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Li Feng Wang · Hai Yan Hu

Thermal vibration of double-walled carbon nanotubes predicted via double-Euler-beam model and molecular dynamics

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Abstract The paper presents how to study the thermal vibration of a double-walled carbon nanotube (DWCNT) by using a model of double-Euler beams, together with the law of energy equipartition, with the energy of van der Waals interaction between layers taken into consideration. The basic finding of the study is the relation, derived via the model of double-Euler beams and the law of energy equipartition, between the temperature and the root-of-mean-squared (RMS) amplitude of the thermal vibration at any cross section of the DWCNT. The molecular dynamics simulations of thermal vibration of the DWCNT in argon atmosphere show that the model of double-Euler beams can predict the RMS amplitude of the thermal vibration of the DWCNT reasonably well.

1 Introduction

The development of nanotechnology enables one to construct small devices based on carbon nanotubes and activated by thermal fluctuation. The thermal vibration can serve as a source of self-excitation and noise in determining the natural frequencies and the resonance properties of the carbon nanotubes. The need of modeling and analyzing the thermal vibration of carbon nanotubes has attracted much attention. For example, Treacy et al. [1] estimated the Young's modulus of isolated carbon nanotubes by measuring, in a transmission electron microscope, the amplitude of their intrinsic thermal vibrations. Krishnan et al. [2] presented the relationship between Young's modulus, the size, and the stand deviation of the vibration amplitude at the tip of a carbon nanotube at a given temperature by using the model of an Euler beam. Xu et al. [3] studied thermally driven large-amplitude fluctuations in carbon-nanotube-based devices. Their molecular dynamic simulations show that the axial oscillation of large amplitude can be effectively excited for the local van der Waals potential barrier accessible by the thermal fluctuation. Hsieh et al. [4] investigated the variations in the Young's modulus of single-walled carbon nanotubes with tube radius and temperature via molecular dynamic simulations of intrinsic thermal vibrations. Wang et. al. [5] studied the thermal vibration of single-walled carbon nanotubes based on the model of Timoshenko beam, together with the law of energy equipartition and molecular dynamic simulations. Feng and Jones [6] calculated the free thermal vibrations of cantilevered carbon nanotubes by using molecular dynamics and explained the resulting power spectral density of the tip displacement with statistical mechanics and beam theory. Most recently, they found that the quality factor of the cantilever carbon nanotube is independent of its length and that the intrinsic signal-to-noise ratio for a cantilever carbon nanotube improves with an increase in length [7].

L. F. Wang (✉) · H. Y. Hu
State Key Laboratory of Mechanics and Control of Mechanical Structures,
Nanjing University Aeronautics and Astronautics, Nanjing 210016, China
E-mail: walfe@nuaa.edu.cn
Tel.: +86-25-8489-2003-8004
Fax: +86-25-8489-2003-8004

Recent years have witnessed numerous applications of the multi-beam model to analyzing the vibration and wave propagation of carbon nanotubes [8]. For example, Yoon et al. [9,10] studied the flexural vibration and wave propagation of a multi-walled carbon nanotube based on the models of Euler beam and Timoshenko beam. To the best of the authors knowledge , however, neither experimental studies nor numerical simulations have been available for the validation of the model of double-Euler beams in studying the thermal vibration of a DWCNT.

Different from other free vibration, the thermal vibration of a nanostructure should yield the law of energy equipartition when the quantum effect is not dominant. The primary objective of this study is to check the validity of the model of double-Euler beams together with the law of energy equipartition, with the effects of interlayer van der Waals interaction taken into consideration, in studying the thermal vibration, simulated via the molecular dynamics, of a DWCNT in argon atmosphere. For this purpose, Sect. 2 presents the RMS amplitude of the stochastically driven vibration of a model of double-Euler beams to be used to model a DWCNT. Section 3 gives the molecular dynamic simulation for the thermal vibration of DWCNTs in argon atmosphere based on the Brenner potential and Lennard–Jones pair potential. Section 4 outlines a comparison between the analytical results and numerical results. Finally, the paper ends with Sect. 5 with some conclusions.

