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Thermal Effect on Wave Propagation in Double Walled Carbon Nanotubes Using Strain Gradient Elasticity

Amara Khaled [1,2], Bouazza Mokhtar[2,3], Besseghier Abderahmane[4,2], Tounsi Abedlouahed[2] and Adda Bedia el abbas[2]

[1] Department of Civil Engineering, University centre of Ain Témouchent, Ain Témouchent 46000, Algeria
amara3176@yahoo.fr

[2] Laboratory of Materials and Hydrology, University of Sidi Bel Abbes, Sidi Bel Abbes 22000, Algeria
mech2003@hotmail.com

[3] Department of Civil Engineering, University of Bechar, Bechar 8000, Algeria
bouazza_mokhtar@yahoo.fr

[4] Department of Civil Engineering, University centre of Tissemssilt, Tissemssilt, 38000, Algeria
Zm14000@yahoo.fr

Abstract: The present paper examine the vibrational characteristics of double-walled carbon nanotubes (DWNTs) embedded in a polymer matrix based on the theory of strain gradient elasticity. The mechanical properties of carbon nanotubes and polymer matrix are treated as the functions of temperature change. The research work reveals the significance of the effect of small scale on wave propagation in DWNTs. It is demonstrated that some properties of transverse vibrations of DWNTs are dependent on the change of temperature.

Keywords: Carbon nanotubes; Vibration; Thermal effect; Strain gradient elastisity.

1. Introduction

When you submit your paper print it in two-column format, including figures and tables. In addition, designate one author as the "corresponding author". This is the author to whom proofs of the paper will be sent. Proofs are sent to the corresponding author only. The Introduction should provide a clear statement of the problem, the relevant literature on the subject, and the proposed approach or solution. It should be understandable to colleagues from a broad range of scientific

Carbon nanotubes (CNTs) are cylindrical macromolecules consisted of carbon atoms in a periodic hexagonal structure.

Research on the mechanical properties of carbon nanotubes has been proposed since CNTs were discovered by Iijima [1]. The results from the research show that CNTs exhibit superior mechanical properties. Although there are various reports in the literature on the exact properties of CNTs, theoretical and experimental results have shown an extremely high elastic modulus, greater than 1 TPa (the elastic modulus of diamond is 1.2 TPa), for CNTs. Reported strengths of CNTs are 10–100 times higher than the strongest steel at a fraction of the weight. Thus, mechanical behavior of CNTs has been the subject of numerous recent studies [2–12].

The modelling for the analytical analysis of CNTs is mainly classified into two categories. The first one is the atomic modelling, including the techniques such as classical molecular dynamics (MD) [13,14], tight binding molecular dynamics (TBMD) [15] and density functional theory (DFT) [16], which is only limited to systems with a small number of molecules and atoms and therefore only restrained to the study of small-scale modelling. On the other hand, continuum modelling is practical in analyzing CNTs with large-scale sizes. Yakobson et al. [17] studied axially compressed buckling of single walled carbon nanotubes using molecular dynamics simulations. These authors compared their simulation results with a simple continuum shell model and found that all changes in buckling pattern can be predicted using a continuum model.

Application of the non local continuum theory to nano technology was initially addressed by Peddieson et al [18] in which the static deformations of beam structures based on a simplified nonlocal model obtained by Eringen [19] were analyzed. Recently, the nonlocal beam models have been further applied to the investigations of static and vibration properties of single walled CNTs (SWCNTs) or multiwalled CNTs (MWCNTs) [20–28].

In early investigations on transverse vibration and wave propagation in CNTs, the effect of initial stress in CNTs on the vibration frequency and wave speeds is not considered.

Corresponding Author: Bouazza Mokhtar, University of Bechar, bouazza_mokhtar@yahoo.fr.

More recently, the effect of initial loading on the vibration of CNTs has attracted attention [29] Zhang et al [30] studied transverse vibration of double-walled CNTs (DWCNTs) under compressive axial load and pointed out that the natural frequencies decreased with increasing the axial load while the associated amplitude ratio of the inner to the outer tube of DWCNTs were independent of the axial load. Wang and Cai [31] investigated the effects of initial stress on noncoaxial resonance of CNTs. In their results, it was shown that the influence of initial stress in CNTs was obvious on their natural frequency but was not obvious on their intertube resonant frequency. Sun and Liu [32] studied the vibrational characteristics of CNTs with initial axial loading using the Donnell equations. In their results, it is shown that the resonant frequency is related to the tension or compression forms of initial axial stress. Lu [33] developed a nonlocal Euler beam model with axial initial stress.

