Chirality and small scale effects on embedded thermo elastic carbon nanotube conveying fluid

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Abstract. This paper presents the mechanical buckling properties of fluid conveying thermo elastic embedded single walled carbon nanotube (SWCNT) with small scale and chirality effect. The analytical formulation is developed based on Eringen’s non local elasticity theory. The nonlocal form of governing equations that contains partial differential equations for (SWCNT) single walled carbon nanotube is derived by considering thermal and chirality effect. The analytical solution is obtained by using Euler–Bernoulli beam theory. The equivalent Young’s modulus and shear modulus of chirality SWCNT is derived. The computed non dimensional wave frequency, phase velocity and group velocity are presented in the form of dispersion curves and the physical characteristic are studied.

1. Introduction

Nano materials has extensive mechanical, chemical and electronic properties and it has been developed recently because of the fact that it is applied in all fields of science, engineering and technology. The interaction between Carbon Nanotubes (CNTs) and polymer matrix have gained great attention due to their vital mechanical properties. The CNT resting on a polymeric matrix will create a remarkable volume fraction in the interfacial layer between CNT and the bulk polymer matrix. Therefore, a thorough understanding of the dynamical and mechanical behaviours of Nano sized structures and their interacting medium is of importance in the analysis and design of Nano or micro structures such as micro- and Nano-electromechanical systems (MEMS and NEMS).

Eringen. [1-3] introduced the new nonlocal continuum field theories and discussed their applicability in CNT models. Aydogdu [4] revealed the common features of presented papers on Eringen’s nonlocal elasticity which are related to the investigation of nanobeams nanowires and nanotubes. Semmah et al.[5] have verified the thermal buckling analysis of a zigzag SWCNT via nonlocal Timoshenko beam theory. They verified the effect of the nonlocal parameter, the ratio of the length to the diameter, rotary inertia and the chirality of SWCNT on the thermal buckling properties. Naceri et al. [6] explained the thermal effect on the vibration characteristics of armchair SWCNTs via nonlocal Levinson beam theory. Theoretical formulations carried out by including the small scale effect, the temperature change and the chirality of armchair carbon nanotube. Ebrahimi, and Dabbagh. [7] checked the magnetic field effects on thermally affected propagation of acoustical waves in rotary double nanobeam systems. Zhang et al. [8] developed a method for transverse vibrations of an elastic beam under distributed transverse pressure on basis of the Bernoulli Euler beam theory and thermal elasticity. Ansari et al.[9] discussed CNT’s embedded on polymer matrix is getting important structural idea among researchers. Besseghier et al. [10] developed the vibration analysis of DWCNTs embedded in elastic support. PradhanandPhadika [11] investigated the vibration of single layered and multi-layered graphene sheets embedded in polymer matrix and has been carried out with continuum models. Bensattalah et al. [12] have used nonlocal Timoshenko beam theory to study the vibration of SWCNTs embedded in an elastic medium, considering the thermal and chirality effects. Popov and Doren[13] studied the Young’s and shear moduli of various SWNT’s and they estimated the analytical formulas derived within a lattice-dynamical model for nanotubes.
Our study is mainly concerned with the non local thermo elastic waves in a fluid conveying single walled carbon nanotube resting on polymer matrix incorporated with chirality and small scale effect. We have researched the basic equations based on the Eringen’s non local elasticity theory. The governing equations having the partial differential equations for single walled carbon nanotube is derived by considering thermal effect along with the nonlocal parameters. The computed non dimensional wave frequency, phase velocity and group velocity are studied.

2. Atomic configuration of CNT

Carbon nanotubes are constructed via graphene sheet with \( \hat{T} \) vector. \( \vec{C}_h \) is the chiral vector perpendicular to \( \hat{T} \). Chiral vector \( \vec{C}_h \) is expressed via \( \vec{a}_1 \) and \( \vec{a}_2 \) as follows

\[
\vec{C}_h = n \vec{a}_1 + m \vec{a}_2
\]

where \( n \) and \( m \) is the translation values of medium over the circumference. Fig.1 gives the translation \( (n, m) \) lattice via base vectors \( \vec{a}_1 \) and \( \vec{a}_2 \). The CNT is classified in to zigzag, armchair and chiral if the translation indices \( m = 0 \), \( m = n \) and \( m = n \), respectively. The chiral angle \( \theta \) between \( n \) and \( m \) is expressed via [14]

\[
\theta = \arccos \frac{2m + n}{2\sqrt{m^2 + n^2 + nm}}
\]

and the diameter via the integers \( (n, m) \) of SWCNTs is as Meo [15]

\[
d = a\sqrt{3(n^2 + m^2 + nm)}/\pi
\]