2 Model of double-Euler beams for DWCNT

This section starts with the following dynamic equation of a model of double beams with uniform cross section for a DWCNT placed along direction x in the frame of coordinates (x, y, z). The vibration of the carbon nanotube in y direction is uncoupled from that in z direction in the linear vibration range. The section deals with the case when both nested individual tubes of the DWNT vibrate in the same plane to represent the vibration of the DWCNT in any direction. The displacements of section x of the inner tube and outer tube in direction y at the moment t, $w_i(x,t)$, $i = 1, 2$, are described by [9,11]

$$c_{12}(w_2 - w_1) = E_1 I_1 \frac{\partial^4 w_1}{\partial x^4} + \rho A_1 \frac{\partial^2 w_1}{\partial t^2}, \tag{1a}$$

$$c_{12}(w_1 - w_2) = E_2 I_2 \frac{\partial^4 w_2}{\partial x^4} + \rho A_2 \frac{\partial^2 w_2}{\partial t^2}, \tag{1b}$$

where E_1 and E_2 are Young's moduli of inner tube and outer tube, I_1 and I_2 are the moments of inertia for the cross section of inner tube and outer tube, A_1 and A_2 are the cross-sectional areas of inner tube and outer tube, ρ is the mass density, and c_{12} is the coefficient of the van der Waals interaction pressure per unit axial length and can be estimated based on an effective interaction width

$$c_{12} = 2R_1 C_{12}. \tag{2}$$

Here, the van der Waals interaction coefficient C_{12} obtained through the Lennard–Jones pair potential by He et al. [12] is used.

The study focuses on the case when both nested individual nanotubes of the DWCNT are clamped at $x = 0$ and free at $x = L$, where L is the length of the DWCNT. Hence, the boundary conditions of the DWCNT are

$$w_1(0,t) = 0, \quad \frac{\partial w_1(0,t)}{\partial x} = 0, \quad \frac{\partial^2 w_1(L,t)}{\partial x^2} = 0, \quad \frac{\partial^3 w_1(L,t)}{\partial x^3} = 0, \tag{3a}$$

$$w_2(0,t) = 0, \quad \frac{\partial w_2(0,t)}{\partial x} = 0, \quad \frac{\partial^2 w_2(L,t)}{\partial x^2} = 0, \quad \frac{\partial^3 w_2(L,t)}{\partial x^3} = 0. \tag{3b}$$

Equations (1) and (3) indicate that both nested carbon nanotubes share the same vibration mode, but may vibrate in phase or out of phase.

To study the free vibration of the DWCNT, let the dynamic deflections of the inner tube and the outer tube be given by

$$w_1 = \hat{w}_1 e^{j\omega t}, \quad w_2 = \hat{w}_2 e^{j\omega t}, \tag{4}$$

where $\hat{w}_1$ and $\hat{w}_2$ represent the deflection amplitudes of the inner tube and the outer tube, respectively. It is straightforward to derive that the inner tube and the outer tube of DWCNT have the following vibration modes:

$$\begin{aligned} w_{1n}(x,t) &= \hat{w}_{1n}(x)\mathrm{e}^{j\omega_n t} = a_{1n} f_n(x)\mathrm{e}^{j\omega_n t} \\ &= \frac{D_n \chi}{2}\left[\cos\lambda_n x - \cosh\lambda_n x + \frac{\sin\lambda_n L - \sinh\lambda_n L}{\cos\lambda_n L + \cosh\lambda_n L}\left(\sin\lambda_n x - \sinh\lambda_n x\right)\right]\mathrm{e}^{j\omega_n t}, \end{aligned} \tag{5a}$$

$$\begin{aligned} w_{2n}(x,t) &= \hat{w}_{2n}(x)\mathrm{e}^{j\omega_n t} = a_{2n} f_n(x)\mathrm{e}^{j\omega_n t} \\ &= \frac{D_n}{2}\left[\cos\lambda_n x - \cosh\lambda_n x + \frac{\sin\lambda_n L - \sinh\lambda_n L}{\cos\lambda_n L + \cosh\lambda_n L}\left(\sin\lambda_n x - \sinh\lambda_n x\right)\right]\mathrm{e}^{j\omega_n t}, \end{aligned} \tag{5b}$$

where $j \equiv \sqrt{-1}$, $\lambda_n^4 \overset{\text{def}}{=} \frac{\rho A}{EI}\omega_n^2$, $\lambda_n L = 1.875, 4.694, 7.855, 10.996, 14.137, \ldots$, $\chi_n = a_{1n}/a_{2n}$ is the amplitude ratio of vibration modes of the inner tube to the outer tube, and D_n is a constant determined from temperature.

