

# An elastic shell model for characterizing single-walled carbon nanotubes

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## Abstract

This paper proposes a two-dimensional elastic shell model to characterize the deformation of single-walled carbon nanotubes using the in-plane rigidity, Poisson ratio, bending rigidity and off-plane torsion rigidity as independent elastic constants. It was found that the off-plane torsion rigidity of a single-walled carbon nanotube is not zero due to the off-plane change in the  $\pi$ -orbital electron density on both sides of the nanotube. It was concluded that a three-dimensional elastic shell model of single-walled carbon nanotubes can be established with well-defined effective thickness.

## 1. Introduction

Continuum mechanics modeling [1–5], numerical analysis [1, 6–8] and experimental characterization [9, 10] have been widely used for understanding the properties of carbon nanotubes (CNTs). The good agreement achieved between continuum models and simulations/experiments seems to show that continuum mechanics models are applicable to CNTs [1, 5, 11–15]. However, their validity has not been fully verified in terms of the relationship between the molecular structure of single-walled CNTs (SWCNTs) and their equivalent continuum characteristics. A typical example is that the obtained effective thickness of SWCNTs varies from 0.0617 to 0.69 nm [1, 4, 16–31]. According to Vodenitcharova–Zhang’s criterion based on the concept of force equilibrium and equivalence [4], the effective thickness of SWCNTs should be smaller than the theoretical diameter of carbon atoms, which is about 0.142 nm [32]. Thus those greater than 0.142 nm [16, 17, 19, 21, 23, 24, 26–29] are unreasonable, while others below 0.142 nm [18, 20, 22, 25, 30, 31] are possible, but their validity needs to be confirmed.

In an attempt to address the continuum–atomic modeling [33–37], Zhang *et al* [38, 39] directly related the interatomic potential of an SWCNT to a continuum model by equating the strain energy in the equivalent continuum model to that in atomic bonds. An isotropic constitutive model was derived for SWCNTs subjected to in-plane deformation with the in-plane rigidity,  $K_{\text{extension}}$ , and the in-plane shear rigidity,  $K_{\text{shear}}$ .

By comparing  $K_{\text{extension}}$  and  $K_{\text{shear}}$  of SWCNTs with their counterparts of three-dimensional (3D) thin shells [40, 41] with thickness  $h$ , it is easy to obtain the following relationships:

$$K_{\text{extension}} = \frac{Eh}{1 - \nu^2} \quad \text{and} \quad K_{\text{shear}} = Gh, \quad (1)$$

where  $E$  is the Young’s modulus,  $G = E/2(1 + \nu)$  is the shear modulus, and  $\nu$  is the Poisson ratio. Therefore,  $\nu$  can be obtained from  $\frac{K_{\text{extension}}}{K_{\text{shear}}} = \frac{2}{1 - \nu}$ . These studies seem to have demonstrated a promising approach to establishing a continuum SWCNT model.

Recently, Huang *et al* [42] took one step forward to consider both in-plane and off-plane deformations of SWCNTs. Using the Tersoff–Brenner potential [43, 44], which was shown to be appropriate for SWCNTs [45], and the modified Cauchy–Born rule [38, 39], they obtained two-dimensional (2D) isotropic constitutive relations for SWCNTs controlled by  $D_{\text{bending}}$  (bending rigidity),  $D_{\text{torsion}}$  (off-plane torsion rigidity),  $K_{\text{extension}}$  and  $K_{\text{shear}}$ . The authors explained that the deformation of SWCNTs was solely caused by the changes of their in-plane  $\sigma$  bond. In particular,  $D_{\text{bending}}$  is due to the energy increase via the  $\sigma$ -bond angle change, while  $D_{\text{torsion}}$  is independent of the  $\sigma$ -bonds, and thus vanishes.

