Large deformation analysis for functionally graded carbon nanotube-reinforced composite plates using an efficient and simple refined theory

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Abstract. In this paper, the nonlinear cylindrical bending behavior of functionally graded nanocomposite plates reinforced by single-walled carbon nanotubes (SWCNTs) is studied using an efficient and simple refined theory. This theory is based on assumption that the in-plane and transverse displacements consist of bending and shear components in which the bending components do not contribute toward shear forces and, likewise, the shear components do not contribute toward bending moments. The material properties of SWCNTs are assumed to be temperature-dependent and are obtained from molecular dynamics simulations. The material properties of functionally graded carbon nanotube-reinforced composites (FG-CNTCRs) are assumed to be graded in the thickness direction, and are estimated through a micromechanical model. The fundamental equations for functionally graded nanocomposite plates are obtained using the Von-Karman theory for large deflections and the solution is obtained by minimization of the total potential energy. The numerical illustrations concern the nonlinear bending response of FG-CNTRC plates under different sets of thermal environmental conditions, from which results for uniformly distributed CNTRC plates are obtained as comparators.

Keywords: functionally graded materials; nanocomposites; nonlinear behavior; refined plate theory

1. Introduction

Carbon nanotubes (CNTs) have demonstrated exceptional mechanical, thermal and electrical properties, and are considered as one of the most promising reinforcement materials for high performance structural and multifunctional composites with tremendous application potentials (Thostenson *et al.* 2001, Esawi and Farag 2007). Since Ajayan *et al.* (1994) first studied polymer composites reinforced by aligned CNT arrays, many investigators (Cadek *et al.* 2002, Odegard *et al.* 2003, Thostenson and Chou 2003, Griebel and Hamaekers 2004, Mokashi *et al.* 2007) have examined material properties of carbon nanotube-reinforcement composites (CNTRC). Fidelus *et al.* (2005) investigated thermo-mechanical properties of epoxy based nanocomposites based on low weight fractions of randomly oriented single- and multi-walled CNTs. Hu et al. (2005)

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evaluated the macroscopic elastic properties of carbon nanotube-reinforced composites through analyzing the elastic deformation of a representative volume element under various loading conditions. Wuite and Adali (2005) presented a multi-scale analysis of the deflection and stress behavior of CNT reinforced polymer composite beams. The micromechanics models used in the study include straight CNTs aligned in one direction, randomly oriented CNTs and a two parameter model of agglomeration. Vodenitcharova and Zhang (2006) studied the pure bending and bending-induced local buckling of a nanocomposite beam reinforced by a singlewalled carbon nanotube. Recently, Salehi-Khojin and Jalili (2008) considered the buckling of boron nitride nanotube reinforced piezoelectric polymeric composites subjected to combined electro-thermomechanical loadings. Ray and Batra (2007) proposed a new 1-3 piezoelectric composite comprised of armchair SWCNTs embedded in a piezoceramic matrix for the active control of smart structures.

The traditional approach to fabricating nanocomposites implies that the nanotube is distributed either uniformly or randomly such that the resulting mechanical, thermal, or physical properties do not vary spatially at the macroscopic level. Functionally graded materials (FGMs) are a new generation of composite materials in which the microstructural details are spatially varied through nonuniform distribution of the reinforcement phase. They have found a wide range of applications in many industries (Suresh and Mortensen 1998). The static bending, elastic buckling, postbuckling, linear and nonlinear free vibration of FGM structures have been extensively investigated (Yang and Shen 2003, Benatta et al. 2008, Sallai et al. 2009, Na and Kim 2009, Wu et al. 2007, Ke et al. 2009, Yang and Chen 2008, Matsunaga 2009, Yang et al. 2003, Chen 2005). By using the concept of FGM, Shen (2009) suggested that the interfacial bonding strength can be improved through the use of a graded distribution of CNTs in the matrix and examined the nonlinear bending behavior of simply supported, functionally graded nanocomposite plates reinforced by SWCNTs subjected to a transverse uniform or sinusoidal load in thermal environments. Kaci et al. (2012) used the same methodology to study the nonlinear cylindrical bending of simply supported functionally graded nanocomposite plates reinforced by single-walled carbon nanotubes (SWCNTs). Also Shen and Zhang (2010) investigated the thermal buckling of composite plate reinforced by CNT (FG distribution). The obtained results of the paper shown that the FG distribution of CNTs causes critical buckling temperature to be higher than the UD distribution of CNTs. Shen (2011) investigated the buckling and postbuckling of nanocomposite plates with functionally graded nanotube reinforcements subjected to uniaxial compression in thermal environments. The effective material properties of the nanocomposite plates were derived by the use of extended rule of mixture. They found that the linear functionally graded nanoreinforcement has a quantitative effect on the uniaxial buckling load as well as postbuckling strength of the plates.