It turns out that the DWCNT has two natural frequencies of order n in contrast to the single natural frequency of order n of a single-walled carbon nanotube. The two natural frequencies of order n and the associated amplitude ratio of the carbon nanotubes are given by [9]

$$\omega_{nL}^2 = \frac{1}{2}\left(\alpha_n - \sqrt{\alpha_n^2 - 4\beta_n}\right), \tag{6a}$$

$$\omega_{nH}^2 = \frac{1}{2}\left(\alpha_n + \sqrt{\alpha_n^2 - 4\beta_n}\right), \tag{6b}$$

where

$$\alpha_n = \frac{E_1 I_1 \lambda_n^4 + c_{12}}{\rho A_1} + \frac{E_2 I_2 \lambda_n^4 + c_{12}}{\rho A_2}, \tag{6c}$$

$$\beta_n = \frac{E_1 I_1 E_2 I_2 \lambda_n^8}{\rho^2 A_1 A_2} + c_{12}\lambda_n^4 \frac{E_1 I_1 + E_2 I_2}{\rho^2 A_1 A_2}. \tag{6d}$$

In Eq. (6), ω_{nL} stands for the lower natural frequency of order n in a coaxial vibration, whereas ω_{nH} stands for the higher natural frequency of order n in a non-coaxial vibration. For each of the natural frequencies, the associated amplitude ratio of natural vibration modes of the inner tube to the outer tube is

$$\begin{aligned} \chi_{nL} &= \frac{a_{1n}}{a_{2n}} = 1 + \frac{E_2 I_2 \lambda_n^4}{c_{12}} - \frac{\rho\omega_{nL}^2 A_2}{c_{12}}, \\ \chi_{nH} &= \frac{a_{1n}}{a_{2n}} = 1 + \frac{E_2 I_2 \lambda_n^4}{c_{12}} - \frac{\rho\omega_{nH}^2 A_2}{c_{12}}. \end{aligned} \tag{7}$$

The total energy $\tilde{E}_n$ corresponding to the nth mode $\omega_n = \omega_{nL}$ or ω_{nH} can be found by calculating the elastic energy at the instant of maximal deflection when the cantilever carbon nanotube is momentarily stationary for $\mathrm{e}^{j\omega_n t} = 1$ as follows:

$$\begin{aligned} \tilde{E}_{nL}^{\text{elastic}} &= \left[\frac{E_1 I_1}{2}\int_0^L \left(\frac{\partial^2 \hat{w}_{1n}}{\partial x^2}\right)^2 \mathrm{d}x + \frac{E_2 I_2}{2}\int_0^L \left(\frac{\partial^2 \hat{w}_{2n}}{\partial x^2}\right)^2 \mathrm{d}x + \frac{1}{2}c_{12}\left(\hat{w}_{1n} - \hat{w}_{2n}\right)^2\right] \\ &= D_{nL}^2\left[\chi_{nL}^2 \frac{E_1 I_1}{2}\int_0^L \left(\frac{\partial^2 f_n}{\partial x^2}\right)^2 \mathrm{d}x + \frac{E_2 I_2}{2}\int_0^L \left(\frac{\partial^2 f_n}{\partial x^2}\right)^2 \mathrm{d}x + \frac{1}{2}c_{12} f_n^2 \left(\chi_{nL} - 1\right)^2\right], \end{aligned} \tag{8a}$$

$$\tilde{E}_{nH}^{\text{elastic}} = D_{nH}^2\left[\chi_{nH}^2 \frac{E_1 I_1}{2}\int_0^L \left(\frac{\partial^2 f_n}{\partial x^2}\right)^2 \mathrm{d}x + \frac{E_2 I_2}{2}\int_0^L \left(\frac{\partial^2 f_n}{\partial x^2}\right)^2 \mathrm{d}x + \frac{1}{2}c_{12} f_n^2 \left(\chi_{nH} - 1\right)^2\right]. \tag{8b}$$