However, a 3D thin shell theory [40, 41] gives very different deformation mechanisms of SWCNTs modeled as 3D shells where off-plane deformations, i.e., bending and off-plane torsion, are realized via the in-plane deformation across the wall thickness. Accordingly  $D_{\text{bending}}$  and  $D_{\text{torsion}}$  of a 3D shell are related to its thickness  $h$  and the material constants

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by [40, 41]

$$D_{\text{bending}} = \frac{Eh^3}{12(1-\nu^2)} \quad \text{and} \quad D_{\text{torsion}} = \frac{Gh^3}{12}. \quad (2)$$

Combining equations (1) and (2) leads to the following equations:

$$\frac{D_{\text{torsion}}}{D_{\text{bending}}} = \frac{K_{\text{shear}}}{K_{\text{extension}}} = \frac{1-\nu}{2} \quad \text{or} \quad (3)$$

$$\frac{D_{\text{bending}}}{K_{\text{extension}}} = \frac{D_{\text{torsion}}}{K_{\text{shear}}} = \frac{h^2}{12}$$

which gives the existence condition of a 3D isotropic shell model with well-defined effective thickness for SWCNTs. In other words, the existence of a 3D shell model is not guaranteed, as assumed previously. Instead, it is entirely determined by whether the values of elastic constants obtained in atomistic models or experiments can meet the requirements of equation (3). For example, in [42],  $D_{\text{torsion}}$  was reported to be zero, which cannot satisfy equation (3), and thus leads to an effective thickness of SWCNTs varying with loading conditions [42]. This conclusion challenges the validity of 3D shell models for SWCNTs. It is therefore necessary to clarify the issue to see if  $D_{\text{torsion}}$  is zero and, more importantly, whether a 3D shell model with well-defined thickness will be applicable to SWCNTs. To achieve these goals, we propose a 2D shell model for SWCNTs in the present work, which is independent of debatable values of the effective thickness and all the classic formulae (1)–(3) for a 3D shell. This model offers an efficient tool to extract the values of elastic constants for SWCNTs via the 2D shell-model–discrete-model fitting, and thus enables us to examine the issue regarding the definition of the effective thickness and the existence of a 3D continuum model for SWCNTs. Similar to the previous 3D shell models for SWCNTs [11, 13, 46], the present 2D elastic shell also uses bending rigidity and in-plane rigidity to avoid the application of the concept of effective thickness. By comparing our results with the discrete models of phonon dispersion relations of SWCNTs corresponding to  $D_{\text{bending}}$  and  $D_{\text{torsion}}$ , we found that the vibration behavior of SWCNTs predicted by the discrete models can be reasonably reproduced by our 2D thin shell model with a nonzero off-plane torsion rigidity of  $D_{\text{torsion}} \approx 0.8$  eV. Furthermore we found that this 2D model becomes equivalent to a 3D elastic shell when the effective thickness of a (10, 10) SWCNT is  $h \approx 0.1$  nm.

## 2. Modeling: formulation, comparison and discussion

### 2.1. Model formulation

To resolve the problems regarding the definition of effective thickness of SWCNTs and the existence of a 3D shell model for SWCNTs we shall avoid using the controversial effective thickness of SWCNTs by visualizing SWCNTs as 2D isotropic shells formed by rolling up 2D, almost isotropic graphite sheets. Such 2D shells are different from classical 3D shells [40, 41] in that  $D_{\text{bending}}$ ,  $D_{\text{torsion}}$ ,  $K_{\text{extension}}$ , and  $K_{\text{shear}}$

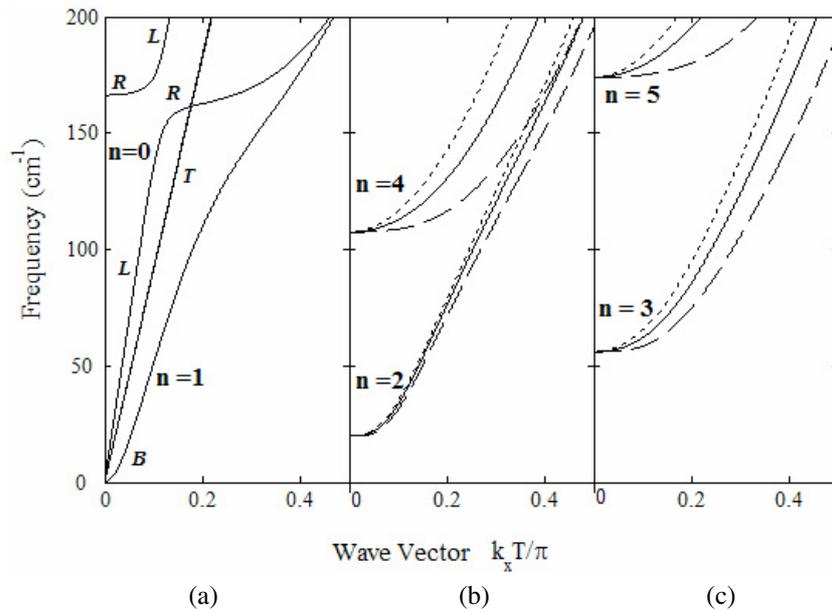
governing their constitutive relation (e.g., equation (5.9) of [41] with  $D_{\text{bending}}(1-\nu)$  replaced by  $2D_{\text{tension}}$ ) are independent parameters not necessarily related to the specific thickness via classical formulae (equations (1) and (2)), and thus do not have to satisfy equation (3). Substituting such constitutive relations into the equations of motion (e.g., equation (5.2) of [41]) leads to the following equations for free vibration of SWCNTs of radius  $R$  and mass density per unit area  $\rho$ .

