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Thermal effect on transverse vibrations of double-walled carbon nanotubes

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Abstract

Based on the theory of thermal elasticity mechanics, a double-elastic beam model is developed for transverse vibrations of double-walled carbon nanotubes with large aspect ratios. The thermal effect is incorporated in the formulation. With this double-elastic beam model, explicit expressions are derived for natural frequencies and associated amplitude ratios of the inner to the outer tubes for the case of simply supported double-walled carbon nanotubes. The influence of temperature change on the properties of transverse vibrations is discussed. It is demonstrated that some properties of transverse vibrations of double-walled carbon nanotubes are dependent on the change of temperature.

1. Introduction

Carbon nanotubes (CNTs) discovered in 1991 [1] are cylindrical macromolecules composed of carbon atoms in a periodic hexagonal arrangement. As they are found to have remarkable mechanical, physical and chemical properties, CNTs hold exciting promise as structural elements in nanoscale devices or reinforcing elements in superstrong nanocomposites [2, 3]. Recently, CNTs have received a great deal of attention in various branches of science. By the use of a variety of experimental, theoretical and computer simulation approaches, extensive research studies of the properties of CNTs have been carried out [4–13].

As a thorough understanding of the mechanical responses of individual CNTs is of great importance for their potential applications [14, 15], the study of the vibrational behavior of CNTs is of practical interest. For the sake of the difficulties in experimental characterization of nanotubes and time-consuming and computationally expensive atomistic simulations, elastic continuum models have been widely used to study the vibrational behavior of CNTs [16–24]. In these continuum models, the single-elastic-beam model [16, 17] assumes that all originally concentric tubes of a multi-walled carbon nanotube (MWNT) remain coaxial during vibration while the multiple-elastic-beam model [20, 21] considers the

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intertube radial displacements of MWNTs which give rise to complicated intertube resonant frequencies and noncoaxial vibrational modes.

Lately, a great deal of research indicates that the mechanical properties of CNTs are related to temperature change. Zhang *et al* [25] conducted an experimental study of thermal effects on the Raman spectra of single-walled carbon nanotubes (SWNTs). They found that the lineshapes of the radial breathing mode features are sensitive to temperature. Raravikar et al [26] studied the temperature dependence of the radial breathing mode Raman frequency of SWNTs by using MD simulation and found that the coefficients of thermal expansion are positive in both radial and axial directions as the temperature is varied from 300 to 800 K. Schelling and Keblinski [27] obtained similar results through MD simulation. Pipes and Hubert [28] investigated the thermal expansion of helical CNTs arrays and the effective coefficients of thermal expansion of the array are determined. Based on the interatomic potential and the local harmonic model, Jiang et al [29] presented an analytical method to determine the coefficient of thermal expansion for SWNTs. Thev concluded that all the coefficients of thermal expansion are negative at low and room temperature and become positive at high temperature. Consequently, the investigation of the thermal effect on the mechanical properties of CNTs is of great importance and necessity. Ni et al [30] conducted an analysis of buckling behavior of SWNTs subjected to axial compression under a thermal environment. Zhang and Shen [31] investigated the temperature-dependent elastic properties of SWNTs by molecular dynamics simulation. Yao and Han [32, 33] studied the thermal effects on torsional and axially compressed buckling of MWNTs.

In this paper, based on the theory of thermal elasticity, a double-elastic-beam model is developed for transverse vibrations of double-walled carbon nanotubes (DWNTs), which accounts for the thermal effect in the formulation. 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 temperature change on them are investigated.

