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Small Scale Effect on Thermal Vibration of Single-Walled Carbon Nanotubes with Nonlocal Boundary Condition

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Abstract: In this study, a single beam model has been developed to analyze the thermal vibration of Single-Walled Carbon Nanotubes (SWCNT). The nonlocal elasticity takes into account the effect of small size into the formulation and the boundary condition. With exact solution of the dynamic governing equations, the thermal-vibrational characteristics of a cantilever SWCNT are obtained. Influence of nonlocal small scale effects, temperature change and vibration modes of the CNT on the frequency are investigated. The present study shows that the additional boundary conditions from small scale do not change natural frequencies at different temperature change. Thus for simplicity, one can apply the local boundary condition to replace the small scale boundary condition.

Keywords: Euler-Bernoulli beams theory, exact solution, nonlocal elasticity, resonant frequency, thermal effect, vibrational mode

INTRODUCTION

Ever since Carbon Nanotubes (CNTs) discovery in 1991 by Sumio Ijima of the NEC Laboratory in Tsukuba, Japan (Iijima, 1991), there has been intensive research on the potential applications of these unique nanostructure elements. Nanostructures can be modeled using atomistic or continuum mechanics. Compared to the atomistic approach, the continuum mechanics approach is widely used due to its computational efficiency and simplicity. Due to the presence of small scale effects at the nano scale, size-dependent continuum mechanics models such as the nonlocal elasticity theory initiated by Eringen is widely used. Unlike the local theories which assume that the stress at a point is a function of strain at that point, the nonlocal elasticity theory assumes that the stress at a point is a function of strains at all points in the continuum. Based on the nonlocal constitutive relation of Eringen, a number of studies have been published attempting to analyze the vibration (Aydogdu, 2009; Benzair *et al*., 2008; Janghorban and Zare, 2011; Aranda-Ruiz *et al*., 2012) responses of nanotubes. A review on the application of nonlocal models in the modeling of carbon nanotubes and graphenes is presented by Arash and Wang (2012). All of these models were based on Euler–Bernoulli beam theory, Timoshenko beam theory and higher-order shear deformation beam theories. It should be noted that the Euler-Bernoulli beam theory is suitable for slender beams. During the past several years, some researches indicated that the thermal effects on the mechanical behaviors of the carbon nanotubes are obvious. Jiang *et al*. (2004) developed a method to determine the thermal expansion coefficient for the nanotubes. In their research, it is concluded that the thermal expansion coefficient is negative for the low or room temperature but positive for the high temperature. Then some works on the mechanical characteristics of the carbon nanotubes with thermal effects are reported in literature (Yao and Han, 2007; Shen and Zhang, 2010; Wen-Hwa *et al*., 2012). To solve various boundary value problems, Generalized Differential Quadrature (GDQ) method is employed to discretize the governing differential equations of different nonlocal beam theories corresponding to four common sets of boundary conditions namely as simply supported-simply supported, clamped-clamped, clamped-simply supported and clamped free, however the small scale effect of boundary conditions has no any investigation on free vibration of CNTs.

In this study, a thermal vibration model is proposed to analyze the natural frequency of single-walled carbon nanotubes with clamped-free ends using Euler–Bernoulli theory. Based on the nonlocal constitutive relations of Eringen, an exact solution of governing equation is obtained. Influence of nonlocal small scale effects, temperature and modes of vibration of the CNT on the frequency are investigated and discussed. Difference of frequency results is shown for models with classical elasticity theory and nonlocal elasticity theory.

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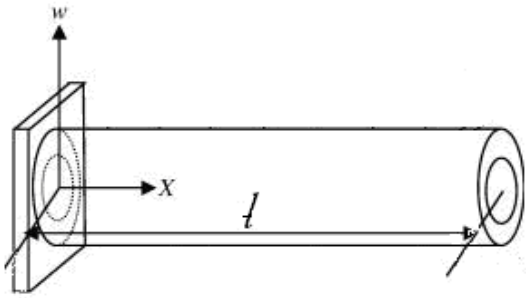

Fig. 1: Model of a cantilever SWCNT of length l

Basic equations: Many studies showed that the classic Euler-elastic beam offers a simple and reliable model for an overall mechanical deformation of CNTs, provided the characteristic wavelength is much larger than the diameter of CNTs. Therefore, the present study the thermal effect on the vibration of SWCNTs described by the Bernoulli–Euler beam model. In the present theory the plane cross sections of the beam remain plane during flexure and that the radius of curvature of a bent beam is large compared to the beam's depth. In addition, CNT is assumed to be clamped-free ends, shown in Fig. 1.