$$\begin{aligned} & R^2 \frac{\partial^2 u}{\partial x^2} + \frac{1-\nu}{2} \frac{\partial^2 u}{\partial \varphi^2} + \frac{R(1+\nu)}{2} \frac{\partial^2 v}{\partial x \partial \varphi} - \nu R \frac{\partial w}{\partial x} \\ &= \frac{\rho}{K_{\text{extension}}} R^2 \frac{\partial^2 u}{\partial t^2} \\ & \frac{R}{2} (1+\nu) \frac{\partial^2 u}{\partial x \partial \varphi} + \frac{R^2}{2} (1-\nu) \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial \varphi^2} - \frac{\partial w}{\partial \varphi} \\ &+ \frac{D_{\text{bending}}}{K_{\text{extension}}} \left( \frac{D_{\text{torsion}}}{D_{\text{bending}}} \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{R^2 \partial \varphi^2} \right) \\ &+ \frac{D_{\text{bending}}}{K_{\text{extension}}} \left( \frac{\partial^3 w}{R^2 \partial \varphi^3} + \left( \frac{D_{\text{torsion}}}{D_{\text{bending}}} + \nu \right) \frac{\partial^3 w}{\partial x^2 \partial \varphi} \right) \\ &= \frac{\rho}{K_{\text{extension}}} R^2 \frac{\partial^2 v}{\partial t^2} \\ & \nu R \frac{\partial u}{\partial x} + \frac{\partial v}{\partial \varphi} - w - \frac{D_{\text{bending}}}{K_{\text{extension}}} \left[ R^2 \frac{\partial^4 w}{\partial x^4} + 2 \left( \frac{D_{\text{torsion}}}{D_{\text{bending}}} + \nu \right) \right. \\ &\quad \times \left. \frac{\partial^4 w}{\partial x^2 \partial \varphi^2} + \frac{1}{R^2} \frac{\partial^4 w}{\partial \varphi^4} \right] - \frac{D_{\text{bending}}}{K_{\text{extension}}} \left[ \left( \frac{2D_{\text{torsion}}}{D_{\text{bending}}} + \nu \right) \right. \\ &\quad \times \left. \frac{\partial^3 v}{\partial x^2 \partial \varphi} + \frac{1}{R^2} \frac{\partial^3 v}{\partial \varphi^3} \right] = \frac{\rho}{K_{\text{extension}}} R^2 \frac{\partial^2 w}{\partial t^2} \end{aligned} \quad (4)$$