2. Double-elastic-beam model with thermal effect

The treatment of beam flexure developed here is on the basis of the Bernoulli–Euler theory. This theory is based upon the assumption that plane cross sections of a beam remain plane during flexure and that the radius of curvature of a bent beam is large compared with the beam's depth. Using the Bernoulli–Euler beam theory, the general equation for transverse vibrations of an elastic beam under distributed transverse pressure is expressed by [34, 35]

$$p(x) = EI\frac{\partial^4 w}{\partial x^4} - N\frac{\partial^2 w}{\partial x^2} + \rho A\frac{\partial^2 w}{\partial t^2},$$
(1)

where x is the axial coordinate, t is time, p(x) is the distributed transverse pressure per unit axial length (measured positive in the direction of the deflection), N is the axial force, w is the deflection of the beam, I and A are the moment of inertia and the area of the cross section of the beam, and E and ρ are Young's modulus and the mass density. Thus, EI denotes the bending stiffness of the beam and ρA represents the mass density per unit axial length.

On the basis of the theory of thermal elasticity mechanics, we have the following stress–strain relation [36]:

$$\boldsymbol{\sigma} = \lambda(\operatorname{tr}\boldsymbol{\varepsilon})\boldsymbol{\delta} + 2\mu\boldsymbol{\varepsilon} - (3\lambda + 2\mu)\alpha\theta\boldsymbol{\delta}, \qquad (2)$$

where σ and ϵ are, respectively, stress and strain tensors, λ and μ are Lame constants, δ is the Kronecker delta, the symbol 'tr' denotes the trace of a tensor, and α and θ are the coefficients of thermal expansion and temperature change, respectively.

Another assumption behind the Bernoulli–Euler beam model is that the beam consists of fibers parallel to the x axis, each in a state of uniaxial tension or compression. For the case of a uniaxial stress state, equation (2) reduces to

$$\sigma = E\varepsilon - \frac{E}{1 - 2v}\alpha\theta,\tag{3}$$

where σ is the axial stress, ε is the axial strain, α denotes the coefficient of thermal expansion in the direction of the *x* axis, and *E* and *v* are Young's modulus and Poisson's ratio, respectively. It is noted that use is made of the following equations:

$$\lambda = \frac{vE}{(1+v)(1-2v)}, \qquad \mu = \frac{E}{2(1+v)}.$$

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For the axial force N, we have

$$N = \sigma A = N_{\rm m} + N_t, \tag{4}$$

where

$$N_{\rm m} = \sigma_{\rm m} A, \qquad N_t = -\frac{EA}{1-2v} \alpha \theta,$$
 (5)

in which $\sigma_{\rm m}$ is the axial stress due to the mechanical loading. Substituting equation (4) into (1), we obtain

$$\left(\sigma_{\rm m}A - \frac{EA}{1-2v}\alpha\theta\right)\frac{\partial^2 w}{\partial x^2} + p(x) = EI\frac{\partial^4 w}{\partial x^4} + \rho A\frac{\partial^2 w}{\partial t^2}.$$
 (6)

It is known that DWNTs are distinguished from traditional elastic beams by their hollow two-layer structure and associated intertube van der Waals forces. As CNTs have high thermal conductivity, it may be regarded that the change of temperature is uniformly distributed in the CNT. Thus, equation (6) can be used for each of the inner and outer tubes of the DWNTs. Assuming that the inner and outer tubes have the same thickness and effective material constants, we have

$$p_{12} + \left(\sigma_{\rm m}A_1 - \frac{EA_1}{1 - 2v}\alpha\theta\right)\frac{\partial^2 w_1}{\partial x^2} = EI_1\frac{\partial^4 w_1}{\partial x^4} + \rho A_1\frac{\partial^2 w_1}{\partial t^2}$$
(7a)
$$-p_{12} + \left(\sigma_{\rm m}A_2 - \frac{EA_2}{1 - 2v}\alpha\theta\right)\frac{\partial^2 w_2}{\partial x^2} = EI_2\frac{\partial^4 w_2}{\partial x^4} + \rho A_2\frac{\partial^2 w_2}{\partial t^2},$$
(7b)

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

For small-deflection linear vibration, the van der Waals pressure at any point between two tubes should be a linear function of the jump in deflection at that point. Thus, the interaction pressure per unit axial length is given by [37, 38]

$$p_{12} = c(w_2 - w_1), \tag{8}$$

where c is the intertube interaction coefficient per unit length between two tubes, which can be estimated by [38]

$$c = \frac{320(2R_1) \operatorname{erg} \operatorname{cm}^{-2}}{0.16a^2}$$

where R_1 is the radius of the inner tube, and the value of parameter *a* is chosen to be 0.142 nm which is the length of a C–C bond.

