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Nonlinear vibration properties of a zigzag single-walled carbon nanotube embedded in a polymer matrix

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Abstract. In the current study, the nonlinear vibration properties of an embedded zigzag single-walled carbon nanotube (SWCNT) are investigated. Winkler-type model is used to simulate the interaction of the zigzag SWCNTs with a surrounding elastic medium. The relation between deflection amplitudes and resonant frequencies of the SWCNT is derived through harmonic balance method. The equivalent Young's modulus and shear modulus for zigzag SWCNT are derived using an energy-equivalent model. The amplitude – frequency curves for large-amplitude vibrations are graphically illustrated. The simulation results show that the chirality of zigzag carbon nanotube as well as surrounding elastic medium play more important roles in the nonlinear vibration of the single-walled carbon nanotubes.

Keywords: zigzag carbon nanotube; nonlinear vibration; harmonic balance method

1. Introduction

In the last few years, carbon nanotubes (CNTs) have attracted extensive research activities due to their exceptional mechanical, physical, chemical and thermal properties. CNTs were first discovered by Iijima (1991) in 1991. To make the full potential applications of CNTs, understanding their mechanical behavior is essential and has become a hot topic. In particular, considerable efforts have been devoted to understand the mechanical behavior of CNTs recently (Fu *et al*. 2006, Yoon *et al*. 2003, Amin *et al*. 2009, Mahdavi *et al*. 2009, Heireche *et al*. 2008a, b, c, Tounsi *et al*. 2008, Murmu and Adhikari 2011, Tounsi *et al*. 2013a, b, Pradhan and Mandal 2013).

During the past decade, several methods have been pursued to investigate and characterize the mechanical behavior of CNTs. Since experiment is difficult to conduct on nanoscale and

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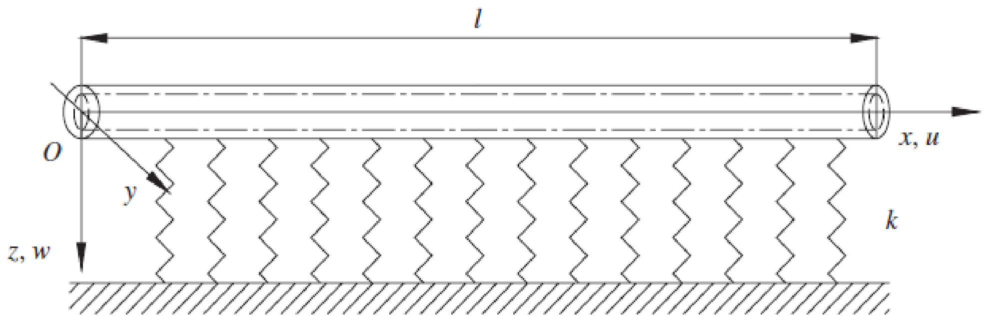

Fig. 1 Model of an embedded carbon nanotube

molecular dynamics simulation is not time-and cost-effective. Thus, elastic continuum modeling of nanostructures has become very important issue (Behfar *et al*. 2005, Popov *et al*. 2000, Sohi and Naghdabadi 2007, Sun and Liu 2008, Besseghier *et al*. 2011, Gafour *et al*. 2006). These studies, among others, have demonstrated the powerfulness of continuum mechanics, i.e., using simple formula offered by these continuum models, key parameters that affect the mechanical behavior of CNTs can be easily discovered to predict new physical phenomena. Most existing studies in literature are linear analysis on the vibrations of CNTs. However, there are much fewer studies on the nonlinear mechanical behavior of CNTs. Fu *et al*. (2006) investigated the nonlinear free vibration of embedded multi-walled CNTs considering inter-tube radial displacement and the related internal degrees of freedom. Xu *et al*. (2006) studied the vibration of a double-walled CNTs induced by nonlinear interlayer van der Waals (vdW) forces which were described as the nonlinear function of interlayer spacing. Nonlinear vibrations of nanotubes have been studied also in (Fu *et al*. 2006) in the case of a single nanotube and in (Fu *et al*. 2009) in the case of DWCNTs where geometric nonlinearity and simply supported boundary conditions were considered.