From the law of energy equipartition, there is an averaged energy of $kT/2$ per degree of freedom for all of the relevant lateral vibration modes. Because there are both elastic and kinetic energy degrees of freedom for

all of the relevant lateral vibration modes, then on average, both $\langle \tilde{E}_{nL} \rangle = kT$ and $\langle \tilde{E}_{nH} \rangle = kT$ hold for each vibration mode, with $\tilde{E}_{nL}$ or $\tilde{E}_{nH}$ yielding the Boltzmann distribution. It is straightforward to show that each mode of a stochastically driven oscillator has a Gaussian probability profile, and the standard deviation of the vibration amplitude coefficients D_n of the model of double-Euler beams is given by [2,5]

$$D_{nL}^2 = \tilde{E}_n^{\text{elastic}} \Bigg/ \left[\chi_{nL}^2 \frac{E_1 I_1}{2} \int_0^L \left(\frac{\partial^2 f_n}{\partial x^2} \right)^2 \mathrm{d}x + \frac{E_2 I_2}{2} \int_0^L \left(\frac{\partial^2 f_n}{\partial x^2} \right)^2 \mathrm{d}x + \frac{1}{2} c_{12} f_n^2 \left(\chi_{nL} - 1 \right)^2 \right]$$

$$= kT \Bigg/ \left[\chi_{nL}^2 \frac{E_1 I_1}{2} \int_0^L \left(\frac{\partial^2 f_n}{\partial x^2} \right)^2 \mathrm{d}x + \frac{E_2 I_2}{2} \int_0^L \left(\frac{\partial^2 f_n}{\partial x^2} \right)^2 \mathrm{d}x + \frac{1}{2} c_{12} f_n^2 \left(\chi_{nL} - 1 \right)^2 \right], \tag{9a}$$

$$D_{nH}^2 = kT \Bigg/ \left[\chi_{nH}^2 \frac{E_1 I_1}{2} \int_0^L \left(\frac{\partial^2 f_n}{\partial x^2} \right)^2 \mathrm{d}x + \frac{E_2 I_2}{2} \int_0^L \left(\frac{\partial^2 f_n}{\partial x^2} \right)^2 \mathrm{d}x + \frac{1}{2} c_{12} f_n^2 \left(\chi_{nH} - 1 \right)^2 \right]. \tag{9b}$$

Then, the RMS amplitudes of the nth mode at x read

$$\hat{\sigma}_{1nL}(x) = D_{nL} \chi_{nL} f_n(x), \quad \hat{\sigma}_{2nL}(x) = D_{nL} f_n(x), \tag{10a}$$

$$\hat{\sigma}_{1nH}(x) = D_{nH} \chi_{nH} f_n(x), \quad \hat{\sigma}_{2nH}(x) = D_{nH} f_n(x). \tag{10b}$$

As all vibration modes are independent, their contributions can be added incoherently. To average coherently over all the vibration modes, it is possible to simply add the variances $\sigma_{1nL}^2(x)$, $\sigma_{1nH}^2(x)$ or $\sigma_{2nL}^2(x), \sigma_{2nH}^2(x)$ to get the other Gaussian distribution with the standard deviation given by

$$\hat{\sigma}_1(x) = \sqrt{\sum_{n=1}^{\infty} \hat{\sigma}_{1nL}^2(x) + \sum_{n=1}^{\infty} \hat{\sigma}_{1nH}^2(x)}, \tag{11a}$$

$$\hat{\sigma}_2(x) = \sqrt{\sum_{n=1}^{\infty} \hat{\sigma}_{2nL}^2(x) + \sum_{n=1}^{\infty} \hat{\sigma}_{2nH}^2(x)}. \tag{11b}$$

The RMS amplitudes of the stochastic vibration for the inner tube and the outer tube of the DWCNT at x are $\hat{\sigma}_1(x)$ and $\hat{\sigma}_2(x)$, respectively.

3 Molecular dynamic model for DWCNT

In order to check the applicability of the above model of double-Euler beams, together with the law of energy equipartition, to studying the thermal vibration of a DWCNT, this section presents the model of molecular dynamics of a DWCNT in an argon atmosphere as shown in Fig. 1. In the corresponding molecular dynamics model, the interatomic actions can be described by the Tersoff–Brenner potential with the first set of parameters [13]. In addition, the C–C bond length in the model is 0.142 nm.