Introduction of equation (8) into equations (7a) and (7b) yields

$$c(w_{2} - w_{1}) + \left(\sigma_{m}A_{1} - \frac{EA_{1}}{1 - 2v}\alpha\theta\right) = EI_{1}\frac{\partial^{4}w_{1}}{\partial x^{4}}$$

+ $\rho A_{1}\frac{\partial^{2}w_{1}}{\partial t^{2}}$ (9a)
 $-c(w_{2} - w_{1}) + \left(\sigma_{m}A_{2} - \frac{EA_{2}}{1 - 2v}\alpha\theta\right) = EI_{2}\frac{\partial^{4}w_{2}}{\partial x^{4}}$

$$+\rho A_2 \frac{\partial^2 w_2}{\partial t^2}.$$
(9b)

With the thermal effect included, these two differential equations describe the transverse vibrations of DWNTs, and they are coupled together by the van der Walls interaction. When the thermal effect is ignored, equations (9a) and (9b) reduce to the result obtained by Zhang *et al* [39] for DWNTs.

3. Solution of the problem

Let us consider a DWNT of length *L*. Suppose that its ends are simply supported, the boundary conditions are given by

$$w_{1}(0,t) = \frac{\partial^{2} w_{1}(0,t)}{\partial x^{2}} = w_{1}(L,t) = \frac{\partial^{2} w_{1}(L,t)}{\partial x^{2}} = 0$$
(10a)
$$w_{2}(0,t) = \frac{\partial^{2} w_{2}(0,t)}{\partial x^{2}} = w_{2}(L,t) = \frac{\partial^{2} w_{2}(L,t)}{\partial x^{2}} = 0.$$
(10b)

The homogeneous partial differential equations (9a) and (9b) with the governing boundary conditions (10a) and (10b) can be solved by the Bernoulli–Fourier method assuming the solutions in the form

$$w_1(x,t) = \sum_{n=1}^{\infty} X_n(x) T_{1n}(t)$$
(11a)

$$w_2(x,t) = \sum_{n=1}^{\infty} X_n(x) T_{2n}(t), \qquad (11b)$$

where $T_{1n}(t)$ and $T_{2n}(t)$ are the unknown time functions, and $X_n(x)$ is the known mode shape function for a simply supported single beam, which is expressed as

$$X_n(x) = \sin(k_n x),$$
 $k_n = \frac{n\pi}{L},$ $n = 1, 2, 3,$

Introduction of equations (11a) and (11b) into equations (9a) and (9b) leads to

$$\begin{split} &\sum_{n=1}^{\infty} \left(\rho A_1 \frac{\partial^2 T_{1n}}{\partial t^2} + \left(E I_1 k_n^4 + c \right. \\ &+ \left(N_{m1} - \frac{E A_1}{1 - 2v} \alpha \theta \right) k_n^2 \right) T_{1n} - c T_{2n} \right) X_n = 0 \\ &\sum_{n=1}^{\infty} \left(\rho A_2 \frac{\partial^2 T_{2n}}{\partial t^2} + \left(E I_2 k_n^4 + c \right. \\ &+ \left(N_{m2} - \frac{E A_2}{1 - 2v} \alpha \theta \right) k_n^2 \right) T_{2n} - c T_{1n} \right) X_n = 0. \end{split}$$