3. Analytical formulations

3.1 Eringen Nonlocal Theory of beam

The motion equation of a material is reads from Eringen [2] as follows
1. Equilibrium equation

\[ \sigma_{mm,m} = - \rho (f_n - u_n) \]  

where \( \sigma_{mm,m} \), \( \rho \), \( f_n \), \( u_n \) shows the stress, density, mass, force on the body and bending vector at \( x' \) via the time variable \( t \).

2. Constitutive form of equation

\[ \sigma_{mm}(x) = \int_{v} \xi(|x - x'|, \tau)\sigma_{mm}^c(x')dv(x') \quad \forall x \in v \]  

\[ \sigma_{mm}^c = C_{mnlk}e_{kl} \]  

where \( \sigma_{mm}^c(x') \) is the stress tensor at \( x' \) in the body, this stress and displacement equation is

\[ e_{mm}(x') = \frac{1}{2} \left( \frac{\partial u_m(x')}{\partial x_m} + \frac{\partial u_n(x')}{\partial x_n} \right) \]  

The kernel function which will add nonlocal effect in the relation is represented by \( \xi(|x - x'|, \tau) \) . The non-local characteristic length \( l \) with the unit \( (length)^{-3} \) is an external characteristic length of the system, hence the non-local modulus has form

\[ \xi = \xi(|x - x'|, \tau), \tau = \frac{e_o a}{l} \]  

Where \( e_o \) is a material constant which has to be calculated for each material differently and \( \sqrt{||x - x'||} \) is the Euclidian distance. Then, “Eq. (2)” can be simplifies to partial differential equation as follows

\[ (1 - \tau^2 l^2 \nabla^2)\sigma_{mm}(x) = \sigma_{mm}^c(x) = C_{mnlk}e_{kl}(x) \]  

where \( C_{mnlk} \) is the elastic modulus tensor and \( e_{mm} \) is the strain tensor. Here \( \nabla^2 \) is the second-order gradient processed on \( \sigma_{mm} \) and \( \tau = \frac{e_o a}{l} \). In Brillouin area at \( ka = \pi \), Eringen computed \( e_o = 0.39 \) using Born-Karman lattice \( a \), \( k \) shows the atomic distance and \( k \) is the wave number (13).

3.2 Formulation of SWCNT with nonlocal relations

The partial differential equation which governs the elastic waves in nanotube conveying fluid via thermal force using Simsek [16] can be expressed as,

\[ \frac{\partial S}{\partial x} + T_i \frac{\partial^2 W}{\partial x^2} + F_n + \delta(x) = \rho A \frac{\partial^2 W}{\partial t^2} + m_e \frac{\partial^4 W}{\partial t^2} \]  

\( \delta(x) \) shows the interactive force between nanotube and polymer matrix. \( A \) is the cross section of CNT and \( m_e \) is a mass of nanotube per unit length. Shear force \( S \) on nanotube cross section is defined in the following equilibrium equation

\[ S = \frac{\partial M}{\partial x} \]  

\( T_i \) denotes the temperature dependent axial force with thermal expansion coefficient \( \alpha_s \). This constant force is defined as

\[ T_i = -EA \alpha_s T \]  

where \( T \) is the temperature change. The force for unit length due to plug flow fluid is taken as
\[ F_p = m_f \left( 2v \frac{\partial^2 w}{\partial x \partial t} + v^2 \frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial t^2} \right) \] (10)

Here \( v \) and \( m_f \) show the flow velocity and mass of fluid. Dynamic bending \( M \) in “Eq. (8)”, is defined for the Euler beam as follows

\[ M = \int_A y \sigma_{xx} \, dA. \] (11)

where \( \sigma_{xx} \) is the nonlocal axial stress defined by nonlocal continuum theory. The constitutive equation of a homogeneous isotropic elastic solid for one-dimensional nanotube is considered as

\[ \sigma_{xx} - (r)^2 \frac{\partial^2 \sigma_{xx}}{\partial x^2} = E \varepsilon_{xx} \] (12)

where \( x \) is the axial coordinate, \( \varepsilon_{xx} \) is the axial strain, \( (e_0a) \) is a nonlocal parameter which represents the impact of nonlocal scale effect on the structure. \( a \) is an internal characteristic length and \( E \) is young modulus.