According to the Euler-Bernoulli beam theory (the classical beam theory), the strain displacement relations are given by:

$$\varepsilon_{xx} = -z\frac{\partial^2 w}{\partial x^2} \tag{1}$$

where x is the longitudinal coordinate measured from the left end of the beam, z the coordinate measured from the mid-plane of the beam, w the transverse displacement. Consider a cantilever SWCNT of length l. Young's modulus E, material density ρ, cross-sectional area A and cross-sectional inertia moment I, The free vibration equation of this beam-modeled CNT considering the thermal can be developed to become:

$$\frac{\partial^2 M}{\partial x^2} - \rho A\frac{\partial^2 w}{\partial t^2} + N_T\frac{\partial^2 w}{\partial x^2} = 0 \tag{2}$$

$$Q = -\frac{\partial M}{\partial x} \tag{3}$$

where,

M = The bending moment
Q = The shear force
N_T = The additional axial force arising due to thermal effects. On the basis of the theory of thermal elasticity mechanics, the axial force NT can be written as Zhang *et al*. (2008):

$$N_T = -\frac{EA}{1-2\nu}\alpha_x T \tag{4}$$

where, α_x is the coefficient of thermal expansion in the direction of x axis and v is the Poisson's ratio, respectively. T denotes the change in temperature. In the present study, it is assumed that only axial loads due to temperature change exist on the SWCNT and temperature change is considered at low or room temperature. It should be noted that the Young's modulus is assumed to insensitive to temperature change.

The boundary conditions of the nonlocal cantilever beam theory are of the form as follows:

$$w = 0 \quad , \quad \frac{\partial w}{\partial x} = 0 \text{ at } x = 0 \tag{5}$$

$$M = 0 \quad , \quad Q = 0 \text{ at } x = l \tag{6}$$

As written, the governing equations and boundary conditions appear of the same form as the local beam theory, but it must be recognized that the bending moment and shear force expressions for the nonlocal beam theory are different due to the nonlocal constitutive relations as will be demonstrated below (Eringen and Edelen, 1972)

$$\sigma_{xx} - (e_0 a)^2\frac{\partial^2\sigma_{xx}}{\partial x^2} = E\varepsilon_{xx} \tag{7}$$

where σ_{xx} is the normal stress, ε_{xx} is the normal strain and $e_0 a$ is the scale coefficient that incorporates the small scale effect. Note that a is the internal characteristic length (e.g., lattice parameter, C–C bond length and granular distance) and e_0 is a constant appropriate to each material.

Considering M = $\int_A \sigma_{xx}\, zdA$, multiplying Eq. (7) by zdA and integrating the result over the area A yields:

$$M - (e_0 a)^2\frac{\partial^2 M}{\partial x^2} = -EI\frac{\partial^2 w}{\partial x^2} \tag{8}$$

By substituting the equilibrium Eq. (2) and (3) into Eq. (8), one obtains:

$$M = -EI\frac{\partial^2 w}{\partial x^2} + (e_0 a)^2[\rho A\frac{\partial^2 w}{\partial t^2} - N_T\frac{\partial^2 w}{\partial x^2}] \tag{9}$$

$$Q = EI\frac{\partial^3 w}{\partial x^3} - (e_0 a)^2[\rho A\frac{\partial^3 w}{\partial x\partial t^2} - N_T\frac{\partial^3 w}{\partial x^3}] \tag{10}$$

In view of Eq. (9) and (10), the governing equations for the nonlocal Euler beams are given by:

$$EI\frac{\partial^4 w}{\partial x^4} + \rho A\frac{\partial^2 w}{\partial t^2} - N_T\frac{\partial^2 w}{\partial x^2} - (e_0 a)^2[\rho A\frac{\partial^4 w}{\partial x^2\partial t^2} - N_T\frac{\partial^4 w}{\partial x^4}] = 0 \tag{11}$$