It follows from the above that

$$\frac{\partial^2 T_{1n}}{\partial t^2} + (F_1 + \eta \sigma_{\rm m} - Q\alpha\theta)T_{1n} - H_1T_{2n} = 0 \qquad (12a)$$

$$\frac{\partial^2 T_{2n}}{\partial t^2} + (F_2 + \eta \sigma_{\rm m} - Q\alpha\theta)T_{2n} - H_2T_{1n} = 0, \qquad (12b)$$

where

$$F_{1} = \frac{EI_{1}k_{n}^{4}}{\rho A_{1}} + H_{1}, \qquad H_{1} = \frac{c}{\rho A_{1}}, \qquad \eta = \frac{k_{n}^{2}}{\rho}$$
$$F_{2} = \frac{EI_{2}k_{n}^{4}}{\rho A_{2}} + H_{2}, \qquad H_{2} = \frac{c}{\rho A_{2}}, \qquad Q = \frac{E}{1 - 2v}\eta.$$

The solutions of equations (12a) and (12b) can be expressed by

$$T_{1n}(t) = C_{1n} e^{i\omega_n t}, \qquad T_{2n}(t) = C_{2n} e^{i\omega_n t}, \qquad i = \sqrt{-1},$$
(13)

where ω_n denotes the natural frequency of the DWNT, and C_{1n} and C_{2n} represent the amplitude coefficients of the inner and outer tubes, respectively. Substituting equation (13) into equations (12*a*) and (12*b*), we obtain

$$(F_1 + \eta \sigma_{\rm m} - Q\alpha\theta - \omega_n^2)C_{1n} - H_1C_{2n} = 0$$
(14*a*)

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$$(F_2 + \eta \sigma_{\rm m} - Q\alpha\theta - \omega_n^2)C_{2n} - H_2C_{1n} = 0.$$
(14b)

Non-trivial solutions for the constants C_{1n} and C_{2n} can be obtained only when the determinant of the coefficients in equations (14*a*) and (14*b*) vanishes. Consequently, we have

$$\omega_n^4 - (F_1 + F_2 + 2\eta\sigma_{\rm m} - 2Q\alpha\theta)\omega_n^2 + (F_1 + \eta\sigma_{\rm m} - Q\alpha\theta)$$
$$\times (F_2 + \eta\sigma_{\rm m} - Q\alpha\theta) - H_1H_2 = 0 \tag{15}$$

which is the frequency characteristic equation. It is found that the discriminant of this biquadratic algebraic equation is positive

$$\Delta = (F_1 - F_2)^2 + 4H_1H_2 > 0.$$

Thus the characteristic equation (15) has two different, real, and positive roots

$$\omega_{nI}^{2} = \frac{1}{2}(F_{1} + F_{2} + 2\eta\sigma_{m} - 2Q\alpha\theta) -\sqrt{(F_{1} - F_{2})^{2} + 4H_{1}H_{2}}$$
(16a)
$$\omega_{nII}^{2} = \frac{1}{2}(F_{1} + F_{2} + 2\eta\sigma_{m} - 2Q\alpha\theta)$$

$$+\sqrt{(F_1 - F_2)^2 + 4H_1H_2}),\tag{16b}$$

where ω_{nI} is the lower natural frequency and ω_{nII} is the higher natural frequency. For each of the natural frequencies, the associated amplitude ratio of the vibrational modes of the inner to the outer tubes is given by

$$B_n = \frac{C_{1n}}{C_{2n}} = \frac{H_1}{F_1 + \eta \sigma_m - Q\alpha\theta - \omega_n^2}$$
$$= \frac{F_2 + \eta \sigma_m - Q\alpha\theta - \omega_n^2}{H_2}.$$
(17)

Introducing equations (16a) and (16b) into equation (17), respectively, we obtain

$$B_{nI} = \frac{1}{2H_2}(F_2 - F_1 + \sqrt{(F_1 - F_2)^2 + 4H_1H_2}) \quad (18a)$$

$$B_{n\Pi} = \frac{1}{2H_2} (F_2 - F_1 - \sqrt{(F_1 - F_2)^2 + 4H_1H_2}). \quad (18b)$$

It can be observed that the amplitude ratio B_{nI} dependent on the lower natural frequency ω_{nI} is always positive, which indicates that the inner and outer tubes execute synchronous vibrations, while the amplitude ratio B_{nII} dependent on the higher frequency ω_{nII} is always negative, which indicates that the inner and outer tubes execute asynchronous vibrations. It can also be found that the amplitude ratios B_{nI} and B_{nII} are independent of the change of temperature.