The investigation of dynamic behavior of CNTs has been the subject of numerous experimental, molecular dynamics (MD), and elastic continuum modeling studies. Since controlled experiments at nanoscales are difficult, and molecular dynamics simulations are limited to systems with a maximum atom number of about 109 by the scale and cost of computation, the continuum mechanics methods are often used to investigate some physical problems in the nanoscale [34–36]. Recently, continuum elastic-beam models have been widely used to study vibration [37–38] and sound wave propagation [39–41] in CNTs. In the literature [42,43], multi-walled carbon nanotubes (MWNTs) have been modeled as a single-elastic beam, which neglected Vander Waals force of interaction between two adjacent tubes [44–46]. Recently, therole of Vander Waals force interaction between two adjacent tubes in transverse vibration and wave propagation in MWNTs using the multiple-Euler-beam model has been studied [47–52]. In many proposed applications and designs, however, CNTs are often embedded in another elastic medium [48-50].

In this study, based on the strain gradient theory of thermal elasticity, a double-elastic-beam model is developed for wave propagation in double-walled carbon nanotubes (DWNTs) embedded in an elastic medium (polymer matrix), which accounts for the thermal effect in the formulation. The effects of surrounding elastic medium and Vander Waals forces between the inner and outer nanotubes are taken into consideration. In example calculations, the mechanical properties of carbon nanotubes and polymer matrix are treated as the functions of temperature change. Explicit expressions are derived for natural frequencies and associated amplitude ratios of the inner to the outer tubes for the case of simply supported DWNTs, and the influences of both temperature change and small length scale on them are investigated.

2. Materials and methods

2.1 Strain gradient beam model with thermal effect

Using the Euler Bernoulli theory, the general equation for transverse vibrations of an elastic beam can be obtained as [51–53]

$$\frac{\partial Q}{\partial x} + N_t\frac{\partial^2 w}{\partial x^2} + f(x) + p(x) = \rho A\frac{\partial^2 w}{\partial t^2} \qquad (1)$$

$$Q = \frac{\partial M}{\partial x} \qquad (2)$$

N_t denotes an additional axial force and is dependent on temperature T and thermal expansion coefficient α of nanotube. This force can be expressed as

$$N_t = -EA\alpha T \qquad (3)$$

The axial stress corresponding to strain gradient elasticity is given by

$$\sigma = E\left(\varepsilon + (e_0 a)^2\frac{\partial^2\varepsilon}{\partial x^2}\right) \qquad (4)$$

Where e_0 is a constant that is appropriate to the material and a is an internal characteristic length.

For the case where the thermal effect is taken into account, Eq 4 becomes

$$\sigma = E\left(\varepsilon + (e_0 a)^2\frac{\partial^2\varepsilon}{\partial x^2}\right) - E\alpha T \qquad (5)$$

Considering the definition of the resultant bending moment and the kinematics relation in a beam structure, we have

$$M = \int_A y\sigma dA \qquad (6)$$

$$\varepsilon = -y\frac{\partial^2 w}{\partial x^2} \qquad (7)$$

Where y is the coordinate measured from the midplane along the direction of the beam's height.

Substituting Eqs 6 and 7 into Eq 5 leads to:

$$M = -EI\left(\frac{\partial^2 w}{\partial x^2} + (e_0 a)^2\frac{\partial^4 w}{\partial x^4}\right) \qquad (8)$$

Differentiating Eq (8) twice and substituting Eq (1) into the resulting equation

$$-EI\left(\frac{\partial^4 w}{\partial x^4} + (e_0 a)^2\frac{\partial^6 w}{\partial x^6}\right) = \rho A\frac{\partial^2 w}{\partial t^2} + EA\alpha T\frac{\partial^2 w}{\partial x^2} - f(x) - p(x) \qquad (9)$$

This is the general equation for transverse vibrations of an elastic beam under distributed transverse pressure and the thermal effect with the surrounding elastic medium on the basis of Strain gradient elasticity.