The van der Waals interaction either between two argon atoms, two carbon atoms belonging to different layer of carbon nanotube, or between a carbon atom and an argon atom is described by the Lennard–Jones pair potential

$$V(r) = 4\varepsilon \left[(\sigma/r)^{12} - (\sigma/r)^6 \right], \tag{12}$$

where $\varepsilon_{\text{Ar-Ar}} = 1.032 \times 10^{-2}$ eV, $\sigma_{\text{Ar-Ar}} = 3.822$ Å $\varepsilon_{\text{C-Ar}} = \sqrt{\varepsilon_{\text{C-C}} \varepsilon_{\text{Ar-Ar}}}$ and $\varepsilon_{\text{C-C}} = 3.19 \times 10^{-3}$ eV, $\sigma_{\text{C-C}} = 3.345$ Å, $\sigma_{\text{C-Ar}} = (\sigma_{\text{C-C}} + \sigma_{\text{Ar-Ar}})/2$ [14,15].

In the numerical simulations of the thermal vibration of carbon nanotubes, the following Verlet algorithm in velocity form with time step 1 fs is used:

$$R(t + \delta t) = R(t) + \delta t V(t) + \frac{1}{2} \delta t^2 a(t), \tag{13a}$$

$$V(t + \delta t) = V(t) + \frac{1}{2} \delta t [a(t) + a(t + \delta)], \tag{13b}$$

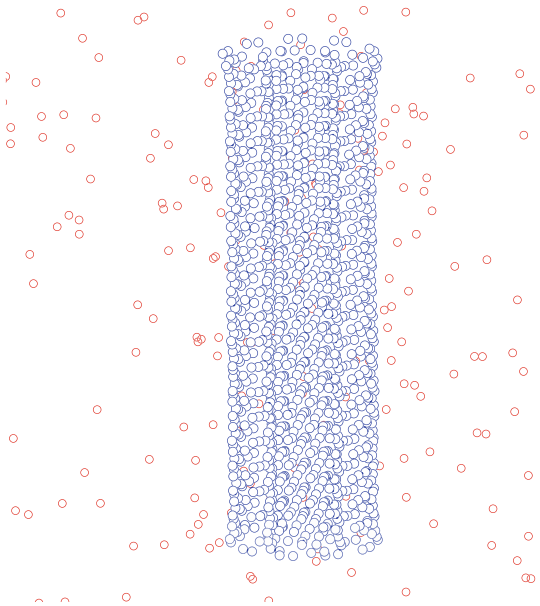

Fig. 1 Model of molecular dynamics of a DWCNT in argon atmosphere

where a represents the acceleration of atoms, V the velocity of atoms, R the position of atoms, and δt the time step. In numerical simulations, the periodic boundary conditions are applied to argon atmospheres. The displacements of carbon nanotube of the sections of inner wall or out wall are observed every 1 ps, while the total simulation time is $T_{\text{tat}}(\text{ps})$. The RMS amplitudes of the thermal vibration of the cross section x of the inner tube and the outer tube are

$$\tilde{w}_1(x) = \sqrt{\sum_{i=1}^{T_{\text{tot}}} w_{i1}^2(x) \,/ T_{\text{tot}}}\,, \quad \tilde{w}_2(x) = \sqrt{\sum_{i=1}^{T_{\text{tot}}} w_{i2}^2(x) \,/ T_{\text{tot}}}\,, \tag{14}$$

where $w_{i1}(x)$ and $w_{i2}(x)$ are the vibration amplitudes of the cross section x of the inner tube and the outer tube at the observation moment i.