The literature lacks a comprehensive study on nonlinear free vibration of embedded CNTs with considering the chirality effect. The present work tries to fill this gap where the effect of chirality on the nonlinear vibration response of embedded zigzag CNTs is studied.

In this paper, based on the continuum mechanics and a single-elastic beam model, the nonlinear free vibration analysis of embedded zigzag CNT is investigated The novelty of this present work in contrast to Fu *et al*. (2006) is that the chirality of zigzag carbon nanotube is included in the theoretical formulation. The equivalent Young's modulus for zigzag SWCNT is derived using an energy-equivalent model (Wu *et al*. 2006, Zidour *et al*. 2012, Baghdadi *et al*. 2014, Semmah *et al*. 2014, Zidour *et al*. 2014, Benguediab *et al*. 2014, Naceri *et al*. 2011, Tokio, 1995). The obtained results in this work can provide useful guidance for the study and design of the next generation of nanodevices that make use of the thermal vibration properties of zigzag carbon nanotubes.

2. Basic equations

Consider a zigzag CNT of length L, Young's modulus E_z, density ρ, cross sectional area A, and cross-sectional inertia moment I, embedded in an elastic medium (as shown in Fig. 1) with constant k determined by the material constants of the surrounding medium. Assume that the displacement of zigzag CNT along x direction is $u(x, t)$, and the displacement along z direction is

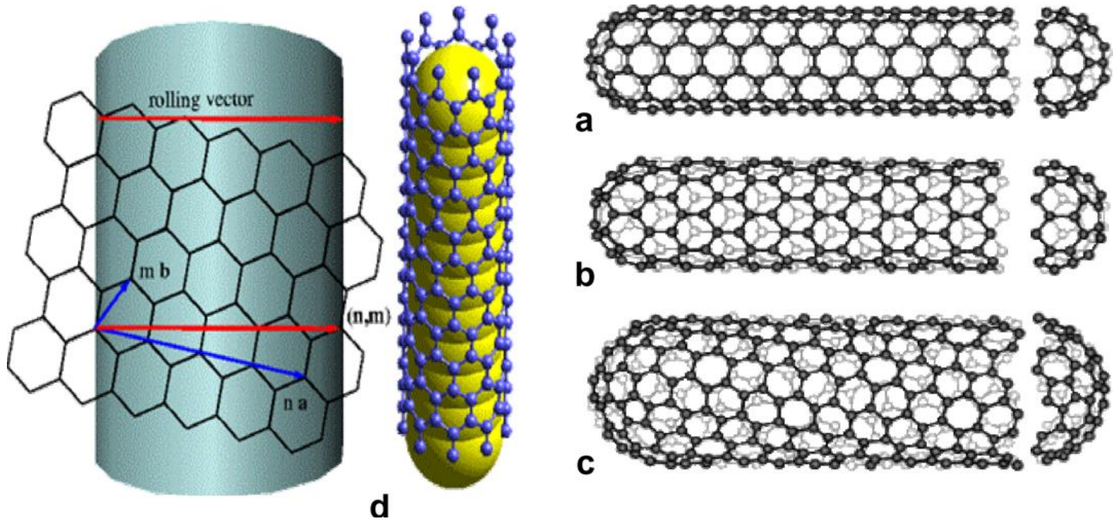

Fig. 2 (a) An armchair, (b) a zigzag and (c) a chiral nanotube and (d) a graphene being rolled into a cylinder

