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A new nonlocal beam model for free vibration analysis of chiral single-walled carbon nanotubes

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Abstract. In this letter, nonlocal Timoshenko beam theory has been implemented to investigate the free vibration response of chiral single-walled carbon nanotubes (SWCNTs). According to nonlocal Timoshenko vibration equation for (SWCNTs), The analytical solution is derived and two solutions for vibration are obtained. Influence of nonlocal small-scale coefficient, the vibrational mode number, the chirality of carbon nanotube and aspect ratio of the (SWCNTs) on frequency of the (SWCNTs) are studied and discussed. The results indicate significant dependence of natural frequencies on the chirality of single-walled carbon nanotube with increase the nonlocal small-scale coefficient, the vibrational mode number and the nanotube aspect ratio of length to diameter.

Keywords: single-walled carbon nanotubes; vibration; nonlocal elasticity; chirality; small-scale

1. Introduction

Recent studies have indicated that carbon nanotubes (CNTs) possess superior electronic, thermal and mechanical properties (Dresselhaus 2001, Bachtold 2001), Since the single-walled carbon nanotube (SWNT) and multi-walled carbon nanotube (MWNT) are found by Iijima (1991, 1993), studies (Dai 1996, Thostension 2001) have showed that they have good properties so they can be used for nanoelectronics, nanodevices and nanocomposites. In order to make good use of these nanomaterials, it is important to have a good knowledge of their mechanical properties.

Since experiments at nanoscales are difficult, and molecular dynamics (MD) simulations are limited to systems of computation, the continuum mechanics methods are often used to investigate some physical problems in the nanoscale (Wong 1997, Ru 2000). Recently, the continuum mechanics approach has been widely and successfully used to study the mechanical behaviour of CNTs, such as the static (Tounsi 2008, Naceri 2011, Benferhat 2016), the buckling (Zidour 2012, Benhenni2018, Rabahi 2019, Karami2018, Mokhtar 2018, Cherif 2018, Bouadi 2018, Bensatallah 2016), free vibration (Tounsi 2009a, Bensatallah 2018), wave propagation (Tounsi 2009b, Maachou 2011, Khalifa 2018, Ahouel 2016, Zemri 2015 and Amara 2010) and thermo-mechanical analysis of (CNTs) (Larbi 2015, Adim 2018, Bellifa 2017, Youcef 2018, Yazid 2018, Benhenni 2019, Khetir 2017, Karami 2017, karami 2018, kadari 2018, Besseghir 2017, Al-Basyouni 2015, and Ansari 2011). More recently, Murmu and Adhikari (2010) have developed a

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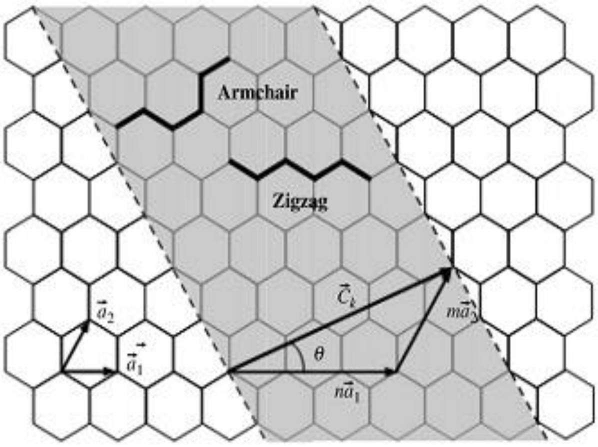

Fig. 1 Schematic diagram of the chiral vector and the chiral angle

nonlocal double-elastic beam model, and applied it to investigate the small scale effect on the free vibration and the axial instability of the double-nanobeam system. Murmu and Adhikari (2010) have analyzed the longitudinal vibration of double nanorod systems using the nonlocal elasticity. He et al. (2006) investigated effect of van der Waals (vdW) interaction modeling on the vibration characteristics of multi-walled (CNTs).