Recently, Tounsi and his co-workers (Benachour *et al.* 2011, Hadji *et al.* 2011) developed a new refined plate theory to investigate the free vibration and static bending of functionally graded plates. This theory which looks like higher-order theory uses only four unknown functions in order to derive four governing equations for functionally graded plates. The most interesting feature of this theory is that it does not require shear correction factor, and accounts for parabolic distribution of the transverse shear strains, and satisfies the zero traction boundary conditions on the surfaces of the plate without using shear correction factor.

Although several studies on the nonlinear bending of functionally graded plates have been carried out based on variety of plate theories, no studies can be found for the nonlinear bending of FG-CNTRC plates based on the refined plate theory (Benachour *et al.* 2011, Hadji *et al.* 2011).

Therefore, the aim of this study is to extend the refined plate theory (Benachour *et al.* 2011, Hadji *et al.* 2011) to the nonlinear cylindrical bending of FG-CNTRC plates subjected to a pressure loading. The material properties of the FG-CNTRC are assumed to be graded in the thickness direction and estimated though the rule of mixture in which the CNT efficiency parameter is determined by matching the elastic modulus of CNTRCs obtained from MD simulation with the numerical results calculated from the rule of mixture. The constitutive equations for rectangular FG-CNTRC plates were obtained using the Von-Karman theory for large deflections and the solution was obtained by minimization of the total potential energy. To illustrate the accuracy of the present theory, the obtained results are presented to show the influence of material properties, plate geometry and mechanical loading on the resulting transverse deflection and stress state. Also, the results show that the linear analysis yields wrong results not only quantitatively but also qualitatively.

2. Theoretical formulation

2.1 Material properties of functionally graded CNTRC plates

Fig. 1 shows the CNTRCs of thickness h where the distribution of CNTs is uniform across the thickness direction in Fig. 1(a) (UD-CNTRC) and is non-uniform and graded along the thickness direction in Fig. 1(b) (FG-CNTRC), respectively. It is assumed that the CNTRC is made from a mixture of SWCNT and an isotropic matrix. We first determine the effective material properties of CNTRC. It was pointed out by many investigators (Han and Elliott 2007, Zhang and Shen 2006a) that the material properties of the SWCNT and CNTRC are anisotropic. According to the rule of mixture, the effective Young's modulus, the shear modulus and the thermal expansion coefficient of CNTRC can be expressed as (Shen 2009, Kaci *et al.* 2012)

$$E_{11} = \eta_1 V_{CN} E_{11}^{CN} + V_m E^m \tag{1a}$$

$$\frac{\eta_2}{E_{22}} = \frac{V_{CN}}{E_{22}^{CN}} + \frac{V_m}{E^m}$$
(1b)

$$\frac{\eta_3}{G_{12}} = \frac{V_{CN}}{G_{12}^{CN}} + \frac{V_m}{G^m}$$
(1c)

$$\alpha_{11} = V_{CN} \alpha_{11}^{CN} + V_m \alpha^m \tag{1d}$$

$$\alpha_{22} = (1 + \nu_{12}^{CN})V_{CN}\alpha_{22}^{CN} + (1 + \nu^m)V_m\alpha^m - \nu_{12}\alpha_{11}$$
(1e)

where E_{11}^{CN} , E_{22}^{CN} , G_{12}^{CN} , α_{11}^{CN} and α_{22}^{CN} are the Young's modulus, shear modulus and thermal expansion coefficient, respectively, of the carbon nanotube, and E^m , G^m and α^m are corresponding properties for the matrix. v_{12}^{CN} and v^m are Poisson's ratios, respectively, of the carbon nanotube and matrix. To account for the scale-dependent material properties Eq. (1) includes η_i (j = 1, 2, 3) which is called the CNT efficiency parameter, and will be determined