$w(x, t)$ in terms of the spatial coordinate x and the time variable t. The free vibration equation of embedded zigzag CNT considering the geometric nonlinearity of the structure is (Fu *et al*. 2006)

$$E_z I \frac{d^4 w}{dx^4} + \rho A \frac{d^2 w}{dt^2} + kw = \left[\frac{E_z A}{2L} \int_0^L \left(\frac{dw}{dx} \right)^2 dx \right] \frac{d^2 w}{dx^2} \tag{1}$$

where the equivalent Young's modulus of a zigzag CNT is expressed using an energy-equivalent model (Wu *et al*. 2011, Zidour *et al*. 2012) as follows

$$E_z = \frac{4\sqrt{3}KC}{9Ct_z + 4Ka_z^2 t_z (\lambda_{z1}^2 + 2\lambda_{z2}^2)}, \tag{2}$$

and K and C are the force constants. t_z is the thickness of the nanotube and the parameters λ_{z1} and λ_{z2} are given by

$$\lambda_{z1} = \frac{-3\sqrt{4 - 3\cos^2(\pi/2n)}\cos(\pi/2n)}{8\sqrt{3} - 2\sqrt{3}\cos^2(\pi/2n)}, \quad \lambda_{z2} = \frac{12 - 9\cos^2(\pi/2n)}{16\sqrt{3} - 4\sqrt{3}\cos^2(\pi/2n)}, \tag{3}$$

Fig. 2 shows the lattice indices of translation (n, m) along with the base vectors. The radius of the zigzag nanotube $(n, 0)$ in terms of the chiral vector components can be obtained from the relation (Wu *et al*. 2006)

$$R = \frac{na_z}{2\pi}\sqrt{3}, \tag{4}$$

where a_z is the length of the carbon–carbon bond which is $1.42A°$ and n is the index of translation, which decide the structure around the circumference.

For a simply supported nanotube at the two ends, the deflection $w(x, t)$ may be given as