The study of vibration and wave propagation in (CNTs) is a major topic of current interest, which is used to understand the dynamic behaviour of (CNTs) further. Continuum elastic-beam models have been widely used to study vibration (Aissani 2015, Ansari 2012) and sound wave propagation (Herieche 2008) in (CNTs). Malan (2002) studied vibration of (CNT) using a thin-walled hollow cylinder model. A Flugge type shell theory was used by Wang et al. (2005) to study free vibration of multi-walled (CNTs).

In structural analysis of nano beam, two models are usually employed, namely Euler–Bernoulli and Timoshenko beam models. Both models assume that plane sections remain plane. But in Euler beam model, the sections remain perpendicular to the neutral axis whereas this assumption is removed in Timoshenko beam model to account for the effect of shear and rotary effect. Some researchers have applied nonlocal theory of elasticity to nanoscale materials by employing the nonlocal Euler-Bernoulli beam model (Heireche 2009).

This study is concerned with the use of the nonlocal Timoshenko elastic beam model to analyse the wave propagation of single-walled carbon nanotubes (SWCNTs). Two solutions for vibration are obtained. Influence of the chirality of carbon nanotube, nonlocal small-scale coefficient, the vibrational mode number, and aspect ratio of the (SWCNTs) are studied and discussed.

2. Geometry of single-walled carbon nanotube (SWCNT)

A single-walled carbon nanotube (SWCNT) is theoretically assumed to be made by rolling a graphene sheet (Fig.1). The fundamental structure of carbon nanotubes can be classified into three categories as zigzag, armchair and chiral in terms of the chiral vector ($\vec{C}_h$) and the chiral angle θ shown in (Fig.1).

The chiral vector can be expressed in terms of base vectors ($\vec{a}_1$) and ($\vec{a}_2$) (Fig.1):

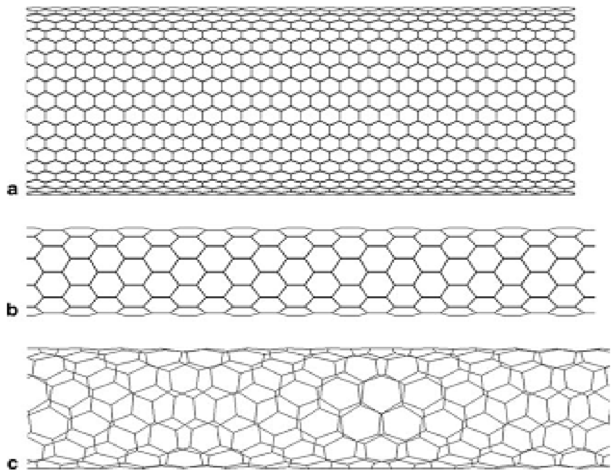

Fig. 2 Carbon nanotube: (a) armchair (b) zig-zag and (c) chiral

$$\vec{C}_h = m\vec{a}_1 + n\vec{a}_2 \tag{1}$$

The integer pair (n, m) specify the structure of carbon nanotubes.

The relationship between the integers (n, m) and the radius is given by (Bensatallah 2016):

$$R = a\sqrt{3(n^2 + m^2 + nm)} / 2\pi, \tag{2}$$

where (a) is the length of the carbon–carbon bond which is ($1.42\ \boldsymbol{A}^{\circ}$).
The relationship between the integers (n, m) and the chiral angle is given by (Zidour 2012):

$$\tan\theta = \frac{\sqrt{3}m}{2n + m} \tag{3}$$

It is simple to evaluate that (θ =0°) for zig-zag configuration and (θ =30°) for armchair configuration (Fig. 2).