It is known that double walled carbon nanotubes are distinguished from traditional elastic beam by their hollow two layer structures and associated intertube Van der Waals forces. Thus Eq (9) can be used to each of the inner and outer tubes of the double walled carbon nanotubes.

Assuming that the inner and outer tubes have the same thickness and effective material constants, we have

$$-EI_1\left(\frac{\partial^4 w_1}{\partial x^4} + (e_0 a)^2\frac{\partial^6 w_1}{\partial x^6}\right) = \rho A_1\frac{\partial^2 w_1}{\partial t^2} + EA_1\alpha T\frac{\partial^2 w_1}{\partial x^2} - p_{12} \qquad (10a)$$

$$-EI_2\left(\frac{\partial^4 w_2}{\partial x^4} + (e_0 a)^2\frac{\partial^6 w_2}{\partial x^6}\right) = \rho A_2\frac{\partial^2 w_2}{\partial t^2} + EA_2\alpha T\frac{\partial^2 w_2}{\partial x^2} - f + p_{12} \qquad (10b)$$

Where subscripts 1 and 2 are used to denote the quantities associated with the inner and outer tubes, respectively, p_{12} denotes the Van der Waals pressure per unit axial length exerted on the inner tube by the outer tube.

For small amplitude sound waves, the Van der Waals pressure should be a linear function of the difference of the deflections of the two adjacent layers at the point as follows:

$$p_{12} = c(w_2 - w_1) \qquad (11)$$

Where c is the intertube interaction coefficient per unit length between two tubes, wich can be estimated by [29]

(12)

$$C = \frac{320(2R_1)erg\,cm^2}{0.16d^2} \qquad (d = 0.142nm)$$

Where R1 is the radius of the inner tube. In addition the pressure per unit axial length, acting on the outermost tube due to the surrounding elastic medium, can be described by a Winkler type model [17,29]

$$f = -kw_2 \tag{13}$$

Where the negative sign indicates that the pressure f is opposite to the deflection of the outermost tube, and k is spring constant of the surrounding elastic medium (polymer matrix). It is noted that the spring constant k is proportional to the Young's modulus of the surrounding elastic medium E_m [17].

In the above formula, E, α and E_m are, respectively, express Young's modulus and thermal expansion coefficients of CNTs and polymer matrix, under temperature changes environments, which may be a function of temperature change as follow [45,56,57]:

$$E = E^0(1 - 0.0005T),\ \alpha = \alpha^0\,(1 + 0.002T)$$
$$\text{and}\ E_m = E_m^0(1 - 0.0003T) \tag{14}$$

Because k is proportional to the Young's modulus of the surrounding elastic medium E_m [17], we can write

$$k = k^0(1 - 0.0003T) \tag{15}$$

Where E^0 and α^0 express elastic modulus and thermal expansion coefficients of CNTs under a room temperature environment, respectively. k^0 and E_m^0 are spring constant and Youn's modulus of polymer matrix under a room temperature environment, respectively.

Introduction of Eqs (11) and (13) into Eq (10a) and b yields

$$-EI_1\left(\frac{\partial^4 w_1}{\partial x^4} + (e_0 a)^2\frac{\partial^6 w_1}{\partial x^6}\right) = \rho A_1\frac{\partial^2 w_1}{\partial t^2} + EA_1\alpha T\frac{\partial^2 w_1}{\partial x^2} - C(w_2 - w_1) \tag{16a}$$

$$-EI_2\left(\frac{\partial^4 w_2}{\partial x^4} + (e_0 a)^2\frac{\partial^6 w_2}{\partial x^6}\right) = \rho A_2\frac{\partial^2 w_2}{\partial t^2} + EA_2\alpha T\frac{\partial^2 w_2}{\partial x^2} + kw_2 + C(w_2 - w_1) \tag{16b}$$

2.2 Solution procedure

Let us consider a double walled nanotube of length L in which the two ends are simply supported, so vibrational modes of the DWNT are of the form [20, 39].

$$w_1 = a_1 e^{i\omega t}\sin\lambda_n x, \quad w_2 = a_2 e^{i\omega t}\sin\lambda_n x \tag{17}$$
$$\text{and}\ \lambda_n = \frac{n\pi}{L}, (n = 1,2, \ldots.)$$

Where a_1 and a_2 are the amplitudes of deflections of the inner and outer tubes, respectively.