The nonlocal relations in “Eq. (12)” can be written with temperature environment as follows

\[ \sigma_{xx} - (r)^2 \frac{\partial^2 \sigma_{xx}}{\partial x^2} = E \varepsilon_{xx} - E \alpha T \] (13)

In the context of Euler–Bernoulli beam model, the axial strain \( \varepsilon_{xx} \) for small deflection is defined as

\[ \varepsilon_{xx} = -y \frac{\partial^2 w}{\partial x^2} \] (14)

where \( y \) is the flexural co-ordinate via positive direction of bending. Inserting “Eq. (13)” and (14), in “Eq. (11)”, the bending moment \( M \) is

\[ M - (r)^2 \left[ \frac{\partial^2 M}{\partial x^2} \right] = EI \frac{\partial^4 w}{\partial x^2} \] (15)

\[ I = \int_A y^2 \, dA \] shows the moment of inertia. Inserting “Eq. (7)” and “Eq. (9)” into “Eq. (15)”, the nonlocal dynamic bending \( M \) and shear force \( S \) can be expressed as follows:

\[ M - (r)^2 \left[ (m_r + \rho A) \frac{\partial^2 w}{\partial t^2} + F_p - f(x) + \frac{\partial w}{\partial x} + EA \alpha T \right] = EI \frac{\partial^4 w}{\partial x^2} \] (16)

and

\[ S - (r)^2 \left[ (m_r + \rho A) \frac{\partial^4 w}{\partial x^2 \partial t^2} + F_p \frac{\partial w}{\partial x} - \delta(x) \frac{\partial w}{\partial x} + EA \alpha T \right] = EI \frac{\partial^4 w}{\partial x^2} \] (17)

The simplified form of above equation via pressure and thermal environment is derived as

\[ \delta(x) = EI \frac{\partial^4 w}{\partial x^2} + EA \alpha T \frac{\partial^2 w}{\partial x^2} + m_r v^2 \frac{\partial^3 w}{\partial x^2} + 2m_r v \frac{\partial^2 w}{\partial x \partial t} + (\rho A + m_r + m_f) \frac{\partial^2 w}{\partial t^2} \]

\[ - \left( r)^2 \left[ \frac{\partial w}{\partial x} + m_r \frac{\partial^2 w}{\partial x^2} + m_f v \frac{\partial^4 w}{\partial x^2 \partial t^2} + 2m_f v \frac{\partial^3 w}{\partial x^2 \partial t} + m_r \frac{\partial^4 w}{\partial t^4} + \delta(x) \frac{\partial^2 w}{\partial x^2} \right) \right] \] (18)

The pressure of the CNT due to polymer matrix in unit axial length is reads from Winkler-type model by Yoon [17-18]
\[ \delta(x) = -kw \] (19) where \( k \) is the spring constant [12].

Introduction of “Eq. (19)” into “Eq. (18)” yields

\[ EI \frac{\partial^4 w}{\partial x^4} + m_1 v^2 \frac{\partial^2 w}{\partial x^2} + E\alpha T \frac{\partial^2 w}{\partial t^2} + 2m_1 v \frac{\partial^3 w}{\partial x^2 \partial t} + \rho A \frac{\partial^3 w}{\partial t^3} + \left( m_c + m_f \right) \frac{\partial^2 w}{\partial x \partial t^2} = kw \] (20)