Fig. 1 Geometry of carbon nanotube-reinforced composites: (a) UD-CNTRC; and (b) FG-CNTRC

later by matching the elastic modulus of CNTRCs observed from the MD simulation results with the numerical results obtained from the rule of mixture. V_{CN} and V_m are the carbon nanotube and matrix volume fractions and are related by

$$V_{CN} + V_m = 1 \tag{2a}$$

We assume the volume fraction V_{CN} follows as

$$V_{CN} = \left(1 - \frac{2z}{h}\right) V_{CN}^* \tag{2b}$$

in which

$$V_{CN}^{*} = \frac{W_{CN}}{W_{CN} + (\rho_{CN} / \rho_{m}) - (\rho_{CN} / \rho_{m})W_{CN}}$$
(2c)

where W_{CN} is the mass fraction of nanotube, and ρ_{CN} and ρ_m are the densities of carbon nanotube and matrix, respectively. In such a way, the two cases of uniformly distributed (UD), i.e., $V_{CN} = V_{CN}^*$, and functionally graded (FG) CNTRCs will have the same value of mass fraction of nanotube.

The Poisson's ratio is assumed to be uniformly distributed, i.e.

$$\nu_{12} = V_{CN}^* \nu_{12}^{CN} + V_m \nu^m \tag{2d}$$

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2.2 Displacement field and strains

The four variable refined plate theory used by Tounsi and his co-workers (Benachour *et al.* 2011, Hadji *et al.* 2011) accounts for quadratic variation of the transverse shear strains across the thickness of the plate, and satisfies the zero traction boundary conditions on the top and bottom surfaces of the plate. The displacement field of this theory in the case of the cylindrical bending problem is as follows

$$u(x, y, z) = u_0(x, y) - z \frac{\partial w_b}{\partial x} + z \left[\frac{1}{4} - \frac{5}{3} \left(\frac{z}{h} \right)^2 \right] \frac{\partial w_s}{\partial x}$$

$$v(x, y, z) = 0$$

$$w(x, y, z) = w_b(x, y) + w_s(x, y)$$
(3)

where u_0 is the mid-plane displacement of the plate in the x direction; w_b and w_s are the bending and shear components of transverse displacement, respectively.

The nonlinear von Karman strain-displacement relations are used as follows

$$\varepsilon_{x} = \varepsilon_{x}^{0} + z k_{x}^{b} + f(z) k_{x}^{s}$$

$$\gamma_{xz} = g(z) \gamma_{xz}^{s}$$

$$\varepsilon_{z} = 0$$
(4)

where

$$\mathcal{E}_{x}^{0} = \frac{\partial u_{0}}{\partial x} + \frac{1}{2} \left(\frac{\partial w_{b}}{\partial x} + \frac{\partial w_{s}}{\partial x} \right)^{2}, \quad k_{x}^{b} = -\frac{\partial^{2} w_{b}}{\partial x^{2}}, \quad k_{x}^{s} = -\frac{\partial^{2} w_{s}}{\partial x^{2}}$$

$$\mathcal{Y}_{xz}^{s} = \frac{\partial w_{s}}{\partial x}, \quad f(z) = -\frac{1}{4}z + \frac{5}{3}z \left(\frac{z}{h}\right)^{2} \quad \text{and} \quad g(z) = \frac{5}{4} - 5 \left(\frac{z}{h}\right)^{2}$$
(5)

2.3 Constitutive relations

The constitutive relations can be expressed as

$$\sigma_x = Q_{11} \left(\varepsilon_x - \alpha_{11} \Delta T \right), \quad \tau_{xz} = Q_{55} \gamma_{xz} \tag{6}$$

where $\Delta T = T - T_0$ is temperature rise from some reference temperature T_0 at which there are no thermal strains.