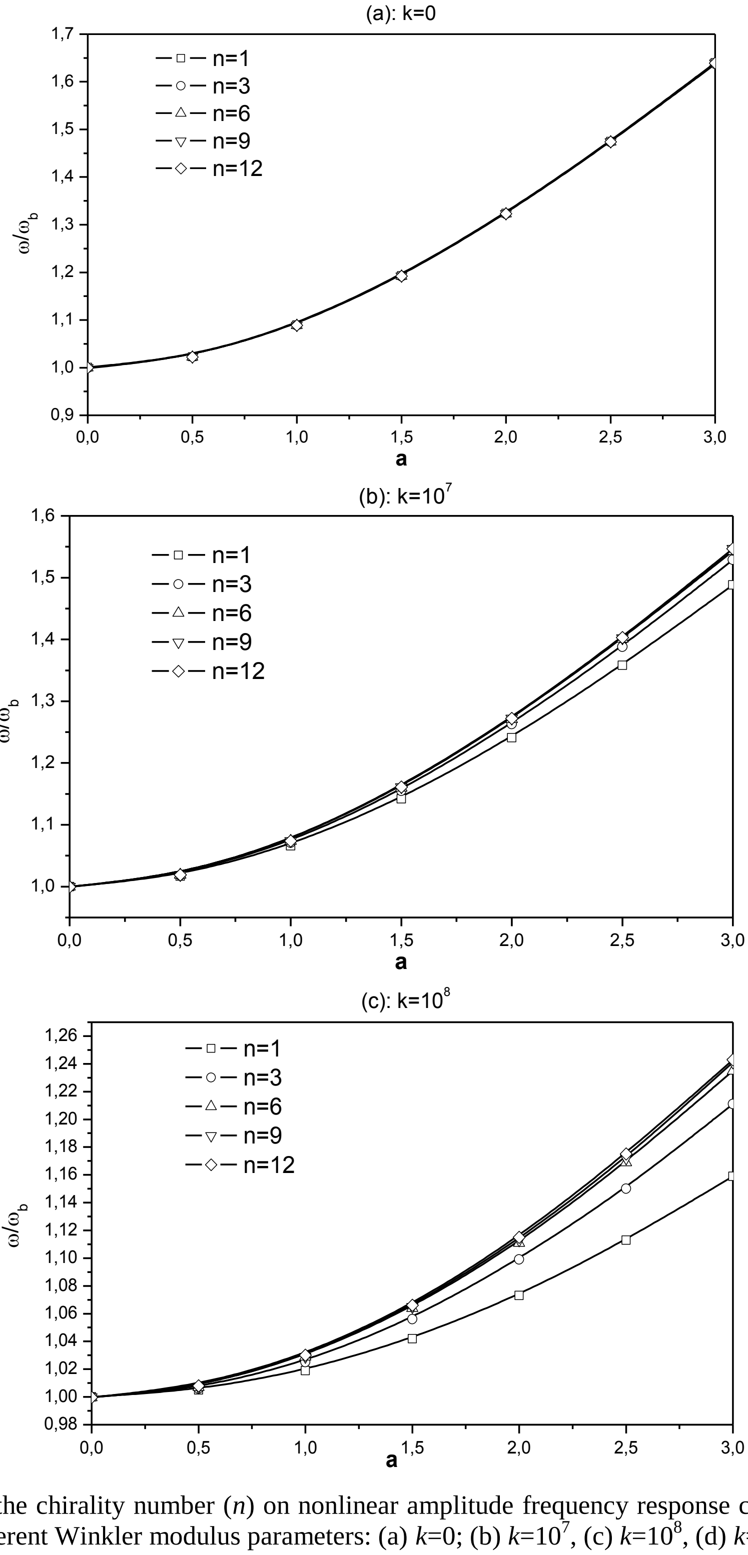

Fig. 3 Effect of the chirality number (*n*) on nonlinear amplitude frequency response curves of zigzag SWCNT for different Winkler modulus parameters: (a) k=0; (b) k=10^7, (c) k=10^8, (d) k=10^9

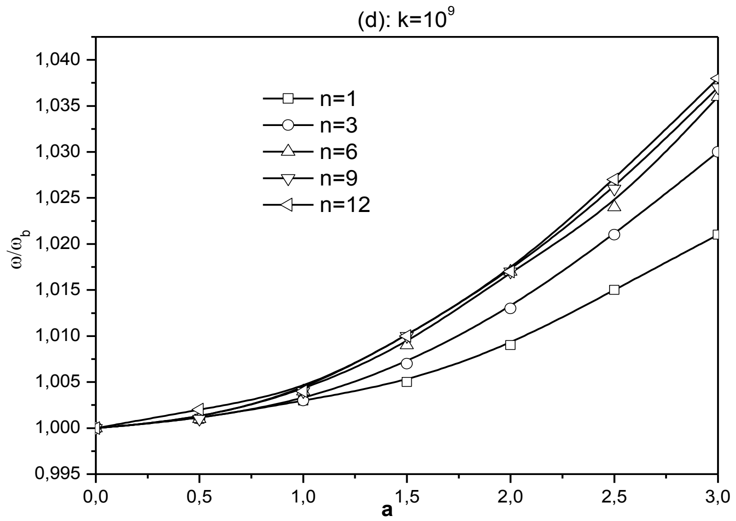

Fig. 3 Continued

$$w(x,t) = W(t)\sin\frac{\pi x}{L} \tag{5}$$

By substituting Eq. (5) into Eq. (1), the nonlinear differential equation for the time function $W(t)$ can be obtained as follows

$$\frac{d^2W}{dt^2} + \left[\frac{\pi^4 E_z I}{L^4 \rho A} + \frac{k}{\rho A}\right]W + \frac{\pi^4 E_z}{4L^4 \rho}W^3 = 0 \tag{6}$$

Introducing the dimensionless parameters

$$r = \sqrt{I/A}\,,\ a = W/r\,,\ \omega_l = \frac{\pi^2}{L^2}\sqrt{\frac{E_z I}{\rho A}}\,,\ \ \omega_k = \sqrt{\frac{k}{\rho A}}\,,\ \ \tau = \omega t\,, \tag{7}$$

By substituting Eq. (7) into Eq. (6), the dimensionless nonlinear vibration governing equation is given as

$$\left(\frac{\omega}{\omega_l}\right)^2 \frac{d^2 a}{d\tau^2} + \left[1 + \left(\frac{\omega_k}{\omega_l}\right)^2\right]a + \alpha\, a^3 = 0 \tag{8}$$

where α=0.25. Eq. (8) is the famous Duffing equation. The method of harmonic balance is adopted to find an analytical solution of good accuracy to the problem.