4 Comparison between analytical and numerical results

To predict the thermal vibration of a DWCNT from the analytical results in Sect. 2, it is necessary to know the elastic properties of the DWCNT in advance. The previous studies based on the Tersoff–Brenner potential gave a great variety of Young's moduli of single-walled carbon nanotubes from the simulated tests of axial tension and compression [16–18]. In our previous studies [19], for the thickness of wall $h = 0.34$ nm, the simulation of pure bending using the first set of parameters in the Tersoff–Brenner potential gave the product of effective Young's modulus $E = 0.39$ TPa and Poisson's ratio $\upsilon = 0.22$ for the armchair (5,5) carbon nanotube, $E = 0.45$ TPa and $\upsilon = 0.20$ for the armchair (10,10) carbon nanotube [19]. In the numerical simulations of this study, Young's moduli and Poisson's ratios obtained from the simulated test of pure bending for those two single-walled carbon nanotubes are used for each layer of the DWCNT. The wall thickness is $h = 0.34$ nm for both inner and outer layers of the DWCNT, the mass density of the carbon nanotubes is $\rho = 2,237\,\text{kg/m}^3$, and the van der Waals coefficient between layers of carbon nanotube is $c_{12} = 103.56$ GPa [12].

Figure 2 shows the RMS amplitudes of the thermal vibration of the first four natural modes of a ((5, 5), (10,10)) armchair carbon nanotube of 24.6 nm length at the temperature of 300 K. In Fig. 2, there is no difference between the first coaxial modes of both inner and outer tubes, and there exists a little difference between the second coaxial modes of those tubes. However, the difference between the inner tube and the outer tube becomes very obvious for the two non-coaxial modes.

Figures 3, 4, and 5 illustrate the RMS amplitudes of the thermal vibration of double-walled armchair ((5,5), (10,10)) carbon nanotubes of different sizes or at different temperatures. Figures 3 and 4 show the RMS amplitudes of the thermal vibration of a ((5,5), (10,10)) armchair carbon nanotube of 4.8 nm length at