Thus, the two n order resonant frequencies of the DWNT with thermal effect can be obtained via strain gradient model by substituting Eq (17) into Eq (16a) and (16b), which yields

$$\omega_{nI}^2 = \frac{1}{2}\left(\alpha_n - \sqrt{\alpha_n^2 - 4\beta_n}\right),\ \omega_{nII}^2 = \frac{1}{2}\left(\alpha_n + \sqrt{\alpha_n^2 - 4\beta_n}\right) \tag{18}$$

With

$$\alpha_n = \frac{C(A_1 + A_2)}{\rho A_1 A_2} + \frac{k + EI_2\lambda_n^4}{\rho A_2} - \frac{2E\alpha T\lambda_n^2}{\rho} + \frac{EI_1\lambda_n^4(1 - (e_0 a)^2\lambda_n^2)}{\rho A_1} \tag{19}$$

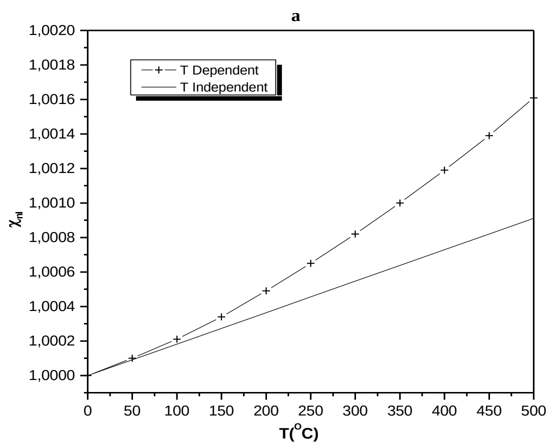
$$\beta_n = \frac{E^2\alpha^2T^2\lambda_n^4}{\rho^2} - CE\alpha T\lambda_n^2\frac{(A_1 + A_2)}{\rho^2 A_1 A_2} - \left[E^2\alpha T\lambda_n^6(A_1 I_2 + A_2 I_1) + E\lambda_n^4\left(kI_1 - C(I_1 + I_2)\right)\right]\frac{(1-(e_0 a)^2\lambda_n^2)}{\rho^2 A_1 A_2} + E^2 I_1 I_2\lambda_n^8\frac{(1-(e_0 a)^2\lambda_n^2)^2}{\rho^2 A_1 A_2} + \frac{k(C - EA_1\alpha T\lambda_n^2)}{\rho^2 A_1 A_2} \tag{20}$$

3. Results and discussion

On the basis of the above equations, we investigate the effect of temperature change and the small length scale on the frequency with numerical examples. The parameters used in calculations of DWNT are given as follows: theYoung's modulus at room temperature E^0 =1.1 TPa with the effective thickness of single-walled carbon nanotubes taken to be t =0.35 nm, and the mass density ρ =2.3 g/cm^3. The thermal expansion coefficient at room temperature α^0 = -1.5x10^{-6} ^{0}C^{-1}. The inner diameter D_{in} =0.7 nm and the outer diameter D_{out}=1.4 nm. The spring constant of polymer matrix under a room temperature environment is k^0=3.3 GPa. The calculations of vibration characteristics were performed by considering the elastic modulus E, the thermal expansion a and the spring constant k independent of temperature as well as dependent on temperature. To examine the influence of temperature change on vibrations of double-walled nanotubes embedded in a polymer matrix, the results including and excluding the thermal effect are compared. It follows that the ratios of the results with temperature change to those with out temperature change are respectively given by

$$\chi_{nI} = \frac{(\omega_{nI})}{(\omega_{nI})^0}, \chi_{nII} = \frac{(\omega_{nII})}{(\omega_{nII})^0}$$

In the following we define $(\omega_{nI})^0$ and $(\omega_{nII})^0$ as the computed frequencies with out thermal effect (T=0). With the aspect ratio L/D_{out} =40, the thermal effects on the lower natural frequency (ω_{nI}) and the higher natural frequency (ω_{nII}) are shown in Figs.1 and 2, respectively, without the surrounding polymer matrix (k=0). As can be seen, the thermal effect on the lower natural frequency ω_{nI} is significant and especially for lower vibrational mode (n=1) while the higher natural frequency ω_{nII} is insensitive to temperature change. It can be seen that temperature dependent parameters lead to an increase in percentage change especially at higher temperature $(T > 50°C)$.