3. Nonlocal Timoshenko beam models of (SWCNT's):

The equations of motion for transversely vibrating based on the nonlocal Timoshenko beam model can be obtained as (Bensatallah 2018):

$$\frac{\partial V}{\partial x} - \rho A\frac{\partial^2 w}{\partial t^2} = 0 \tag{4}$$

$$\frac{\partial M}{\partial x} - V = \rho I\frac{\partial^2 \psi}{\partial t^2} \tag{5}$$

where (x) is the axial coordinate, (w) is the transverse deflection of the (SWCNT), (Ψ) is the rotation angle of cross section of the beam, (ρ) is the mass density of the material, (A) is the area of the cross section of the nanotubs beam, (I) the second moment of inertia and *(V)* is the resultant shear force on the cross section, which satisfies the moment equilibrium condition:

$$V = \int_A \tau dA \tag{6}$$

The resultant bending moment (M) is defined by:

$$M = \int_A y\sigma dA \tag{7}$$

Where (y) is the transverse coordinate measured positive in the direction of deflection. For the nonlocal Timoshenko beam theory, the Hook's law of carbon nanotube can be expressed as (Zidour 2012, Bensatallah 2016):

$$\left[1 - e0a^2 \frac{\partial^2}{\partial x^2}\right]\sigma = E\varepsilon \tag{8}$$

$$\left[1 - e0a^2 \frac{\partial^2}{\partial x^2}\right]\tau = G\gamma \tag{9}$$

where (σ) is the axial stress, (τ) the shear stress, (ε) the axial strain, (γ) the shear strain, (E) the Young's modulus and (G) the shear modulus. (a) the internal characteristic lengths (distance between C–C bonds), (e0) the constant for adjusting the model in matching with experimental results and by other models,

The expressions of the axial strain and the shear strain are (Achenbach 1973)

$$\varepsilon = y\frac{\partial \psi}{\partial x}, \qquad \gamma = \frac{\partial w}{\partial x} + \psi \tag{10}$$

According to Eqs.(6), (7), (8), (9) and (10) we can obtain the following relation:

$$\left[1 - e0a^2 \frac{\partial^2}{\partial x^2}\right]M = EI\frac{\partial \psi}{\partial x} \tag{11}$$

$$\left[1 - e0a^2 \frac{\partial^2}{\partial x^2}\right]V = \beta AG\left(\frac{\partial w}{\partial x} + \psi\right) \tag{12}$$

Where ($I = \int_A y^2 dA$) is the moment of inertia and (β) the shear correction factor which is used to compensate for the error due to the constant shear stress assumption is (9/10) for a circular shape of the cross area (Zidour 2012).

Based on Eqs. (4), (5) and (11), the following relation can be obtained:

$$M = EI\frac{\partial \psi}{\partial x} + e0a^2\left[\rho A\frac{\partial^2 w}{\partial t^2} + \rho I\frac{\partial^3 \psi}{\partial x \partial t^2}\right] \tag{13}$$

Substituting Eq. (4) into Eq. (12), we can obtain

$$V = \beta AG\left(\frac{\partial w}{\partial x} + \psi\right) + e0a^2\left[\rho A\frac{\partial^3 w}{\partial x \partial t^2}\right] \tag{14}$$

Substituting Eq. (14) into Eq. (4), we can obtain

$$\beta AG\left(\frac{\partial^2 w}{\partial^2 x} + \frac{\partial \psi}{\partial x}\right) - \left(1 - e0a^2\frac{\partial^2}{\partial x^2}\right)\left[\rho A\frac{\partial^2 w}{\partial t^2}\right] = 0 \tag{15}$$

Based on Eqs. (13), (14) and (5), it can be derived that

$$EI\frac{\partial^2\psi}{\partial x^2}-\beta AG\left(\frac{\partial w}{\partial x}+\psi\right)-\left(1-e0a^2\frac{\partial^2}{\partial x^2}\right)\left[\rho I\frac{\partial^2\psi}{\partial t^2}\right]=0 \tag{16}$$

Since finding an analytical solution is possible for simply supported boundary conditions for the present problem, the (SWNT) beam is assumed simply supported. as a result, the boundary conditions have the following form (Bensatallah 2016):

$$\begin{gathered} w(x,t)=\overline{W}e^{i\omega t}\sin(\lambda x), \\ \psi(x,t)=\overline{\psi}e^{i\omega t}\cos(\lambda x), \\ \lambda=\frac{N\pi}{L} \end{gathered} \tag{17}$$

Where (W) is the amplitude of deflection of the beam and (Ψ) is the amplitude of the slope of the beam due to bending deformation alone. In addition, (ω) is the frequency.