4. Ultrasonic wave form

In order to analysis the elastic wave charcetric of SWCNT, a harmonic solution of displacement \( w(x, t) \) is reads from Eringen[3] and Narender [19]

\[ w(x, t) = \sum_{n=1}^{N} \hat{w}(x) e^{-jt(k_n - \omega t)} \] (21)

where \( j = \sqrt{-1}, k_n, \omega, n \) and \( N \) are the amplitude, wave number, frequency and Nyquist frequency, respectively. Substitution of “Eq. (21)” into “Eq. (20)”, we get the following coupled equations

\[ \sum_{n=1}^{N} \left[ EI \frac{\partial^4 \hat{w}}{\partial x^4} - T \frac{\partial^2 \hat{w}}{\partial x^2} + m_1 v^2 \frac{\partial^2 \hat{w}}{\partial x^2} - \left( m_c + m_f \right) \frac{\partial^2 \hat{w}}{\partial x \partial t} + \rho A \frac{\partial^3 \hat{w}}{\partial t^3} + \left( k_n - \omega \right) \frac{\partial^2 \hat{w}}{\partial x \partial t} \right] \hat{w} = 0 \] (22)

“Eq. (22)” is reached the following form for all minimal values of \( N \)

\[ \left[ EI \frac{\partial^2 \hat{w}}{\partial x^2} + m_1 v^2 \frac{\partial^2 \hat{w}}{\partial x^2} + E\alpha T \frac{\partial^2 \hat{w}}{\partial t^2} + 2m_1 v \frac{\partial^2 \hat{w}}{\partial x^2 \partial t} \right] \left( m_c + m_f + \rho A \right) \frac{\partial^2 \hat{w}}{\partial x^2} + m_f \frac{\partial^2 \hat{w}}{\partial t^2} = 0 \] (23)

The following non dimensional parameters are used for the convenience of the problem

\[ \frac{x}{l} = \hat{x}; \frac{\hat{w}}{l} = \hat{w}; \frac{\beta}{1} = \frac{\omega}{\sqrt{EI}} ; m = \frac{m_f}{(m_c + m_f)} ; \nu = \frac{m_f}{EI} \tau \frac{\eta}{(m_c + m_f)l^4} ; k = \frac{IE}{(1 + E\alpha)T} \]

\[ \hat{T} = \frac{Tl^2}{EI} ; \alpha_i = \frac{l}{l} \] (24)

The corresponding boundary conditions are
is the wave number, into “Eq. (25)”, we reached

\[ \alpha^2 - \left[ v^2 + T_i - k + (1-m)\beta^2 \tau^2 \right] k^2 + 2i\beta v\sqrt{\mu \rho A} k \] \[ \frac{2}{\alpha^2} \frac{2i\beta v\sqrt{\mu \rho A} k}{\alpha^2} \frac{[\beta^2 \rho A]}{[\beta^2 \rho A]} = 0 \] (25)

Incorporating the solution \( w(x) = e^{ikx} \) \( k \) is the wave number, into “Eq. (25)”, we reached

\[ \left(1 + T_i\right) k^4 + \left[ v^2 + T_i - k + (1-m)\beta^2 \tau^2 \right] k^2 + 2i\beta v\sqrt{\mu \rho A} k \] \[ \frac{2}{\alpha^2} \frac{2i\beta v\sqrt{\mu \rho A} k}{\alpha^2} \frac{[\beta^2 \rho A]}{[\beta^2 \rho A]} = 0 \] (26)
The wave numbers can be calculated by solving the characteristic “Eq. (26)” as

\[ k_n = \pm \sqrt{-\frac{1}{2} \lambda_2(\eta) \pm \sqrt{\frac{1}{2} \lambda_2(\eta)}} \frac{4\lambda_2(\eta)}{2\lambda_2(\eta)} \] (27)

Where \( \lambda_2 = v^2 + T_i - k + (1-m) - \beta^2 \epsilon^2 \eta = \frac{1}{1 + T_i} \), \( \lambda_4 = 2i\beta v\sqrt{\mu \rho A} k \), \( \lambda_0 = -[\beta^2 \rho A] \) and

In order to derive the resonant frequency parameter, we assumes the vibrational modes of clamped SWCNT in the following form

\( \bar{w}(x) = w e^{ikx} \) (28)

\[ \omega_n = \frac{1}{2} \left( T_i \pm \sqrt{T_i^2 - 4k} \right) \] (29)

