}$$

Similar to the approach used for determining the axial buckling load, the critical shearing stress σ_{xy}^{cr} for the onset of instability of MWCNT can be determined by applying Rayleigh's principle [18,21] as

$$\sigma_{xy}^{cr}=\min_{w_i}\frac{\sum_{i=1}^{n}\int_{\Omega_i}\left[F_i(w_i)+G_i(w_i)\right]d\Omega_i+\int_{\Omega_n}H(w_n)d\Omega_n}{h\sum_{i=1}^{n}\int_{\Omega_i}J_i^{Torsional}(w_i)d\Omega_i} \tag{47}$$

where $G_i(w_i)$ and $H(w_n)$ was previously defined in Eqs. (42)-(43), and $J_i^{Torsional}(w_i)$ is defined as

$$J_i^{Torsional}(w_i)=\frac{\partial^2}{\partial x\partial y}\Big[w_{i,x^{(2)}}^2+2w_{i,xy}^2+w_{i,y^{(2)}}^2+$$
$$+\eta^2\left(w_{i,x^{(3)}}^2+3w_{i,x^{(2)}y}^2+3w_{i,xy^{(2)}}^2+w_{i,y^{(3)}}^2\right)\Big] \tag{48}$$

Hence, the torsional critical moment $T_x^{Bucling}$ is given as

$$T_x^{Buckling}=\sigma_{xy}^{Buckling}\left(2\pi h\sum_{i=1}^{n}R_i\right). \tag{49}$$

One can use the numerical methods such as Galerkin or Ritz method to minimize the function given in (41) and (47) to calculate the critical axial load and critical torsional moment.

4. Boundary conditions

Deriving the BCs for a complicated coupled system of differential equations such as given in Eqs. (12)-(14) seems quite difficult. This is why the He's semi-inverse method [19,20] has been used to obtain the functional V, then to obtain the essential and natural BCs more smoothly.

According to the Donnell's nonlocal elastic equations given in (13) one can see that each equation is a PDE of degree 8, then it's necessary to obtain $8n$ BCs for the coupled PDEs given in (12)-(14). One can take variations of functional V with respect to w_i to arrive at the Euler-Lagrange equations (here, Donnell's nonlocal equilibrium Eqs. (13)), and also the natural and essential BCs for the multi-walled carbon nanotube as [18]

$$\delta_{w_1} V = \delta_{w_1} V_1 + \delta_{w_1} V_2 = \int_{\Omega_1} D_1(w_1, w_2)\delta w_1 d\Omega_1 + \partial\Xi_1\big|_\Gamma = 0, \tag{50}$$

$$\delta_{w_i} V = \delta_{w_i} V_{i-1} + \delta_{w_i} V_i + \delta_{w_i} V_{i+1} = \int_{\Omega_i} D_i(w_{i-1}, w_i, w_{i+1})\delta w_i d\Omega_i + \partial\Xi_i\big|_\Gamma = 0, \tag{51}$$

$$\delta_{w_n} V = \delta_{w_n} V_{n-1} + \delta_{w_n} V_n = \int_{\Omega_n} D_n(w_{n-1}, w_n)\delta w_n d\Omega_n + \partial\Xi_n\big|_\Gamma = 0 \tag{52}$$

where $\partial\Xi_i\big|_\Gamma$ denotes the BCs applied or existed on boundary Γ and $\delta_{w_i} V_j$ is defined as

$$\delta_{w_i} V_j = \sum_{\ell,k} \frac{\partial^{(\ell+k)} V_j}{\partial w_{i,x^{(\ell)}y^{(k)}}} \delta w_{i,x^{(\ell)}y^{(k)}} \tag{53}$$

Here, the 8 BCs on each layer of MWCNT are given for the case of axial loadings. The essential BCs can be derived uniquely, But no one can propose a general form of natural BCs applied or existed on the boundary of MWCNT. Here one of the more common and more probable BCs are given as