4. Discussion

To focus on the thermal effect, the axial mechanical load is assumed absent. In this manner we have

$$\omega_{n\mathrm{I}}^{2} = \frac{1}{2} \left(F_{1} + F_{2} - 2Q\alpha\theta - \sqrt{(F_{1} - F_{2})^{2} + 4H_{1}H_{2}} \right)$$

$$\omega_{n\mathrm{II}}^{2} = \frac{1}{2} \left(F_{1} + F_{2} - 2Q\alpha\theta + \sqrt{(F_{1} - F_{2})^{2} + 4H_{1}H_{2}} \right).$$
(19a)
(19b)

When the thermal effect is also ignored, equations (19a) and (19b) reduce to the classical results [20]

$$(\omega_{nI}^0)^2 = \frac{1}{2}(F_1 + F_2 - \sqrt{(F_1 - F_2)^2 + 4H_1H_2})$$
(20a)

$$(\omega_{n\Pi}^0)^2 = \frac{1}{2}(F_1 + F_2 + \sqrt{(F_1 - F_2)^2 + 4H_1H_2}).$$
(20b)

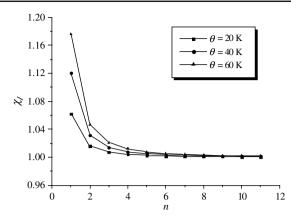


Figure 1. Thermal effects on the lower natural frequency ω_{n1} with the aspect ratio $L/d_2 = 40$ in the case of low or room temperature.

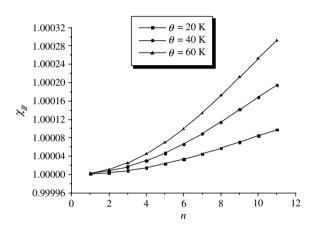


Figure 2. Thermal effects on the higher natural frequency $\omega_{n\rm II}$ with the aspect ratio $L/d_2 = 40$ in the case of low or room temperature.

To examine the influence of temperature change on vibrations of double-walled nanotubes, the results including and excluding the thermal effect are compared. It follows that the ratios of the results with temperature change to those without temperature change are respectively given by

$$\chi_{\mathrm{I}} = \frac{\omega_{n\mathrm{I}}}{\omega_{n\mathrm{I}}^{0}}, \qquad \chi_{\mathrm{II}} = \frac{\omega_{n\mathrm{II}}}{\omega_{n\mathrm{II}}^{0}}.$$

As previously mentioned, Jiang *et al* [29] found that the coefficients of thermal expansion for CNTs are negative at low or room temperature and become positive at high temperature. Consequently, the values of the ratios $\chi_{\rm I}$ and $\chi_{\rm II}$ are herein calculated for both cases of low and high temperatures. The parameters used in calculations for the DWNT are given as follows: the Young's modulus E = 1 TPa with the effective thickness of SWNTs taken to be 0.35 nm and the mass density $\rho = 2.3$ g cm⁻³ [40], the Poisson's ratio $\nu = 0.3$ [41], and the inner diameter $d_1 = 0.7$ nm and the outer diameter $d_2 = 1.4$ nm [42].

For the case of room or low temperature, we suppose $\alpha = -1.6 \times 10^{-6} \text{ K}^{-1}$ [32, 33]. With the aspect ratio $L/d_2 = 40$, the thermal effects on the lower natural frequency ω_{nI} and the higher natural frequency ω_{nII} are shown in figures 1 and 2, respectively. With the vibrational mode number n = 2, the

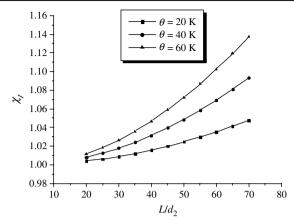


Figure 3. Thermal effects on the lower natural frequency ω_{n1} with the vibrational mode number n = 2 in the case of low or room temperature.