3. Numerical results and discussion

The material and geometric parameters considered here for a zigzag CNT are ρ=1300 kg/m^3

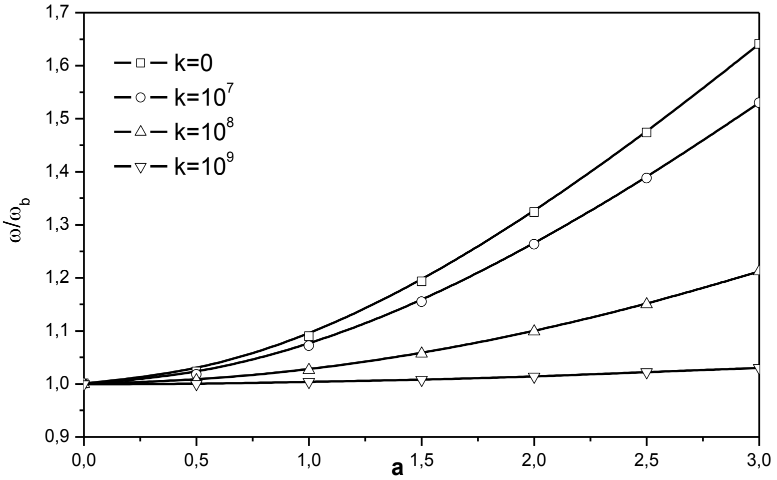

Fig. 4 Effect of the Winkler modulus parameters (k) on nonlinear amplitude frequency response curves of zigzag SWCNT with n=3

(Pantano *et al*. 2003), L=45 nm, the outside diameter is d_1=3 nm, the inside diameter is d_0=2.32 nm. The linear free vibration frequency is assumed to be ω_b in Eq. (8), and $\omega_b^2 = \omega_l^2 + \omega_k^2$.

The effect of the chirality number on the amplitude-frequency response curves for a zigzag SWCNT with different Winkler modulus parameters k are shown in Fig. 3. From the figure it is observed that there is significant influence of the chirality number on the amplitude-frequency response curves for an embedded zigzag SWCNT ($k \neq 0$). However, this effect is not obvious for a zigzag SWNT without a surrounding elastic medium (Fig. 3(a)). Further, it can be seen that the effect of the chirality number, is more significant for lower values of index of translation n and higher Winkler modulus parameters.

The effect of the Winkler modulus parameters k on the amplitude-frequency response curves of the zigzag SWCNT (n=3) are shown in Fig. 4. From the results illustrated in Fig. 4, it is noted that the Winkler modulus parameter k of surrounding elastic medium has a pronounced effect on the nonlinear amplitude frequency response curves of zigzag SWCNT. It can be also seen that the nonlinear free vibration frequency of nanotubes rises rapidly with the increment of the vibration amplitude when the stiffness of medium is relatively small (say $k<10^7$ N/m^2 (Yoon *et al*. 2003, Lanir and Fung 1972)), in which case the variation of spring constant k has little effect on the response curves of zigzag SWCNT. Thus, the effect of surrounding elastic medium can be neglected when the medium is flexible (such as a polymer medium).