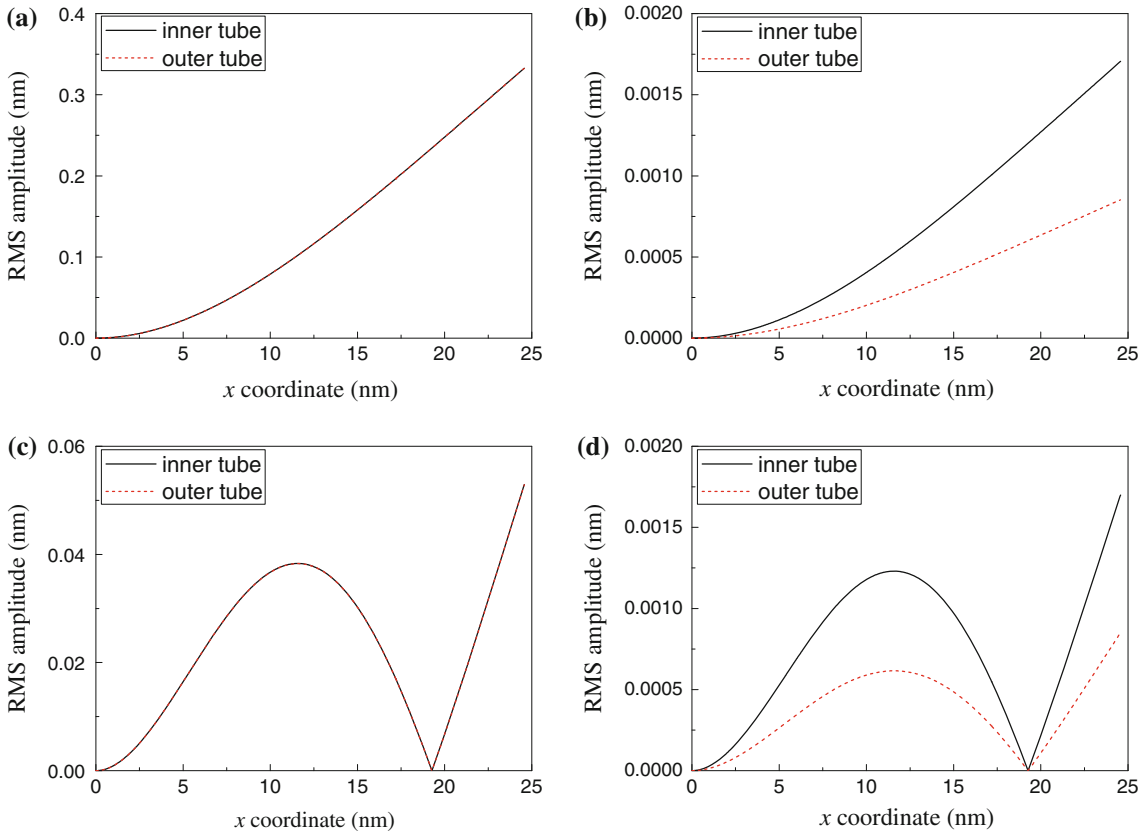

Fig. 2 RMS amplitudes of the first four vibration modes of a ((5,5), (10,10)) DWCNT of 24.6 nm length at the temperature of 300 K, **a** The first coaxial mode, **b** The first non-coaxial mode, **c** The second coaxial mode, **c** The second non-coaxial mode

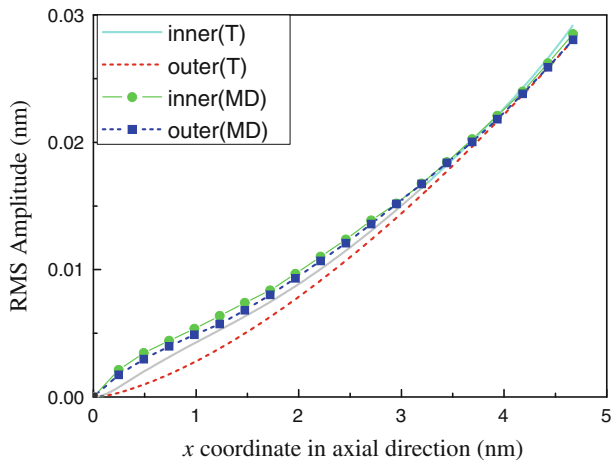

Fig. 3 RMS amplitudes of the thermal vibration of a ((5,5), (10,10)) DWCNT of 4.8 nm length at the temperature of 300 K

the temperatures 300 and 600 K, respectively. Figure 5 gives the RMS amplitudes of the thermal vibration of a ((5,5),(10,10)) armchair carbon nanotube of 9.6 nm length at the temperature of 300 K. In those figures, the symbol T represents the results predicted via the model of double-Euler beams together with the law of energy equipartition, and MD represents the molecular dynamic simulations. The parameters of the model of double-Euler beams are the same as those in the previous case. In the molecular dynamic simulation, different densities of argon are used, but the difference among those results is not obvious. Figures 3, 4, and 5 indicate that the model of double-Euler beams can well predict the RMS amplitudes of the thermal vibration of carbon nanotubes.

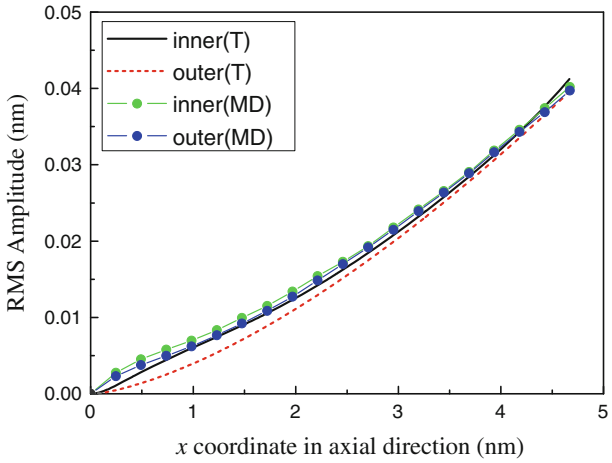

Fig. 4 RMS amplitudes of the thermal vibration of a ((5,5), (10,10)) DWCNT of 4.8 nm length at the temperature of 600 K

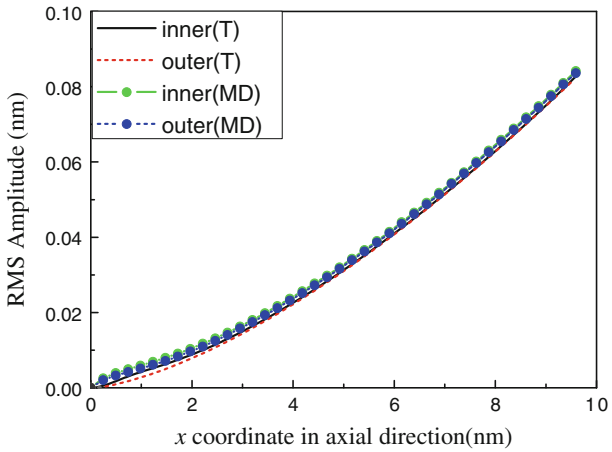

Fig. 5 RMS amplitudes of the thermal vibration of a ((5,5), (10,10)) DWCNT of 9.6 nm length at the temperature of 300 K