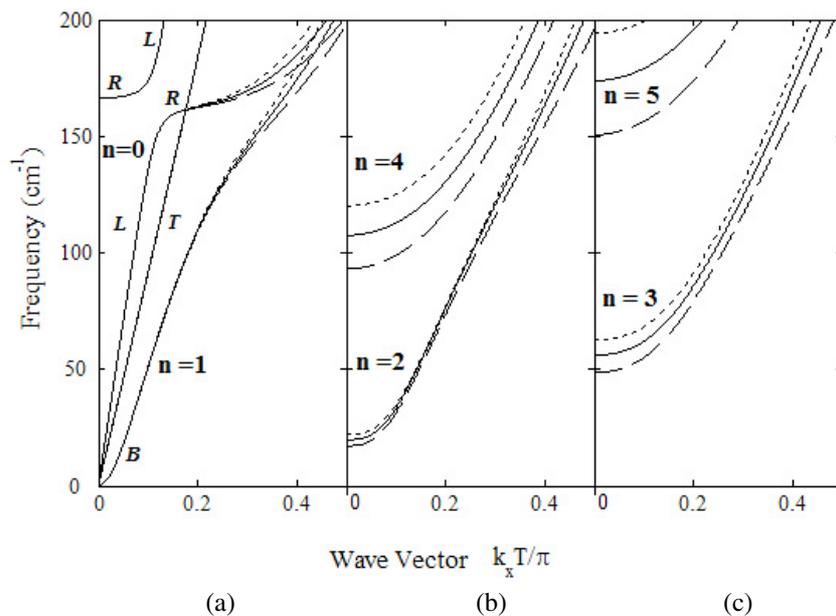
where  $x$  and  $\varphi$  are the axial coordinate and circumferential angular coordinate,  $u$ ,  $v$  and  $w$  are longitudinal, circumferential and (inward positive) radial displacements, and  $t$  is time. For simply supported ends the solution to equation (4) reads  $u(x, \theta, t) = U \cos k_x x \cos n\theta e^{i\omega t}$ ,  $v(x, \theta, t) = V \sin k_x x \sin n\theta e^{i\omega t}$ ,  $w(x, \theta, t) = W \sin k_x x \cos n\theta e^{i\omega t}$ , where  $U$ ,  $V$  and  $W$  are the vibration amplitudes,  $k_x$  is the wavevector in the  $x$ -direction,  $n$  is the circumferential wavenumber and  $\omega$  is angular frequency related to frequency  $f$  by  $\omega = 2\pi f$ . The condition of nonzero solution of  $(U, V, W)$  gives the vibration frequencies and associated modes for SWCNTs. Here, it is noted that in previous studies [1, 16–23, 25, 30, 47–49] the values of  $K_{\text{extension}}$  obtained mainly fall in a range of 330–363 J m<sup>-2</sup> and  $\nu$  varies from 0.14 to 0.34. Thus, in the present work it is reasonable to adopt  $K_{\text{extension}} = 350$  J m<sup>-2</sup> and  $\nu = 0.2$  for SWCNTs.

### 2.2. Model comparison and discussion

In what follows, we shall compare the 2D shell model with available atomistic models for vibration spectra of SWCNTs to (1) validate the values of  $K_{\text{extension}}$  and  $\nu$  used here, (2) extract the values of  $D_{\text{tension}}$  and  $D_{\text{bending}}$ , and (3) finally clarify the aforementioned issues based on equation (3). In doing so, let us first examine the sensitivity of different vibration modes of SWCNTs to their elastic constants. The results for a (10, 10) SWCNT are shown in figure 1 with  $D_{\text{bending}} = 2$  eV [14] and



**Figure 1.** The phonon spectrum of a (10, 10) SWCNT given by the 2D elastic shell model with  $D_{\text{bending}} = 2$  eV and  $D_{\text{torsion}} = 0$  (dashed lines), 0.8 eV (solid lines) and 1.2 eV (dotted lines). The axisymmetric radial ( $R$ ), longitudinal ( $L$ ) and torsional ( $T$ ) vibration modes with  $n = 0$  and beam-like bending mode ( $B$ ) with  $n = 1$  are shown in (a) and the circumferential modes with  $n = 2-5$  are displayed in (b) and (c).