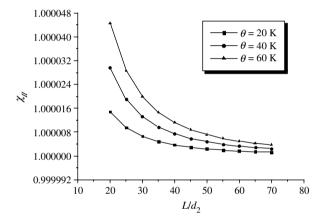


Figure 4. Thermal effects on the higher natural frequency $\omega_{n\text{II}}$ with the vibrational mode number n = 2 in the case of low or room temperature.

thermal effects on ω_{nI} and ω_{nII} represented by the ratios χ_I and χ_{II} are indicated in figures 3 and 4. As can be seen, the thermal effect on the lower natural frequency ω_{nI} is significant while the higher natural frequency ω_{nII} is insensitive to temperature change. The thermal effect on the lower natural frequency ω_{nI} diminishes with increasing the number *n* and becomes more significant with the increase of the aspect ratio L/d_2 and temperature change θ . Moreover, it can be observed from figures 1–4 that the values of ω_{nI} and ω_{nII} accounting for the thermal effect are larger than those ignoring the influence of temperature change.

For the case of high temperature, we suppose $\alpha = 1.1 \times 10^{-6} \text{ K}^{-1}$ [32, 33]. With the aspect ratio $L/d_2 = 40$, the thermal effects on the lower natural frequency ω_{nI} and the higher natural frequency ω_{nII} are obtained, which are illustrated in figures 5 and 6, respectively. With the vibrational mode number n = 2, the thermal effects on ω_{nI} and ω_{nII} are calculated, which are indicated in figures 7 and 8. It is found from figures 5–8 that the thermal effect on the lower natural frequency ω_{nI} is significant while the influence of temperature change on the higher natural frequency ω_{nII} is very insignificant. This is consistent with the case of room

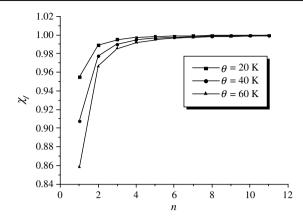


Figure 5. Thermal effects on the lower natural frequency ω_{nI} with the aspect ratio $L/d_2 = 40$ in the case of high temperature.

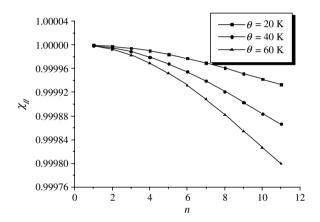


Figure 6. Thermal effects on the higher natural frequency $\omega_{n\Pi}$ with the aspect ratio $L/d_2 = 40$ in the case of high temperature.

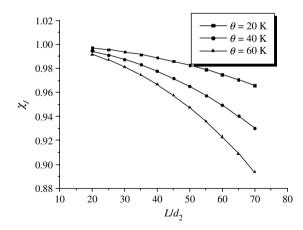


Figure 7. Thermal effects on the lower natural frequency ω_{n1} with the vibrational mode number n = 2 in the case of high temperature.

or low temperature. We can also draw a similar conclusion to the case of room or low temperature that the thermal effect on the lower natural frequency ω_{nI} becomes less significant with the increase of the vibrational mode number *n* and increases with increasing the aspect ratio L/d_2 and temperature change θ . In addition, it is seen from figures 5–8 that the values of

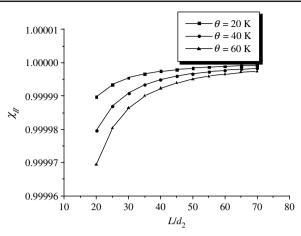


Figure 8. Thermal effects on the higher natural frequency $\omega_{n\text{II}}$ with the vibrational mode number n = 2 in the case of high temperature.