Figure 6a shows the displacement history in the y direction for the free end of the inner tube of a ((5,5), (10,10)) double-walled carbon nanotube of 9.6 nm length. The natural frequencies are computed by the fast Fourier transform (FFT) method. The displacement of inner tube and outer tube carry the same frequency messages. As shown in Fig. 6b, every peak represents one natural frequency of the double-walled carbon nanotube. Figure 6c shows the first five natural frequencies, where DE represents the results predicted by the double-Euler beam model, SE represents the single-Euler beam model, and MD1 and MD2 represent the molecular dynamics results in y direction and z direction. From Fig. 6c, one can see that the natural frequencies predicted by the double-Euler beam model are better than those based on the single-Euler beam model. However, the difference in natural frequencies predicted by using the double-Euler beam model and the molecular dynamics simulation still looks obvious. More accurate models, such as the Timoshenko beam model or a shell model, are needed to predict the natural frequencies of such a double–walled carbon nanotube. In addition, the above results show that the RMS amplitude is not sensitive to the change of a natural frequency.

5 Conclusions

The model of double-Euler beams, together with the law of energy equipartition, enables one to establish the analytical relation between the temperature and the RMS amplitude of thermal vibration at any cross section of a DWCNT. The molecular dynamic simulations for ((5,5), (10,10)) armchair carbon nanotubes show that the model of double-Euler beams offers a reasonable prediction for the thermal vibration of those carbon

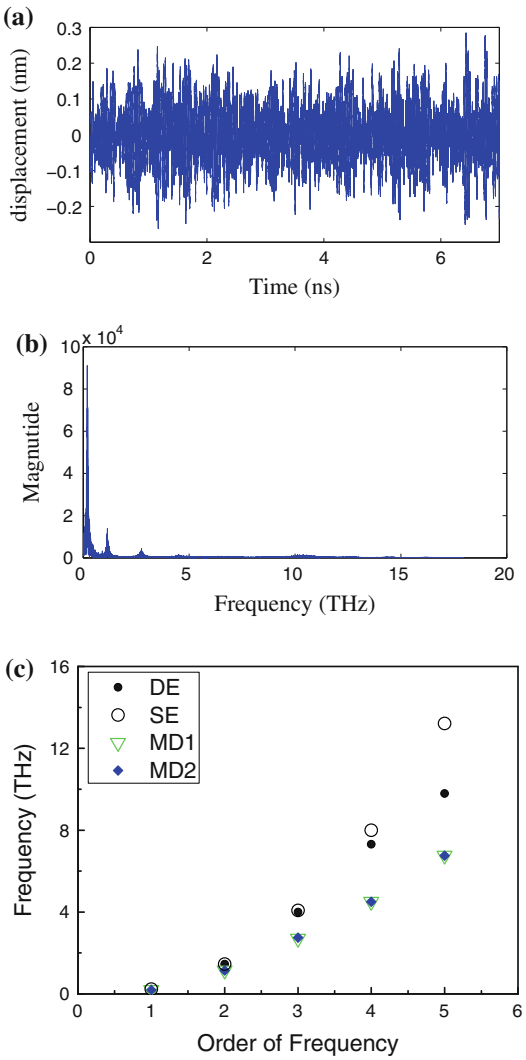

Fig. 6 Natural frequencies of a ((5,5), (10,10)) double-walled carbon nanotube of 9.6 nm long, **a** Displacement in y direction of the free end of the inner tube, **b** Amplitude–frequency curve of atom A, **c** The first five natural frequencies

nanotubes. Furthermore, the study implies that whether the law of energy equipartition holds or not may be used to define the thermal vibration of a nanostructure when the quantum effect is not dominant.

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