4. Conclusions

In this article, the nonlinear vibration properties of embedded zigzag SWCNT are investigated on the basis of the continuum mechanics and the single-elastic beam model. Theoretical formulations include the Winkler modulus parameter and the chirality of zigzag SWCNT. According to this work, the results showed the dependence of the nonlinear vibration characteristics on the chirality of zigzag SWCNT and the surrounding elastic medium. The important conclusions that emerge from this paper can be summarized as follows:

• The nonlinear free vibration of zigzag SWCNT is influenced considerably by surrounding elastic medium.

• The nonlinear vibration characteristics are affected significantly by the chirality of zigzag SWCNT.

• The effect of the chirality of zigzag SWCNT on the amplitude frequency response curves is significantly felt when the stiffness of elastic medium becomes large enough.

The formulation lends itself particularly well to nanostructures studied with advanced shear deformation theories (Ould Larbi *et al*. 2013, Bouderba *et al*. 2013, Tounsi *et al*. 2013c, Bousahla *et al*. 2014, Khalfi *et al*. 2014, Fekrar *et al*. 2014, Ait Amar Meziane *et al*. 2014, Hebali *et al*. 2014, Belabed *et al*. 2014, Zidi *et al*. 2014, Al-Basyouni *et al*. 2015, Bourada *et al*. 2015), which will be considered in the near future.

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References

Ait Amar Meziane, M., Abdelaziz, H.H. and Tounsi, A. (2014), "An efficient and simple refined theory for buckling and free vibration of exponentially graded sandwich plates under various boundary conditions" *J. Sandw. Struct. Mater.*, **16**(3), 293-318.

Al-Basyouni, K.S., Tounsi, A. and Mahmoud, S.R. (2015), "Size dependent bending and vibration analysis of functionally graded micro beams based on modified couple stress theory and neutral surface position", *Compos. Struct.*, **125**, 621-630.

Amin, S.S., Dalir, H. and Farshidianfar, A. (2009), "Carbon nanotube-reinforced composites: frequency analysis theories based on the matrix stiffness", *Comput. Mech.*, **43**, 515-524.

Baghdadi, H., Tounsi, A., Zidour, M. and Benzair, A. (2014), "Thermal effect on vibration characteristics of armchair and zigzag single-walled carbon nanotubes using nonlocal parabolic beam theory", *Full. Nanotub. Carbon Nanostruct.*, **23**, 266-272.

Behfar, K. and Naghdabadi, R. (2005), "Nanoscale vibrational analysis of a multi-layered grapheme sheet embedded in an elastic medium", *Compos. Sci. Technol.*, **65**(7-8), 1159-1164.

Belabed, Z., Houari, M.S.A., Tounsi, A., Mahmoud, S.R. and Anwar Bég, O. (2014), "An efficient and simple higher order shear and normal deformation theory for functionally graded material (FGM) plates", *Compos. Part B*, **60**, 274-283.

Benguediab, S., Tounsi, A., Zidour, M. and Semmah, A. (2014), "Chirality and scale effects on mechanical buckling properties of zigzag double-walled carbon nanotubes", *Compos. Part B: Eng.*, **57**, 21-24.

Benzair, A., Tounsi, A., Besseghier, A., Heireche, H., Moulay, N. and Boumia, L. (2008), "The thermal effect on vibration of single-walled carbon nanotubes using nonlocal Timoshenko beam theory", *J. Phys. D: Appl. Phys.*, **41**(22), 225404.

Besseghier, A., Tounsi, A., Houari, M.S.A., Benzair, A., Boumia, L. and Heireche, H. (2011), "Thermal effect on wave propagation in double-walled carbon nanotubes embedded in a polymer matrix using nonlocal elasticity", *Physica E*, **43**, 1379-1386.

Bouderba, B., Houari, M.S.A. and Tounsi, A. (2013), "Thermomechanical bending response of FGM thick plates resting on Winkler-Pasternak elastic foundations", *Steel Compos. Struct.*, **14**, 85-104.