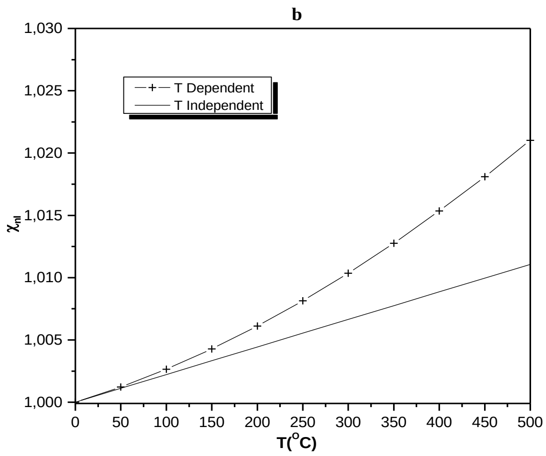


Figure 1: Thermal effects on the lower natural frequency ω_{nI} with the aspect ratio L/D_{out}=40 and e_0a=0; (a) the vibrational mode number n=1, and (b) the vibrational mode number n=6.

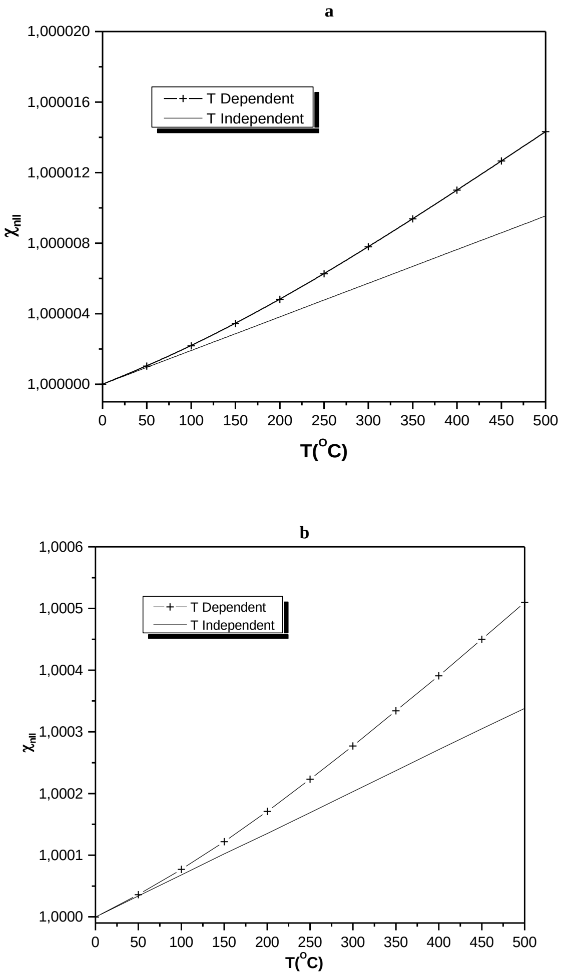


Figure 2: Thermal effects on the higher natural frequency ω_{nII} with the aspect ratio L/D_{out}=40 and e_0a=0; (a) the vibrational mode number n=1, and (b) the vibrational mode number n=6.

To investigate the effects of the surrounding polymer matrix on the vibration response of DWNT in thermal environment, variations of frequency ratio with and without foundation parameter are plotted in Figs. 3 and 4. The calculation is carried out by considering the elastic modulus E, the thermal expansion a and the spring constant k dependent on temperature.It can be observed from the results illustrated in Fig.3 that the presence of the elastic foundation reduces the values of the ratio χ_{nI} in thermal environment with $T > 0$. However, the values of the ratio χ_{nII} are insensitive to the elastic foundation. This implies that there is comparatively less effect of elastic medium on higher natural frequency of DWNT.