Substitution of Eq. (17) into Eqs. (15) and (16) gives two branches of wave dispersion relation and the correspondent frequencies via nonlocal Timoshenko beam model are as follows;

$$\omega_{NT}=\sqrt{\frac{1}{2}\left(\frac{\beta IG\lambda^2+\beta AG+EI\lambda^2}{\rho I\left(1+e0a^2\lambda^2\right)}\pm\sqrt{\left(\frac{\beta IG\lambda^2+\beta AG+EI\lambda^2}{\rho I\left(1+e0a^2\lambda^2\right)}\right)^2-4\frac{E\beta G\lambda^4}{\rho^2\left(1+e0a^2\lambda^2\right)^2}}\right)} \tag{18}$$

3. Results and discussion

Based on the formulations obtained above with the nonlocal Timoshenko beam models, the vibration properties of single-walled carbon nanotubes (SWCNT's) are discussed here. The parameters used in calculations of (SWCNT) are given as follows: the effective thickness of (CNTs) taken to be 0.34 nm (Heireche 2008), the mass density ρ =2.3 g/cm^3 (Zidour 2012) and poisson ratio υ=0.25 nm (Yoon 2003).

To investigate the effect of scale parameter on vibrations of SWCNTs, the results including the effect of nonlocal small-scale coefficient, the vibrational mode number, aspect ratio of the (SWCNTs) and the nonlocal parameter are compared. In addition, the vibration characteristics of different chiral angle of (SWCNTs) are compared in order to explore the effect of chirality. It follows that the ratio of the results with nonlocal parameter to those without nonlocal parameter is given by:

$$\chi_N=\frac{\omega_{NT}}{\omega_{LT}} \tag{19}$$

Where (ωLT, ωNT) is the frequency based on the local and nonlocal Timoshenko beam respectively. In the present study, the (figs. 3–5) illustrate the dependence of the frequency ratios (χ_N) on the chirality of carbon nanotube for different values of small-scale coefficient, vibrational mode number and aspect ratio of the (SWCNTs). The frequency ratio (χ_N) serves as an index to assess quantitatively the scale effect on (CNT) vibration solution. It is clearly seen from (Figs. 3–5) that the frequency ratios (χ_N) are less than unity. This means that the application of the local Timoshenko beam model for (CNT) analysis would lead to an overprediction of the frequency if

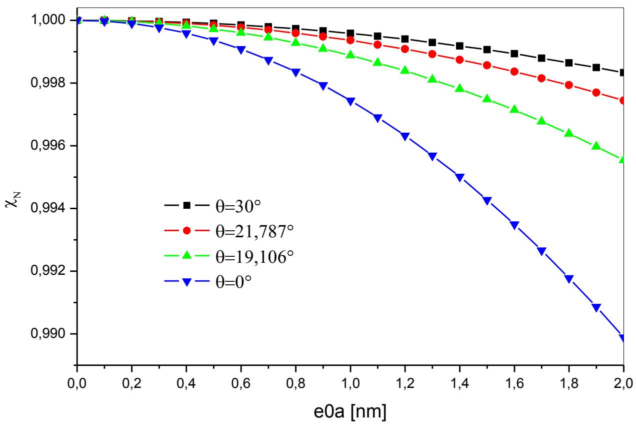

Fig. 3 Effect Relationship between the values of ratio (χ_N), chirality of carbon nanotube and the small-scale coefficients with (*L/d*=40 and N=1)

the scale effect between the individual carbon atoms in (CNTs) is neglected. The frequency ratios (χ_N) exhibit a dependence on the structure characteristic of carbon nanotube. However for (CNTs) with larger values of diameters, this dependence becomes very weak. The reason for this phenomenon is that a carbon nanotube with smaller diameter has a larger curvature, which results in a more significant distortion of (C–C) bonds.