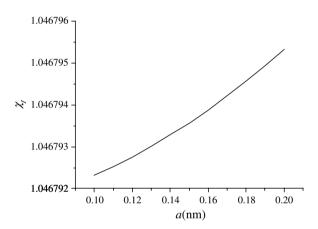


Figure 9. Relationship between values of the ratio χ_1 and parameter *a* with n = 2, $L/d_2 = 40$ and $\theta = 60$ K in the case of low or room temperature.

 ω_{nI} and ω_{nII} considering the thermal effect are smaller than those excluding the influence of temperature change, which is contrary to the case at room or low temperature.

It should be pointed out that the present model can be applied to the various nanotubes with different chirality as the diameter of a SWNT is a function of tube chirality, which can be expressed as

$$d = \frac{\sqrt{3}a}{\pi} \sqrt{(n_1^2 + n_2^2 + n_1 n_2)},$$

where the pair of integers (n_1, n_2) represent the chirality of the SWNT. In addition, it is noted that the parameter a, the C–C bond length, is quoted as 0.142 nm in the present model. However, the C–C bond length is actually not a uniform constant in CNTs but is a function of bond orientation with respect to the nanotube axis as well as tube chirality. In consideration of this, the sensitivity of the present model to the value of the parameter a is discussed, as shown in figures 9–12. It is seen from figures 9–12 that the thermal effects on transverse vibrations of DWNTs with large aspect ratios are insensitive to the value variation of the parameter a. This implies that for a specific diameter the thermal effect on the

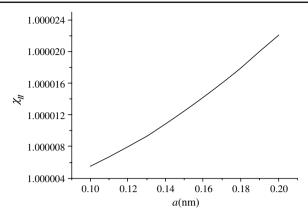


Figure 10. Relationship between the values of ratio χ_{II} and parameter *a* with n = 2, $L/d_2 = 40$ and $\theta = 60$ K in the case of low or room temperature.

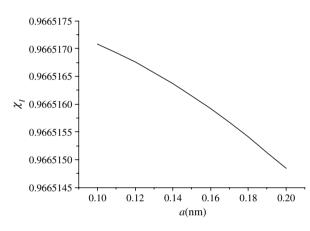


Figure 11. Relationship between the values of ratio χ_1 and parameter *a* with n = 2, $L/d_2 = 40$ and $\theta = 60$ K in the case of high temperature.

transverse vibration of a DWNT with large aspect ratio is almost independent of its chirality.

5. Conclusions

On the basis of the Bernoulli–Euler beam theory and thermal elasticity, the general equation for transverse vibrations of an elastic beam under distributed transverse pressure is formulated. Following this general equation, a double-elastic-beam model is developed for transverse vibrations of DWNTs, which takes the thermal effect into account. For the case of simply supported DWNTs, the natural frequencies and the associated amplitude ratios of the inner to the outer tubes are determined.

It is concluded that the thermal effect on the lower natural frequency ω_{nI} is significant while the higher natural frequency ω_{nII} is insensitive to the change of temperature. The thermal effect on the lower natural frequency ω_{nI} decreases with the increase of the vibrational mode number *n* and increases with increasing the aspect ratio L/d_2 and temperature change θ . It is also shown that the values of ω_{nI} and ω_{nII} accounting for the thermal effect are larger than those ignoring the influence of temperature change for the case of room or low temperature, whereas the values of ω_{nI} and ω_{nII} with the thermal effect

Figure 12. Relationship between the values of ratio χ_{II} and parameter *a* with n = 2, $L/d_2 = 40$ and $\theta = 60$ K in the case of high

are smaller than those excluding the thermal effect for the case of high temperature. In addition, it is found that the amplitude ratios B_{nI} and B_{nII} are independent of the change of temperature. It is also shown that for a specific diameter the thermal effect on the transverse vibration of a DWNT with large aspect ratio is almost independent of its chirality.

Acknowledgment

0.999998

0 999996

0 999994

0 999992

0 999990

0 999988

0.999986 0.999984

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temperature.

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