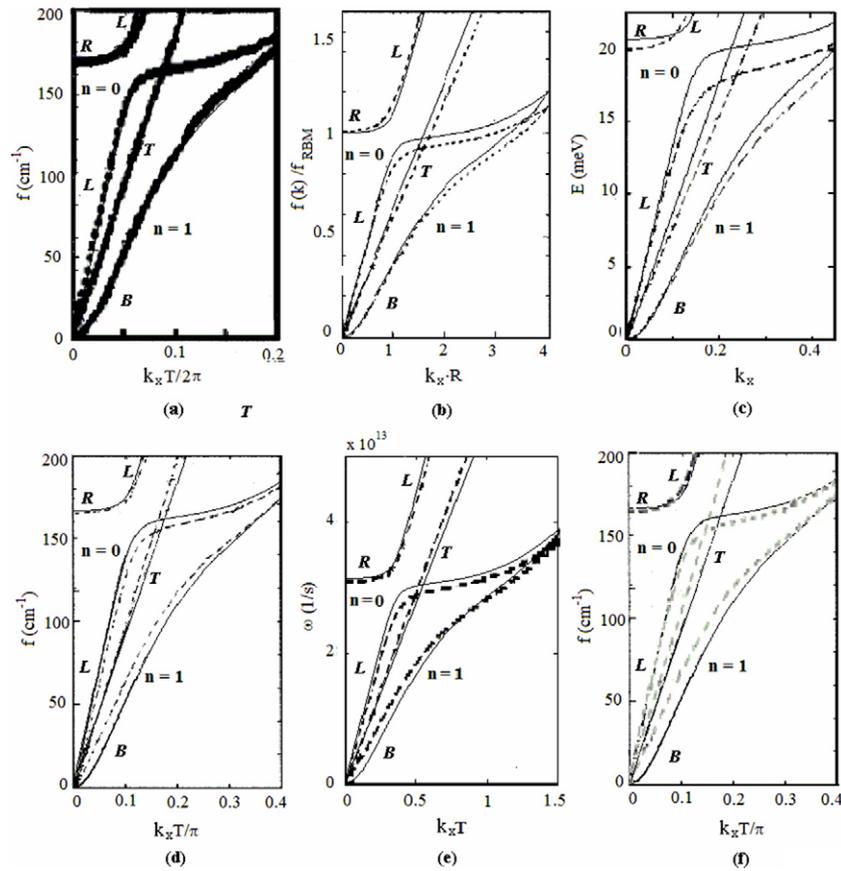


**Figure 2.** The phonon spectrum of a (10, 10) SWCNT given by the 2D elastic shell model with  $D_{\text{torsion}} = 0.8$  eV and  $D_{\text{bending}} = 1.5$  eV (dashed lines), 2 eV (solid lines) and 2.5 eV (dotted lines). The axisymmetric radial ( $R$ ), longitudinal ( $L$ ) and torsional ( $T$ ) vibration modes with  $n = 0$  and beam-like bending mode ( $B$ ) with  $n = 1$  are shown in (a) and the circumferential modes with  $n = 2-5$  are displayed in (b) and (c).

$D_{\text{torsion}} = 0, 0.8, 1.2$  eV, and figure 2 with  $D_{\text{torsion}} = 0.8$  eV and  $D_{\text{bending}} = 1.5, 2, 2.5$  eV. Figures 1(a) and 2(a) show that the axisymmetric radial ( $R$ ), longitudinal ( $L$ ) and torsional ( $T$ ) modes ( $n = 0$ ), and beam-like bending mode ( $B$ ) ( $n = 1$ ) of SWCNTs are governed by  $K_{\text{extension}}$  and  $\nu$  (or  $K_{\text{shear}}$ ) but are independent of  $D_{\text{torsion}}$  and  $D_{\text{bending}}$ . Thus, these vibrations are ideal for validation of the values of  $K_{\text{extension}}$  and  $\nu$  chosen in the present work. For the vibration modes with  $n = 2-5$ , figures 1(b) and (c), and 2(b) and (c) indicate that at  $k_x = 0$  the

vibration frequencies are primarily determined by the value of  $D_{\text{bending}}$ , while at  $k_x > 0$  the strong effects of both  $D_{\text{bending}}$  and  $D_{\text{torsion}}$  are observed. In view of these results, the vibrations with  $n = 2-5$  can be efficiently used to uniquely determine the values of  $D_{\text{torsion}}$  and  $D_{\text{bending}}$  for SWCNTs. With these results we are now ready to perform our analysis via the 2D shell-model–discrete-model fitting.