On the basis of Eq. (5) (9) and (6) (10), the boundary conditions of the cantilever beam, associated with the nonlocal Euler beam theory, are given as follows:

$$w = 0 \quad , \quad \frac{\partial w}{\partial x} = 0 \text{ at x = 0} \tag{12}$$

$$M = -EI\frac{\partial^2 w}{\partial x^2} + (e_0 a)^2[\rho A\frac{\partial^2 w}{\partial t^2} - N_T\frac{\partial^2 w}{\partial x^2}] = 0$$

and

$$Q = EI\frac{\partial^3 w}{\partial x^3} - (e_0 a)^2\left[\rho A\frac{\partial^3 w}{\partial x \partial t^2} - N_T\frac{\partial^3 w}{\partial x^3}\right] = 0 \text{ at x = l} \tag{13}$$

Now we determine the solution of Eq. (11) with different boundary conditions. Let the solution be:

$$w(x,t) = W_0 e^{kx} e^{i\omega t} \tag{14}$$

where, ω is the circular natural frequency and $W(x)$ is the mode shape. Term i is the conventional imaginary number.

Substituting the Eq. (14) into Eq. (11) yields

$$\left[EI + (e_0 a)^2 N_T\right]k^4 + \left[(e_0 a)^2 \rho A\omega^2 - N_T\right]k^2 - \rho A\omega^2 = 0 \tag{15}$$

let

$$s_1 = \left[(e_0 a)^2 \rho A\omega^2 - N_T\right] / \left[EI + (e_0 a)^2 N_T\right]$$

$$s_0 = -\rho A\omega^2 / \left[EI + (e_0 a)^2 N_T\right]$$

yields:

$$k^4 + s_1 k^2 + s_0 = 0 \tag{16}$$

For arbitrary ω, Eq. (16) has four roots

$$k_{1,2} = \pm\sqrt{\frac{-s_1 + \sqrt{s_1^2 - 4s_0}}{2}}$$

$$k_{3,4} = \pm j\sqrt{\frac{s_1 + \sqrt{s_1^2 - 4s_0}}{2}} \tag{17}$$

Thus

$$w(x,t) = \sum_{j=1}^{4} C_j e^{k_j x} e^{i\omega t} \tag{18}$$

The items C_j ($j=1, 2, 3, 4$) are the constants determined from the boundary conditions.

By substituting Eq. (18) into the boundary conditions (12), (13), an eigenvalue problem may be set up as defined by:

$$[D]_{4\times4}\{C_1, C_2, C_3, C_4\}^T = 0 \tag{19}$$

NUMERICAL RESULTS AND DISCUSSION

On the basis of the vibration results obtained, we investigate the small scale effect of boundary condition on the frequency with a numerical example. Consider a (5, 5) armchair SWCNT with diameter d = 1 nm, lengths l= 10d and with the following assumed mechanical parameters: Young's modulus E = 1 TPa, ρ = 2300kg/m^3. It is reported that all the coefficients of thermal expansion for SWCNT are negative at low and room temperature and are positive at high temperature. In the present study, temperature change at low or room temperatures is considered. The coefficient of thermal expansion α_x = -1.6×10^{6}K.

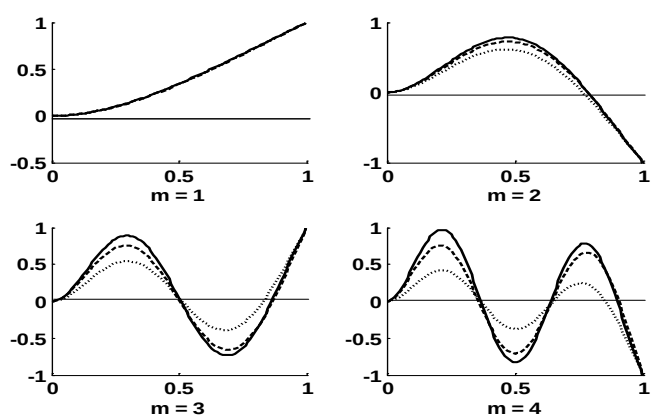

Fig. 2: The fisrt four mode shapes of the cantilever SWCNT with deferent theories for T = 50K and e_0a = 1nm (dashed line: Local Euler; dotted line: Nonlocal euler without nonlocal boundary; continuous line: Nonlocal euler with nonlocal boundary)