$$\begin{aligned}
&\Big\{D\left(w_{i,x^{(7)}} + 4w_{i,x^{(5)}y^{(2)}} + 3w_{i,x^{(3)}y^{(4)}}\right) + \frac{Eh}{R_i^2} w_{i,x^{(3)}} \\
&-\sigma_x h\left[w_{i,x^{(5)}} + w_{i,x^{(3)}y^{(2)}} - \eta^2\left(w_{i,x^{(7)}} + 3w_{i,x^{(5)}y^{(2)}}\right)\right] \\
&-\left(c_{i(i-1)} + c_{i(i+1)} - \delta_{in}k_W\right)\Big[w_{i,x^3} + w_{i,xy^{(2)}} + \\
&-\eta^2\left(w_{i,x^{(5)}} + 3w_{i,x^{(3)}y^{(2)}}\right)\Big] + c_{i(i-1)}\Big[w_{i-1,x^{(3)}} + w_{i-1,xy^{(2)}} \\
&-\eta^2\left(w_{i-1,x^{(5)}} + 3w_{i-1,x^{(3)}y^{(2)}}\right)\Big] + c_{i(i+1)}\Big[w_{i+1,x^{(3)}} + w_{i+1,xy^{(2)}} \\
&-\eta^2\left(w_{i+1,x^{(5)}} + 3w_{i+1,x^{(3)}y^{(2)}}\right)\Big]\Big\}\Big|_{x=0}^{x=L} = 0,
\end{aligned} \tag{54.a}$$

or

$$\delta w_i\big|_{x=0} = 0, \quad \delta w_i\big|_{x=L} = 0; \tag{54.b}$$

$$\begin{aligned}
&\Big\{D\left(w_{i,x^{(6)}} + 4w_{i,x^{(4)}y^{(2)}} + 3w_{i,x^{(2)}y^{(4)}}\right) + \frac{Eh}{R_i^2} w_{i,x^{(2)}} \\
&-\sigma_x h\left[w_{i,x^{(4)}} + w_{i,x^{(2)}y^{(2)}} - \eta^2\left(w_{i,x^{(6)}} + 3w_{i,x^{(4)}y^{(2)}}\right)\right] \\
&-\left(c_{i(i-1)} + c_{i(i+1)} - \delta_{in}k_W\right)\Big[w_{i,x^{(2)}} + w_{i,y^{(2)}} + \\
&-\eta^2\left(w_{i,x^{(4)}} + 3w_{i,x^{(2)}y^{(2)}}\right)\Big] + c_{i(i-1)}\Big[w_{i-1,x^{(2)}} + \\
&-\eta^2\left(w_{i-1,x^{(4)}} + 3w_{i-1,x^{(2)}y^{(2)}}\right)\Big] + c_{i(i+1)}\Big[w_{i+1,x^{(2)}} + \\
&+w_{i+1,y^{(2)}} - \eta^2\left(w_{i+1,x^{(4)}} + 3w_{i+1,x^{(2)}y^{(2)}}\right)\Big]\Big\}\Big|_{x=0}^{x=L} = 0;
\end{aligned} \tag{55.a}$$

or

$$\delta w_{i,x}\big|_{x=0} = 0, \quad \delta w_{i,x}\big|_{x=L}; \tag{55.b}$$

$$\begin{aligned}
&\Big\{D\left[w_{i,x^{(5)}} + 4w_{i,x^{(3)}y^{(2)}}\right] \\
&-\sigma_x h\left[w_{i,x^{(3)}} - \eta^2\left(w_{i,x^{(5)}} + 3w_{i,x^{(3)}y^{(2)}}\right)\right] \\
&+\left(c_{i(i-1)} + c_{i(i+1)} - \delta_{in}k_W\right)\eta^2 w_{i,x^{(3)}} \\
&-c_{i(i-1)}\eta^2 w_{i-1,x^{(3)}} - c_{i(i+1)}\eta^2 w_{i+1,x^{(3)}}\Big\}\Big|_{x=0}^{x=L} = 0,
\end{aligned} \tag{56.a}$$

or

$$\delta w_{i,x^{(2)}}\big|_{x=0} = 0, \quad \delta w_{i,x^{(2)}}\big|_{x=L} = 0; \tag{56.b}$$

$$\left\{D w_{i,x^{(4)}} + \sigma_x h\eta^2 w_{i,x^{(4)}}\right\}\Big|_{x=0}^{x=L} = 0, \tag{57.a}$$

or

$$\delta w_{i,x^{(3)}}\Big|_{x=0}^{x=L} = 0; \tag{57.b}$$

$$\begin{aligned}
&\Big\{D\left(w_{i,y^{(7)}} + 4w_{i,x^{(2)}y^{(5)}} + 3w_{i,x^{(4)}y^{(3)}}\right) \\
&-\sigma_x h\left[w_{i,x^{(4)}y} + w_{i,x^{(2)}y^{(3)}} - \eta^2\left(w_{i,x^{(2)}y^{(5)}} + 3w_{i,x^{(4)}y^{(3)}}\right)\right] \\
&-\left(c_{i(i-1)} + c_{i(i+1)} - \delta_{in}k_W\right)\Big[w_{i,y^{(3)}} + w_{i,x^{(2)}y} + \\
&-\eta^2\left(w_{i,y^{(5)}} + 3w_{i,x^{(2)}y^{(3)}}\right)\Big] + c_{i(i-1)}\Big[w_{i-1,y^{(3)}} + w_{i-1,x^{(2)}y} \\
&-\eta^2\left(w_{i-1,y^{(5)}} + 3w_{i-1,x^{(2)}y^{(3)}}\right)\Big] + c_{i(i+1)}\Big[w_{i+1,y^{(3)}} + w_{i+1,x^{(2)}y} = 0, \\
&-\eta^2\left(w_{i+1,y^{(5)}} + 3w_{i+1,x^{(2)}y^{(3)}}\right)\Big]\Big|_{y=0}^{y=2\pi R_i} = 0;
\end{aligned} \tag{58.a}$$