So far a variety of approaches have been adopted to calculate vibration spectra for SWCNTs [14, 48–57]. The

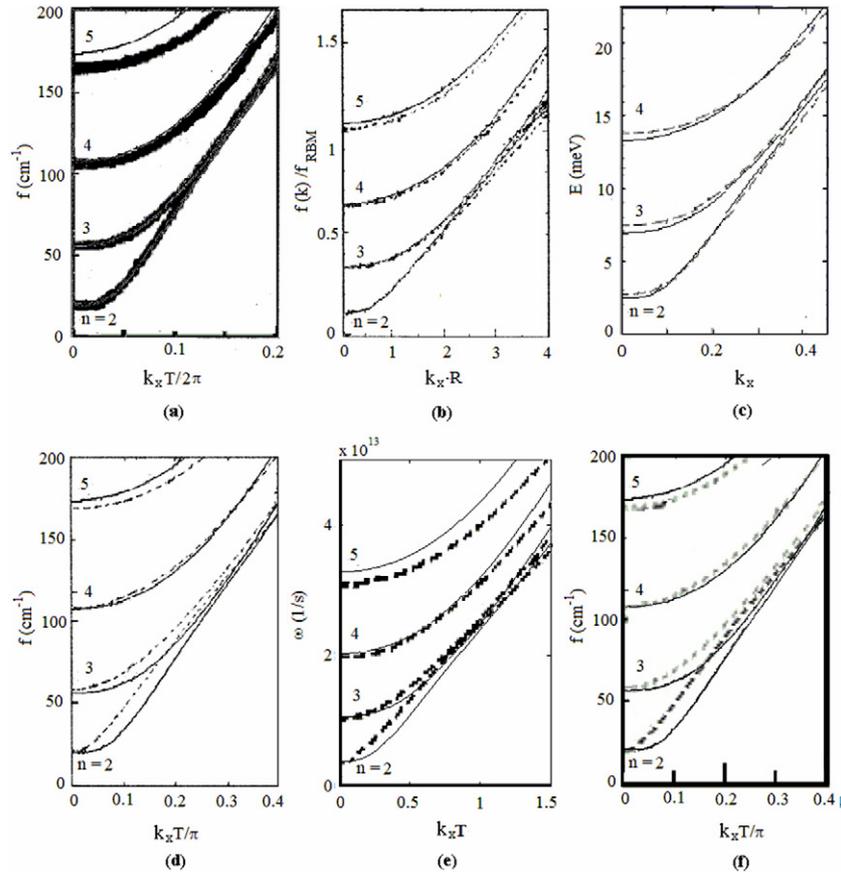


**Figure 3.** The comparison of the 2D elastic shell model (solid thin lines) with (a) the lattice dynamics model (solid coarse lines) in [49], (b) the continuum model (dotted lines) in [51], (c) the lattice dynamics model (dotted lines) in [54], (d) the force constant model (dotted lines) in [50], (e) the lattice dynamics model (dotted lines) in [52] and (f) the lattice dynamics model (dotted lines) in [55] for axisymmetric  $R$ ,  $L$ ,  $T$  modes with  $n = 0$  and  $B$  modes with  $n = 1$  of a (10, 10) SWCNT.

studies on a (10, 10) SWCNT given by a force constant model [50], lattice dynamic models [49, 52, 54, 55], and a continuum model [51] provide detailed results and enable us to compare them with the present shell model for low-frequency vibrations of SWCNTs with long wavelength. It is seen from figure 3 that as far as the asymmetric  $R$ ,  $L$  and  $T$  modes with  $n = 0$  are concerned, the present shell model is consistently in good agreement with the six existing models [49–52, 54, 55], which justifies the values of  $K_{\text{extension}}$  and  $\nu$  used in the present model. Subsequently, for the vibrations with  $n = 2$ –5, which are very sensitive to  $D_{\text{torsion}}$  and/or  $D_{\text{bending}}$ , we found that the best fit of the present shell model to the six existing models leads to unique values of  $D_{\text{bending}} \approx 2$  eV and  $D_{\text{torsion}} \approx 0.8$  eV. For example, in figure 4, at  $k_x = 0$  where the frequency is determined predominantly by  $D_{\text{bending}}$ , the 2D shell model with  $D_{\text{bending}} = 2$  eV is very close to all the six existing models [49–52, 54, 55]. In addition, if, at the same time,  $D_{\text{torsion}}$  is taken as 0.8 eV the 2D shell model matches well with the two lattice dynamics models [49, 54] and the continuum model [51] at  $k_x > 0$  and  $n = 2$ –5 (figures 4(a)–(c)), and the force constant model [50] and other two lattice dynamics models [52, 55] at  $k_x > 0$  and  $n = 4$ –5 (figures 4(d)–(f)). On the other hand, in figures 3(d)–(f) and 4(d)–(f), a notable difference of the present shell model is observed from the latter three atomistic models [50, 52, 55] at  $k_x > 0$  and