Figure 3 show the effect of small scale coefficients and chirality of carbon nanotube on the vibration response of (SWCNT). For the present study, the nonlocal parameter or small-scale coefficient (*e0a*) values of (SWCNT) were taken in the range of 0–2 nm as described by Heireche (2008). The aspect ratio (*L/d)* is taken as 40 and the vibrational mode is *N*=1. From this fig, it is observed that as the small-scale coefficient increases, the scale effect on the frequency ratios (χ_N) increases. Furthermore It can be seen from the figs the dependence of the frequency ratios (χ_N) on the chirality of carbon nanotube, However for $\theta= 30^0$ this dependence becomes very weak and the scale effect on the frequency ratios (χ_N) increases for increasing of carbon nanotube diameter. This increasing is attributed to the larger curvature of smaller diameter, which results in a more significant distortion of (C–C) bonds.

The variation of frequency ratio with vibrational mode number N for various chirality of carbon nanotube is shown in (fig 4) with the aspect ratio (*L/d)* is taken as 40 and nonlocal parameter *e0a*= 2 nm. It can be seen from the fig that as the vibrational mode number increases, the scale effect on the frequency ratios (χ_N) increases. This significance of nonlocal effects in higher modes is attributed to the influence of small wavelength for higher modes. For smaller wavelengths, interactions between atoms are increasing and this leads to an increase in the nonlocal effects.

Figure 5 shows the Relationship between the values of ratio χ_N, chirality of carbon nanotube and the aspect ratio (L/d). In this present computation, a constant value of nonlocal parameter, e0a=2 nm is employed in fundamental vibrational mode. It is clearly seen from the fig that as the aspect ratios of (SWCNT) increases, the frequency ratio (χ_N) increases. However, it is observed, that the scale effect on the frequency ratios (χ_N) is more affected by low aspect ratio values. Therefore, it is clear that the scale effect is significant for short (CNTs).

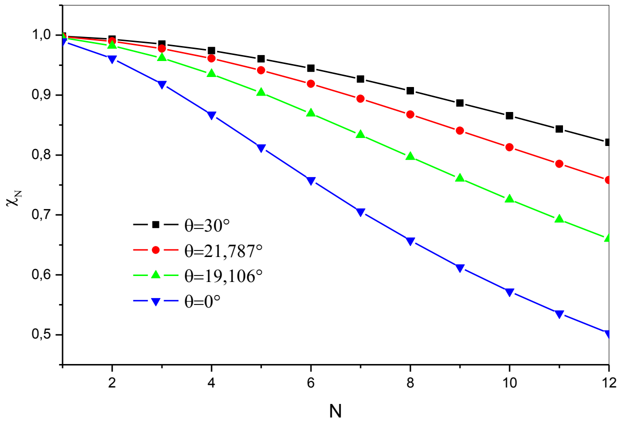

Fig. 4 Relationship between the values of ratio (χ_N), chirality of carbon nanotube and the vibrational mode number (N) with (*e0a*=2 nm and *L/d*=40)