Using the material properties defined in Eq. (1), the stiffness coefficients, Q_{ij} , can be expressed as

$$Q_{11} = \frac{E_{11}}{1 - v_{12}v_{21}}, \quad Q_{55} = G_{12}$$
(7)

where E_{11} , G_{12} , v_{12} and v_{21} have their usual meanings, in particular for an CNTRC layer they are given in detail in Eqs. (1) and (2).

The stress and moment resultants of the FG-CNTRC plate can be obtained by integrating Eq. (6) over the thickness, and are written as

$$(N_x, M_x^b, M_x^s) = \int_{-h/2}^{h/2} \sigma_x(1, z, f(z)) dz$$
 (8a)

$$S_{xz}^{s} = \int_{-h/2}^{h/2} \tau_{xz} g(z) dz.$$
 (8b)

Substituting Eq. (6) into Eq. (8) and integrating through the thickness of the plate, the stress resultants are given as

$$\begin{cases} N_x \\ M_x^b \\ M_x^s \end{cases} = \begin{bmatrix} A_{11} & B_{11} & B_{11}^s \\ B_{11} & D_{11} & D_{11}^s \\ B_{11}^s & D_{11}^s & H_{11}^s \end{bmatrix} \begin{bmatrix} \varepsilon_x^0 \\ k_x^b \\ k_x^s \\ k_x^s \end{bmatrix}, \quad S_{xz}^s = A_{55}^s \gamma_{xz}$$
(9)

where A_{11} , B_{11} , etc., are the plate stiffness, defined by

$$\{A_{11}, B_{11}, D_{11}, E_{11}, F_{11}, H_{11}\} = \int_{-h/2}^{h/2} \{1, z, z^2, z^3, z^4, z^6\} Q_{11} dz$$

$$B_{11}^s = -\frac{1}{4} B_{11} + \frac{5}{3h^2} E_{11}$$

$$D_{11}^s = -\frac{1}{4} D_{11} + \frac{5}{3h^2} F_{11}$$

$$H_{11}^s = \frac{1}{16} D_{11} - \frac{5}{6h^2} F_{11} + \frac{25}{9h^4} H_{11}$$

$$\{A_{55}, D_{55}, F_{55}\} = \int_{-h/2}^{h/2} \{1, z^2, z^4\} Q_{55} dz$$

$$A_{55}^s = \frac{25}{16} A_{55} - \frac{25}{6h^2} D_{55} + \frac{25}{h^4} F_{55}$$

$$(10)$$

2.4 Solution procedure

The total potential energy (Π) of the FG-CNTRC plate is determined by summation of strain energy and the change in potential energy of the uniform externally applied pressure and is written as

$$\Pi = U + V \tag{11}$$

Here, V is the potential energy of a plate under uniform pressure, and is equal to

$$V = \int_{0}^{a} q(w_b + w_s) dx \tag{12}$$

where q is the uniformly distributed load and the integral limit a is the projected length of the FG-CNTRC plate. Also, the strain energy (U) is defined as

$$U = \frac{1}{2} \int_{0}^{a} \int_{-h/2}^{h/2} (\sigma_x \varepsilon_x + \tau_{xz} \gamma_{xz}) dx dz$$
(13)

Now considering the boundary condition for the simply supported FG-CNTRC plate, the principal of minimum potential energy is applied assuming a first guess solution for the considered displacements (i.e., u_0 , w_b and w_s) over the mid-surface of the plate as in Eq. (14).

$$u_0(0) = w_b(0) = w_s(0) = \frac{\partial w_s}{\partial x}(0) = 0$$
 (14a)

$$u_0(a) = w_b(a) = w_s(a) = \frac{\partial w_s}{\partial x}(a) = 0$$
(14b)

$$M_{x}^{b}(0) = M_{x}^{s}(0) = M_{x}^{b}(a) = M_{x}^{s}(a) = 0$$
(14c)

The required mentioned displacement and rotation fields, which satisfy the simply supported boundary conditions, are defined as in Eq. (15)

where C, W_0^b , and W_0^s are arbitrary parameters and are determined minimizing the total potential energy as given in Eq. (16)

$$\frac{\partial \Pi}{\partial (C, W_0^b, W_0^s)} = 0 \tag{16}$$

Eq. (14) provides a set of three nonlinear equilibrium equations in terms of C, W_0^b , and W_0^s which should be solved. The obtained constants are then used to calculate the displacements (Eq. (15)) and subsequently the strain and stresses are found using Eq. (4) and (6).