Bourada, M., Kaci, A., Houari, M.S.A. and Tounsi, A. (2015), “A new simple shear and normal deformations theory for functionally graded beams”, *Steel Compos. Struct.*, **18**(2), 409-423.
Bousahla, A.A., Houari, M.S.A., Tounsi, A. and Adda Bedia, E.A., (2014), “A novel higher order shear and normal deformation theory based on neutral surface position for bending analysis of advanced composite plates”, *Int. J. Comput. Meth.*, **11**(6), 1350082.
Fekrar, A., Houari, M.S.A., Tounsi, A. and Mahmoud, S.R. (2014), “A new five-unknown refined theory based on neutral surface position for bending analysis of exponential graded plates”, *Meccanica*, **49**, 795-810.
Fu, Y.M., Hong, J.W. and Wang, X.Q. (2006), “Analysis of nonlinear vibration for embedded carbon nanotubes”, *J. Sound Vib.*, **296**, 746-756.
Fu, Y.M., Bi, R.G. and Zhang, P. (2009), “Nonlinear dynamic instability of double-walled carbon nanotubes under periodic excitation”, *Acta Mech. Solid Sin.*, **22**(3), 206-212.
Gafour, Y., Zidour, M., Tounsi, A., Heireche, H. and Semmah, A. (2013), “Sound wave propagation in zigzag double-walled carbon nanotubes embedded in an elastic medium using nonlocal elasticity theory”, *Physica E*, **48**, 118-123.
Hebali, H., Tounsi, A., Houari, M.S.A., Bessaim, A. and Adda Bedia, E.A. (2014), “New quasi-3D hyperbolic shear deformation theory for the static and free vibration analysis of functionally graded plates”, *J. Eng. Mech.*, ASCE, **140**, 374-383.
Heireche, H, Tounsi, A, Benzair, A, Maachou, M. and Adda Bedia, EA. (2008a), “Sound wave propagation in single-walled carbon nanotubes using nonlocal elasticity”, *Physica E.*, **40**, 2791-2799.
Heireche, H., Tounsi, A., Benzair, A. and Mechab, I. (2008b), “Sound wave propagation in single-carbon nanotubes with initial axial stress”, *J. Appl. Phys.*, **104**, 014301.
Heireche, H., Tounsi, A. and Benzair, A. (2008c), “Scale eEffect on wave propagation of double–walled carbon nanotubes with initial axial loading”, *Nanotechnol.*, **19**, 185703.
Iijima, S. (1991), “Helica microtubes of graphitic carbon”, *Nature*, **354**, 56.
Khalfi, Y., Houari, M.S.A. and Tounsi, A. (2014), “A refined and simple shear deformation theory for thermal buckling of solar functionally graded plates on elastic foundation”, *Int. J. Comput. Meth.*, **11**(5), 135007.
Lanir, Y. and Fung, Y.C.B. (1972), “Fiber composite columns under compressions”, *J. Compos. Mater.*, **6**, 387-401.
Mahdavi, M.H., Jiang, L.Y. and Sun, X. (2009), “Nonlinear vibration of a single-walled carbon nanotube embedded in a polymer matrix aroused by interfacial van der Waals forces”, *J. Appl. Phys.*, **106**, 114309.
Murmu, T. and Adhikari, S. (2011), “Nonlocal vibration of carbon nanotubes with attached buckyballs at tip", *Mech. Res. Commun.*, **38**, 62.
Naceri, M., Zidour, M., Semmah, A., Houari, M.S.A., Benzair, A. and Tounsi, A. (2011), “Sound wave propagation in armchair single walled carbon nanotubes under thermal environment”, *J. Appl. Phys.*, **110**, 124322.
Ould Larbi, L., Kaci, A., Houari, M.S.A. and Tounsi, A. (2013), “An efficient shear deformation beam theory based on neutral surface position for bending and free vibration of functionally graded beams”, *Mech. Bas. Des. Struct. Mach.*, **41**, 421-433.
Pantano, A., Boyce, M.C. and Parks, D.M. (2003), “Nonlinear structural mechanics based modeling of carbon nanotube deformation”, *Phys. Rev. Lett.*, **91**(14), 145501.
Popov, V.N., Doren, V.E.V. and Balkanski, M. (2000), “Elastic properties of single-walled carbon nanotubes”, *Phys. Rev. B*, **61**(4), 3078-3084.
Pradhan, S.C. and Mandal, U. (2013), “Finite element analysis of CNTs based on nonlocal elasticity and Timoshenko beam theory including thermal effect”, *Physica E.*, **53**, 223-232.
Semmah, A, Tounsi, A., Zidour, M., Heireche, H. and Naceri, M. (2014), “Effect of chirality on critical buckling temperature of a zigzag single-walled carbon nanotubes using nonlocal continuum theory”, *Full. Nanotub. Carbon Nanostruct.*, **23**, 518-522.
Sohi, A.N. and Naghdabadi, R. (2007), “Torsional buckling of carbon nanopeapods”, *Carbon*, **45**(5), 952-957.