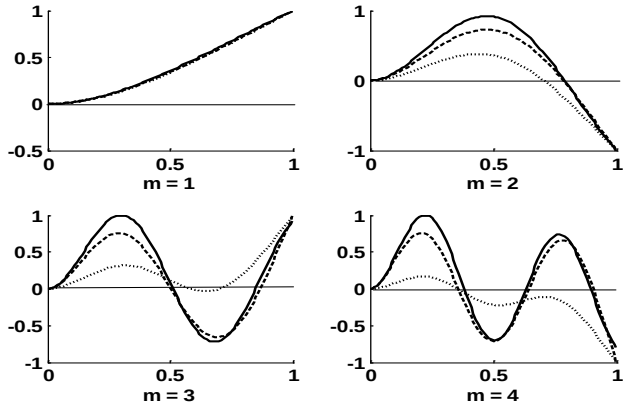

Fig. 3: The fisrt four mode shapes of the cantilever SWCNT with deferent theories for T = 50K and e_0a = 2nm (dashed line: Local euler; dotted line: Nonlocal euler without nonlocal boundary; continuous line: Nonlocal euler with nonlocal boundary)

Table 1: Dependence of the small-scale parameter on the first five free frequencies of the cantilever SWCNT with/without nonlocal boundary conditions (T = 50K) (LE: Local Euler; NE: Nonlocal Euler without nonlocal boundary; NEB: Nonlocal Euler with Nonlocal Boundary)

	e_0a [nm]						
	0	0.5		1		2	
Frequency [GHz] /Small scale / Mode	LE	NE	NEB	NE	NEB	NE	NEB
1	29.444	29.444	29.444	29.444	29.444	29.444	29.444
2	183.35	180.80	180.80	171.89	171.89	147.06	147.06
3	513.12	485.10	485.10	423.99	423.99	307.49	307.49
4	1003.3	898.91	898.91	711.74	711.74	452.00	452.00
5	1659.0	1387.8	1387.8	1008.4	1008.4	599.70	599.70

Table 2: Dependence of the small-scale parameter on the first five free frequencies of the cantilever SWCNT with/without nonlocal boundary conditions. (T = 0K); (LE: Local Euler; NE: Nonlocal Euler without nonlocal boundary; NEB: Nonlocal Euler with Nonlocal Boundary)

	e_0a [nm]						
	0	0.5		1		2	
Frequency [GHz] /Small scale / Mode	LE	NE	NEB	NE	NEB	NE	NEB
1	29.444	29.444	29.444	29.444	29.444	29.444	29.444
2	182.71	180.16	180.16	171.25	171.25	145.79	145.79
3	511.84	485.10	485.10	423.99	423.99	304.94	304.94
4	1003.3	897.63	897.63	711.10	711.10	449.45	449.45
5	1657.8	1386.6	1386.6	1006.5	1006.5	597.15	597.15

For same temperature change T, Fig. 2 and 3 illustrate the dependence of the first four mode shapes on the small scale with/whithout classical and small scale boundary conditions. It is clearly seen from these figures that for different theories, the mode shapes are actually significant difference. Furthermore with either larger values of m or lager values of e_0a, this difference becomes very strong. This means that the application of the nonlocal boundary conditions for CNT analysis would lead to significant change for the mode shapes. The reason for this phenomenon is, for a cantilever SWCNT, the boundary conditions at the free end has an obvious difference between the classical and small scale boundary conditions.

However, the small scale has not effect on frequency of nanotube when the nonlocal elastical theory is considered in boundary conditions. With the temperature change T = 0 K and 50K, the results of the first five frequencies of SWCNTs based on small scale are listed in Table 1 and 2, respectively. It can be seen from Table 1 and 2 that based on nanobeam, the frequencies have not change with/without classical and small scale boundary conditions for the different T and mode number m. This means that the scale effect on boundary conditions can be neglected when the thermal vibration of SWCNT is analyzed based on nonlocal elasticity theory. On basis of virtual work principle, this phenomenon can be explained that the virtual work made from small scale shear force and moment at the both ends cancel each other in viewpoint of energy or work.

CONCLUSION

In this study, the thermal vibration analysis of SWCNT with/without small scale boundary and nonlocal beam theory using exact solution has been performed. Since the additional work made by the moment and shear force at the free end from small scale

effect cancel each other, small scale boundary do not change natural frequencies. With this finding, in the cases of thermal vibration analysis using analytical solution, the boundary conditions due to local elasticity and nonlocal elasticity are also equivalent. Thus for simplicity, we can apply the local boundary condition to replace the small scale boundary condition.

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