or

$$\delta w_i\big|_{y=0} = 0, \quad \delta w_i\big|_{y=2\pi R_i}; \tag{58.b}$$

$$\begin{aligned}
&\Big\{D\left(w_{i,y^{(6)}} + 3w_{i,x^{(4)}y^{(2)}} + 4w_{i,x^{(2)}y^{(4)}}\right) \\
&-\sigma_x h\left[w_{i,x^{(2)}y^{(2)}} - \eta^2\left(w_{i,x^{(2)}y^{(4)}} + 3w_{i,x^{(4)}y^{(2)}}\right)\right] \\
&-\left(c_{i(i-1)} + c_{i(i+1)} - \delta_{in}k_W\right)\left[w_{i,y^{(2)}} - \eta^2\left(w_{i,y^{(4)}} + 3w_{i,x^{(2)}y^{(2)}}\right)\right] \\
&+c_{i(i-1)}\left[w_{i-1,y^{(2)}} - \eta^2\left(w_{i-1,y^{(4)}} + 3w_{i-1,x^{(2)}y^{(2)}}\right)\right] \\
&+c_{i(i+1)}\left[w_{i+1,y^{(2)}} - \eta^2\left(w_{i+1,y^{(4)}} + 3w_{i+1,x^{(2)}y^{(2)}}\right)\right]\Big\}\Big|_{y=0}^{y=2\pi R_i} = 0,
\end{aligned} \tag{59.a}$$

or

$$\delta w_{i,y}\big|_{y=0} = 0, \quad \delta w_{i,y}\big|_{y=2\pi R_i} = 0; \tag{59.b}$$

$$\left\{D\left(w_{i,y^{(5)}}+4w_{i,x^{(2)}y^{(3)}}\right)+\sigma_x h\eta^2 w_{i,x^{(2)}y^{(3)}}\right.$$
$$+\left(c_{i(i-1)}+c_{i(i+1)}-\delta_{in}k_W\right)\eta^2 w_{i,y^{(3)}} \tag{60.a}$$
$$\left.-c_{i(i-1)}\eta^2 w_{i,y^{(3)}}-c_{i(i+1)}\eta^2 w_{i,y^{(3)}}\right\}\Big|_{y=0}^{y=2\pi R_i}=0,$$

or

$$\delta w_{i,y^{(2)}}\Big|_{y=0}=0,\quad \delta w_{i,y^{(2)}}\Big|_{y=2\pi R_i}=0; \tag{60.b}$$

$$\left\{Dw_{i,y^{(4)}}\right\}\Big|_{y=0}^{y=2\pi R_i}=0, \tag{61.a}$$

or

$$\delta w_{i,y^{(3)}}\Big|_{y=0}=0,\quad \delta w_{i,y^{(3)}}\Big|_{y=2\pi R_i}=0. \tag{61.b}$$

It's seen form Eqs. (54)-(61) that the natural boundary conditions are coupled, independent of value of the small scale parameter η. It is to be noted that by modeling the nanotube as an Euler-Bernoulli beam, the natural boundary conditions are uncoupled when $\eta=0$ as stated by Adali [18].

5. Conclusion

The small length scales of nano-structures may call the reasonability of application of classical continuum theories into ambiguity [14-16]. Hence, non-classic continuum theories such as the nonlocal elasticity theory have some merits to consider the small length scales [6-9], however in a macroscopic manner. In this paper, variational equations for multi-walled carbon nanotube based on Donnell's nonlocal elastic shell equilibrium equations [14] are derived. He's semi-inverse method [19,20] is applied to derive the variational functional. The formula for obtaining the buckling axial load and critical torsional is given by applying the Rayleigh's principle on the obtained functional V [18,21] (see Eqs. (41), (45), (47) and (49)). A set of essential and coupled natural boundary conditions (54)-(61) on each layer is derived. The obtained variational results can be used in the implementation of approximate and numerical methods such as the finite-element method in the analysis of the stability of multi-walled nanotubes.

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