3. Numerical results and discussion

Numerical results are presented in this section for FG-CNTRC plates subjected to a transverse uniform load. We first need to determine the effective material properties of CNTRCs. Poly {(*m-phenylene*)-co-[(2.5-dioctoxy-p-phenylene) vinylene]}, referred to as PmPV, is selected for the matrix, and the material properties of which are assumed to be (Shen 2009) $v^m = 0.34$, $\alpha^m = 45(1+0.0005\Delta T) \times 10^{-6}$ /K and $E^m = (3.51-0.0047T)$ GPa, in which

 $T = T_0 + \Delta T$ and $T_0 = 300 \text{ K}$ (room temperature). In such a way, $\alpha^m = 45.0 \times 10^{-6} / \text{ K}$ and $E^m = 2.1 \text{ GPa}$ at $T_0 = 300 \text{ K}$. (10,10) SWCNTs are selected as reinforcements. It has been shown (Zhang and Shen 2006a, Elliott *et al.* 2004, Jin and Yuan 2003, Chang *et al.* 2005, Zhang and Shen 2006b) the material properties of SWCNTs are anisotropic, chirality-and size-dependent and temperature-dependent. Therefore, all effective elastic properties of a SWCNT need to be carefully determined, otherwise the results may be incorrect.

From MD simulation results the size-dependent and temperature-dependent material properties for armchair (10, 10) SWCNT can be obtained numerically (Shen 2009). Typical results are listed in Table 1. It is noted that the effective wall thickness obtained for (10, 10) – tube is h = 0.067 nm (Vodenitcharova and Zhang 2003), and the wide used value of 0.34 nm for tube wall thickness is thoroughly inappropriate to SWCNTs.

The key issue for successful application of the rule of mixture to CNTRCs is to determine the CNT efficiency parameter η_1 . For short fiber composites η_1 is usually taken to be 0.2 (Fukuda and Kawata 1974). However, there are no experiments conducted to determine the value of η_1 for CNTRCs. Recently, Shen (2009) gives an estimation of CNT efficiency parameter η_1 by matching the Young's moduli E_{11} of CNTRCs obtained by the rule of mixture to those from the MD simulations given by Han and Elliott (2007). Through comparison, we find that the Young's moduli obtained from the rule of mixture and MD simulations can match very well if the CNT efficiency parameters η_1 and η_2 are properly chosen, as shown in Table 2. It is clear that different value for the CNT efficiency parameter is possible due to different cases of nanotube volume fractions, and these values will be used in all the following examples. Note that there are no MD results for shear modulus G_{12} in (Han and Elliott 2007), we assume that $\eta_3 = \eta_2$.

It is assumed, unless otherwise stated, that L/h=10 (L=2a), T=300 K, $V_{CN}^*=0.11$. We also take the shear correction factor k=5/6 in first shear deformation plate theory (FSDPT).

The CNTRC plate is subjected to a uniform pressure under thermal environmental condition T = 300 K. Fig. 2 shows the central deflection of the FG- and UD- CNTRC plates as

Temperature (K)	E_{11}^{CN} (TPa)	E_{22}^{CN} (TPa)	G_{12}^{CN} (TPa)	$\alpha_{11}^{CN}(imes 10^{-6} /{ m K})$
300	5.6466	7.0800	1.9445	3.4584
500	5.5308	6.9348	1.9643	4.5361
700	5.4744	6.8641	1.9644	4.6677

Table 1 Temperature-dependent material properties for (10, 10) SWCNT (L = 9.26 nm; R = 0.68 nm; h = 0.067 nm; $v_{12}^{CN} = 0.175$)