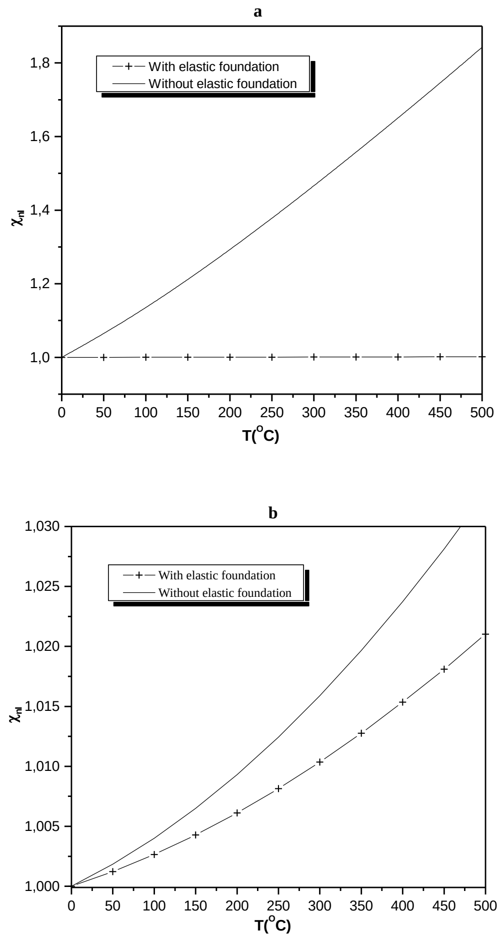


Figure 3: Effect of elastic foundation on the lower natural frequency ω_{nI} with the aspect ratio L/D_{out}=40 and e_0a=0; (a) the vibrational mode number n=1, and (b) the vibrational mode number n=6.

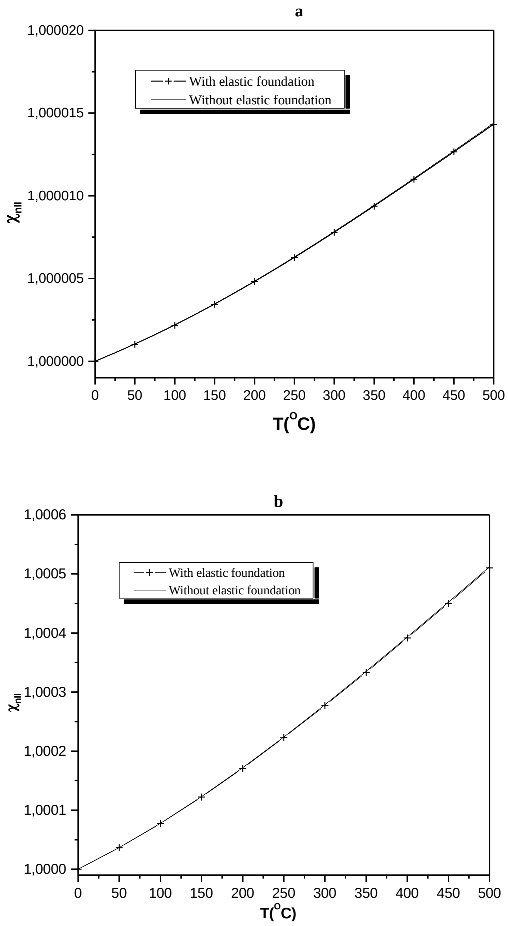


Figure 4: Effect of elastic foundation on the higher natural frequency ω_{nI} with the aspect ratio L/D_{out}=40 and e_0a=0; (a) the vibrational mode number n=1, and (b) the vibrational mode number n=6.

To investigate the effect of scale parameter onvibrations of DWCNTs, the results including and excluding the nonlocal parameter are compared. It follows that the ratios of the nonlocal results to the corresponding local results is given by

$$\xi_{nI} = \frac{(\omega_{nI})_N}{(\omega_{nI})_L}, \xi_{nII} = \frac{(\omega_{nII})_N}{(\omega_{nII})_L}$$

where $(\omega_{nI})_N$ and $(\omega_{nI})_L$ are the frequencies based on nonlocal and local Euler Bernoulli beam model, respectively. Figs. 5 and 6 show the small-scale effect on both lower and higher natural frequencies, respectively, of embedded DWCNT with elastic medium modeled as Winkler-type foundation. The calculationis carried out by considering the elastic modulus E, the thermal expansion a, and the spring constant k dependent on temperature. The nonlocal parameter or small-scale coefficient (e_0a) values of DWCNT were taken in the range of 0 – 2 nm. The aspect ratio L/D_{out} is taken as 40 and the temperature T=100℃ .