In which

\[ T_i = \alpha^2 - \left[ v^2 - k + (1-m)\beta^2 \tau^2 \right] \left( \frac{2\beta v\sqrt{\mu \rho A} k}{\alpha^2} \frac{[\beta^2 \rho A]}{[\beta^2 \rho A]} \right) = 0 \]

\[ \bar{k} = \alpha^2 - \left[ v^2 - T_i + (1-m)\beta^2 \tau^2 \right] \left( \frac{2\beta v\sqrt{\mu \rho A} k}{\alpha^2} \frac{[\beta^2 \rho A]}{[\beta^2 \rho A]} \right) = 0 \]

The phase velocity is read as

\[ C_p = \text{Re} \left( \frac{\omega_n}{k_n} \right) \]

The corresponding wave speed, namely, Phase velocity \( C_p = \text{Re} \left( \frac{\omega_n}{k_n} \right) \) and group velocity

\[ C_g = \text{Re} \left( \frac{\bar{\partial} \omega_n}{\bar{\partial} k_n} \right) \] is reached via “Eq. (28)” and “Eq. (29)”.

5. Results and illustrations

In this paper thermo elastic wave in a fluid conveying single walled carbon nanotube resting on polymer matrix incorporated with chirality and small scale impact is studied. From lee [20] the SWCNT have a young modulus E=1 Tpa, thickness to be 0.35 nm and mass density as 2.3 g/cm3 , the mass density of water \( m = 1000 \text{ kg/m}^3 \), \( EI = 1.1122 \times 10^{-25} \text{Nm}^2 \), \( m_i = 1.52 \times 10^{-16} \text{kgm}^{-2} \) \( m_f = 2.75 \times 10^{-15} \text{kgm}^{-2} \). The dispersion curves are drawn in Figs. 2-3 for the variation of wave frequency versus the wave number of the elastic fluid conveying SWCNT for the varying non local parameter with respect to thermal parameter \( T_i = 0.2, 0.5 \), polymer matrix parameters \( k = 0, 0.2 \) and different chirality value \( (m, n) \), respectively. From Figures. 2-3, it is observed that the wave frequency is increasing with respect to its wave number for the different values of non-local parameters. Figure.
3 reveals dispersion trend in the wave propagation due to the surrounded polymer matrix support. It can be noted that the increasing values of thermal parameter $T_i$ also influence the values of wave frequency in Figures 2 and 3. A comparative illustration is made between the group velocity and wave number of the SWCNT for the thermal and polymer matrix parameters values of vibration is respectively shown in the Figures 4-5 with different chirality value $(m, n)$. From the Figures 4 and 5, it is clear that, at the lower range of wave number the group velocity attain maximum value in both cases of $k = 0$, and $k = 0.2$ but there is a deviation in elastic wave behaviour when $T_i = 0.5$ in Figure 5. The 3D curve in Figures 6-8, clarifies the relation among the quantities bending of CNT, temperature and small scale effect. These curves explain the dependence of bending with temperature and small scale effect with varying spring constants.

Figure 2. Distribution of wave frequency versus wave number with $(m = 2, n = 2) \quad T_i = 0.2 \quad k = 0$.

Figure 3. Distribution of wave frequency versus wave number with $(m = 5, n = 5) \quad T_i = 0.2, k = 0.2$.
Figure 4. Distribution of group velocity versus wave number with \((m = 2, n = 2) \ T^*_c = 0.5, k = 0\)

Figure 5. Distribution of group velocity versus wave number with \((m = 5, n = 5) \ T^*_c = 0.5, k = 0.2\)

Figure 6. 3D Distribution of bending moment of CNT with temperature and small scale value for \(k = 0\) and \((m = 5, n = 5)\)
6. Conclusions

Effect of zigzag and chirality on the dynamic variation of thermal carbon nanotube embedded in polymer matrix is dealt in this study via nonlocal Euler-Bernoulli beam equations. We reached the following conclusions:

- The frequency, group velocity and bending moment are highly dependent on temperature, scale effect and chirality impact.
- In room temperature, frequency ratios $w(x,t)$ varies in linear manner with temperature $\theta$ and is more responsive to the changes of chirality.
- The rate of increases of the frequency ratio is lower for higher values of nonlocal parameter.
- The scale effect shows the maximum energy whenever the elastic medium is absent.

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