Table 2 Comparisons of Young's moduli for PmPV/CNT composites reinforced by (10,10)-tube under T = 300 K

V_{CN}^{*}	MD (Han and Elliott 2007)		Rule of mixture				
	<i>E</i> ₁₁ (GPa)	<i>E</i> ₂₂ (GPa)	<i>E</i> ₁₁ (GPa)	η_1	<i>E</i> ₂₂ (GPa)	η_2	
0.11	94.8	2.2	94.57	0.149	2.2	0.934	
0.14	120.2	2.3	120.09	0.150	2.3	0.941	
0.17	145.6	3.5	145.08	0.149	3.5	1.381	



Fig. 2 Comparison of the central deflection for different theories versus load q



Fig. 3 Effects of nanotube volume fraction on the central deflection w_{max} of the CNTRC plate under uniform transverse load q and T = 300 K

a function of the load q. As it is seen, the results of the present theory show very good agreement with FSDPT both for FG- and UD- CNTRC plates. It can be found that the central deflection of FG-CNTRC plate is larger than those of the UD-CNTRC plate.

The load-deflection curve is presented in Fig. 3 for FG- and UD- CNTRC plates with different values of the nanotube volume fraction $V_{CN}^* = (0.11, 0.14 \text{ and } 0.17)$. It is worthy to note that these two types of plates have the same nanotube mass fraction $W_{CN} = 0.131, 0.165, \text{ and } 0.2$, respectively, by taking the density of carbon nanotube $\rho_{CN} = 1.4 \text{ g/cm}^3$ and the density of matrix $\rho_m = 1.15 \text{ g/cm}^3$ in Eq. (2c). It can be found that the central deflection of FG-CNTRC plate is

larger than those of the UD-CNTRC plate, and the plate has higher deflection when it has lower volume fraction.

Fig. 4 presents the variation of the central deflection of the FG- and UD- CNTRC plates with, for example, $V_{CN}^* = 0.11$ versus the transverse load q. It is seen for the maximum deflections greater than 10 h for FG-CNTRC and 5 h for UD-CNTRC a non-linear solution is required. Increasing the load magnitude causes the nonlinear deflection to be smaller than that of the linear analysis.



Fig. 4 Variation of the non-dimensional central deflection w_{max} of the CNTRC plate versus transverse load q with $V_{CN}^* = 0.11$ and T = 300 K



Fig. 5 Effects of plate length-to-thickness ratio L/h on the nonlinear bending behavior of CNTRC plates under transverse load q with $V_{CN}^* = 0.11$ and T = 300 K



Fig. 6 Effects of nanotube volume fraction on the mid-span axial stress σ_x of the FG-CNTRC plate subjected to q = 50 MPa and T = 300 K with L / h = 10

Fig. 5 presents the load-deflection curves for FG- and UD- CNTRC plates with different values of length-to-thickness ratio L/h (=10, 20 and 50) to show the transverse shear deformation effect on the nonlinear bending behavior of the plates. It can be seen that the moderately thick CNTRC plate (L/h = 10) has lowest central deflections. The results show that the central deflections are increased for both FG- and UD-CNTRC plates by increasing plate length-to-thickness ratio L/h.

Fig. 6 shows through the thickness distributions of the axial stress σ_x of the FG-CNTRC plate for different values of the nanotube volume fraction $V_{CN}^* = (0.11, 0.14, 0.17)$. The plate is subjected to a uniform pressure under thermal environmental condition T = 300 K. Under the application of the pressure loading, the stresses are compressive at the bottom surface and tensile at the top surface.

4. Conclusions

The nonlinear cylindrical bending behavior of functionally graded carbon nanotube-reinforced composite plates subjected to a transverse uniform load in thermal environments has been analyzed by using an efficient and simple refined plate theory. The material properties of FG-CNTRC are assumed to be graded in the thickness and estimated though the rule of mixture. The energy concept along with the present theory and the first-order shear deformation theories are used to predict the large deflection and through the thickness stress of FG-CNTRC plates. The accuracy and efficiency of the present theory have been demonstrated for nonlinear bending analysis of simply supported FG plates.

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