From the results presented in Figs. 5 and 6, it is observed that there is significant in fluence of the small size on the vibration response of embedded DWCNT and especially for vibrational

mode number $n > 4$. The lower natural frequency ω_{nI} considering nonlocal model are always smaller than the local (classical) model. This implies that the employment of the local Euler Bernoulli beam model for DWCNT analysis would lead to an over prediction of the lower natural frequency if the small length scale effects between the individual carbon atoms are neglected.

Further, with increase in e_0a values, the frequencies obtained by nonlocal Euler Bernoulli beam theory become smaller compared tolocal model. Furthermore, it is seen that the nonlocal effects on the vibration response of embedded DWCNT becomes more significant with the increase in the vibrational mode number n. However, the higher natural frequency ω_{nII} is less sensitive to both nonlocal effects and the vibrational mode number .

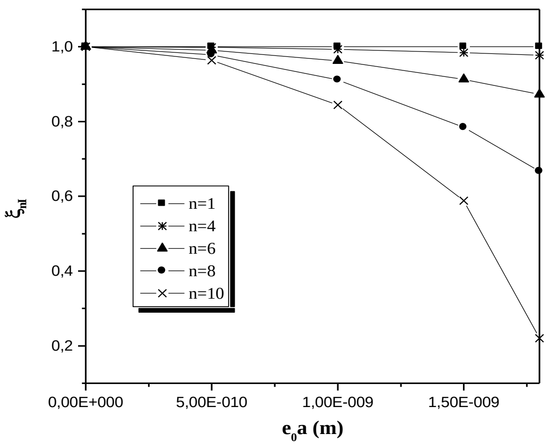


Figure 5: Small scale effect on the lower natural frequency ω_{nI} of embedded DWCNT with elastic medium with the aspect ratio L/D_{out}=40 and temperature T=100 °C.

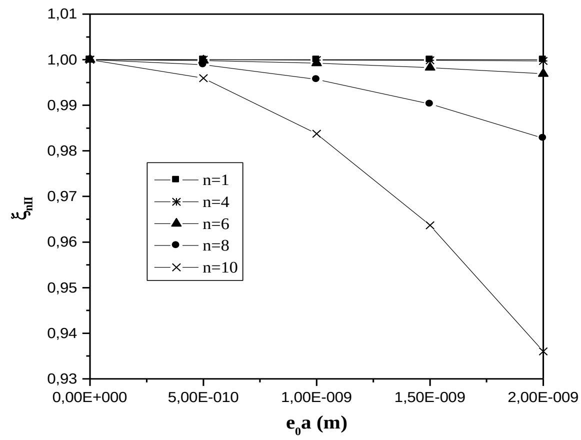


Figure 6: Small scale effect on the higher natural frequency ω_{nI} of embedded DWCNT with elastic medium with the aspect ratio L/D_{out}=40 and T=100 °C.

4. Conclusion

Presented herein is the vibration analysis of DWCNTs embedded in a polymer matrix based on Eringen's nonlocal elasticity theory and the Euler Bernoulli beam theory. The effects of small size, temperature change, Winkler parameter, and Van der Waals forces between the inner and outer nanotubes are taken into account. The mechanical properties of carbon nanotubes and polymer matrix are treated as the functions of temperature change. For the case of simply supported DWCNTs, the natural frequencies are determined and discussed in detail. Itis shown that the higher

natural frequency of DWCNTs is insensitive to the change in temperature, the small scale effect, and the presence of the polymer matrix while theses three effects on the lower natural frequency are significant.
The thermal effect on the lower natural frequency ω_{nI} decreases with the increase in the vibrational mode number n. It is found that the nonlocal effect becomes larger, especially for higher values of vibrational mode number n, and thus the small scale effect cannot be neglected.

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