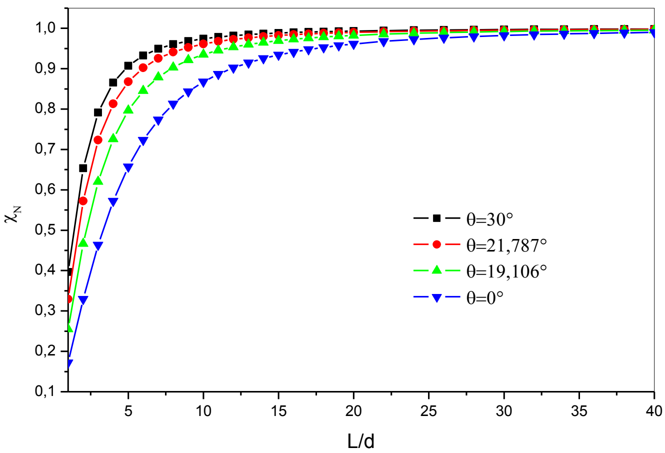

Fig. 5 Relationship between the values of ratio (χ_N), chirality of carbon nanotube and the aspect ratio (L/d) with (*e0a*=2 nm and N=1)

The results of (CNTs) with different length-to-diameter ratios and different angle chiral for the first and the sixth modes based on the nonlocal Timoshenko beam model are listed in (Table 1). A constant value of nonlocal parameter, e0a=2 nm and the values of Young's modulus for different chiral angle are employed. The Young's moduli of (SWCNTs) employed in this study, are simulated using our molecular dynamics simulation program (MD) (Bao 2004). Table 1 show the dependence of the frequency ratio on the chirality of carbon nanotube, Aspect Ratio and, vibrational mode number. In addition, the frequency ratios also increase as the value of diameter of carbon nanotubes increases. Therefore, the scale effect on the frequency ratios (χ_N) decreases.

Table 1 The values of frequency ratios of carbon nanotubes using nonlocal Timoshenko beam model for different, Aspect Ratio and angle chiral for the first and the sixth modes

nanotube	Diameter d (*nm*)	Chiral angle *Θ (°)*	Young's modulus (*GPa*) [39]	Aspect ratio L/d	frequency ratios (χ_N) N=1	frequency ratios (χ_N) N=6
(14,0)	1,0960	0	939.032	10	0,86756	0,27917
				20	0,96129	0,50267
				40	0,98989	0,75823
(12,6)	1,2428	19,106	927.671	10	0,89243	0,31309
				20	0,96950	0,55045
				40	0,99211	0,79679
(14,6)	1,3917	16,996	921.616	10	0,91142	0,34631
				20	0,97546	0,59397
				40	0,99369	0,82800
(16,8)	1,6570	19,106	928.013	10	0,93504	0,40239
				20	0,98250	0,66025
				40	0,99554	0,86924
(18,9)	1,8642	19,106	927.113	10	0,94762	0,44326
				20	0,98610	0,70318
				40	0,99647	0,89243
(20,12)	2,1921	21,787	904.353	10	0,96129	0,50267
				20	0,98989	0,75823
				40	0,99744	0,91869
(24,11)	2,4269	17,896	910.605	10	0,96808	0,54130
				20	0,99173	0,78977
				40	0,99791	0,93218
(20,20)	2,7120	30	935.048	10	0,97420	0,58397
				20	0,99336	0,82114
				40	0,99833	0,94459

4. Conclusion

This paper studies the vibration analysis of (SWCNTs) based on the Timoshenko beam theory. Influence of nonlocal small-scale coefficient, the vibrational mode number, the chirality of carbon nanotube and aspect ratio of the (SWCNTs) on frequency of the (SWCNTs) are studied and discussed. Based on nonlocal Timoshenko beam theory the theoretical formulations include the small scale effect, the the vibrational mode number, the aspect ratio and the chirality of carbon nanotube. The governing equations and the boundary conditions for the (SWCNTs) are solved and two solutions are obtained. According to the study, the results showed the dependence of the vibration characteristics on the chirality of carbon nanotube, small-scale coefficients, Aspect Ratio and mode number. However, the scale effect on the frequency ratios (χ_N) increases with increasing the small-scale coefficient and the vibrational mode number. In addition, the scale effect on the frequency ratios (χ_N) is more affected by low aspect ratio values. Therefore, it is clear that the scale effect is significant for short (CNTs). The scale effect on the frequency ratios (χ_N) also increases as the value of tube diameter decreases.

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