Sun, C. and Liu, K. (2008), "Dynamic torsional buckling of a double-walled carbon nanotube embedded in an elastic medium", *Eur. J. Mech. A/Solid.*, **27**(1), 40-49.

Tokio, Y. (1995), "Recent development of carbon nanotube", *Synth Met.*, **70**, 1511-1518.

Tounsi, A, Heireche, H, Berrabah, HM, Benzair, A. and Boumia, L. (2008), "Effect of small size on wave propagation in double-walled carbon nanotubes under temperature field", *J Appl Phys*, **104**, 104301.

Tounsi, A, Benguediab, S., Adda Bedia, E.A., Semmah, A. and Zidour, M. (2013a), "Nonlocal effects on thermal buckling properties of double-walled carbon nanotubes", *Adv. Nano Res.*, **1**(1), 1-11.

Tounsi, A., Semmah, A. and Bousahla, A.A. (2013b), "Thermal buckling behavior of nanobeam using an efficient higher-order nonlocal beam theory", *J. Nanomech. Micromech.*, ASCE, **3**(3), 37-42.

Tounsi, A., Houari, M.S.A., Benyoucef, S. and Adda Bedia, E.A. (2013c), "A refined trigonometric shear deformation theory for thermoelastic bending of functionally graded sandwich plates", *Aerosp. Sci. Tech.*, **24**, 209-220.

Wu, Y., Zhang, X., Leung, A.Y.T. and Zhong, W. (2006), "An energy-equivalent model on studying the mechanical properties of single-walled carbon nanotubes", *Thin Wall. Struct.*, **44**, 667-676.

Xu, K.Y., Guo, X.N. and Ru, C.Q. (2006), "Vibration of a double-walled carbon nanotube aroused by nonlinear intertube van der Waals forces", *J. Appl. Phys.*, **99**, 064303.

Yoon, J., Ru, C.Q. and Mioduchowski, A. (2003), "Vibration of an embedded multiwall carbon nanotube", *Compos. Sci. Tech.*, **63**, 1533-1542.

Zidi, M., Tounsi, A., Houari, M.S.A., Adda Bedia, E.A. and Anwar Bég, O. (2014), "Bending analysis of FGM plates under hygro-thermo-mechanical loading using a four variable refined plate theory", *Aerosp. Sci. Tech.*, **34**, 24-34.

Zidour, M., Benrahou, K.H., Semmah, A., Naceri, M., Belhadj, H.A., Bakhti, K. and Tounsi, A. (2012), "The thermal effect on vibration of zigzag single walled carbon nanotubes using nonlocal Timoshenko beam theory", *Computat. Mater. Sci.*, **51**, 252-260.

Zidour, M., Daouadji, T.H., Benrahou, K.H., Tounsi, A., Adda Bedia, E.A. and Hadji, L. (2014), "Buckling analysis of chiral single-walled carbon nanotubes by using the nonlocal Timoshenko beam theory", *Mech. Compos. Mater.*, **50**(1), 95-104.

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