$n = 1$ –3. Suzuura *et al* [51] first noticed such discrepancy between their continuum model [51] and the force constant model [50], and explained it as a result of the inappropriate values of force constants used in [50]. Later, Gartstein [54] further examined this issue, and showed that for vibrations with  $n = 1$ –5 his lattice dynamics model, which is irrelevant to the issue of force constant adjustment, agrees well with Popov *et al*'s lattice dynamics model [49] and Suzuura *et al*'s continuum model [51]. This is also well echoed by the present study in figures 3(a) and (c), and 4(a) and (c).

These results clearly show that the present 2D elastic shell model can be efficiently used to give a reliable description for low-frequency vibrations of SWCNTs with long wavelength. The model is valid for individual SWCNTs, no matter what the specific values of the four elastic constants are. Hence, it offers an efficient way to determine the elastic constants for SWCNTs through curve fitting and enables us to examine the long-standing issue regarding the effective thickness of SWCNTs. Specifically, based on the results obtained in the present work, the bending rigidity  $D_{\text{bending}}$  of SWCNTs is found to be about 2 eV and the off-plane torsion rigidity  $D_{\text{torsion}}$  is around 0.8 eV. It is noted that this value of  $D_{\text{torsion}}$  is close to the values given by a local density approximation theory [22] but very different from the vanished  $D_{\text{torsion}}$  obtained in [42]. In particular, with  $K_{\text{extension}} = 350$  J m<sup>-2</sup>,  $\nu = 0.2$ ,  $D_{\text{bending}} = 2$  eV



**Figure 4.** The comparison of the present 2D elastic shell model (solid thin lines) with (a) the lattice dynamics model (solid coarse lines) in [49], (b) the continuum model (dotted lines) in [51], (c) the lattice dynamics model (dotted lines) in [54], (d) the force constant model (dotted lines) in [50], (e) the lattice dynamics model (dotted lines) in [52], and (f) the lattice dynamics model (dotted lines) in [55] for circumferential modes of a (10, 10) SWCNT with  $n = 2-5$ .

and  $D_{\text{torsion}} = 0.8$  eV, equation (3) can be satisfied, which suggests that a 3D elastic thin shell model indeed serves as an approximation for SWCNTs with the effective thickness calculated for a (10, 10) SWCNT via equation (3) as 0.1 nm, which satisfies the Vodenitcharova–Zhang criterion [4].

Based on the local density approximation theory [22, 58], the nonzero off-plane torsion rigidity of SWCNTs is attributed to their  $\pi$ -orbital electron resonance, especially the dihedral angle torsion-induced change in the  $\pi$ -orbital electron density on both sides of SWCNTs, but is independent of  $\sigma$ -bond stretching and angle variation. Thus, the vanished off-plane torsion rigidity  $D_{\text{torsion}} = 0$  reported in [42] is due to the fact that the model used in [42] cannot account for the effect of  $\pi$ -orbital on the deformation of SWCNTs that contributes 100% to the off-plane torsion rigidity of SWCNTs. In addition, it is worth mentioning that for some vibration modes of shell-like structures the influence of boundary conditions imposed on their two ends can effectively propagate into the central part even if their dimension in even changed to even if here; please check. longitudinal direction is very large. For example, the beam-like bending mode ( $n = 1$ ) is strongly dependent on the end conditions of SWCNTs modeled as shells. As indicated before, the frequency of such bending vibration is not controlled by the off-plane rigidities obtained in the present curve fitting; instead, it is

completely determined by the in-plane rigidity  $K_{\text{extension}}$  used in the present work whose value,  $350 \text{ J m}^{-2}$ , has been justified by almost all previous studies [1, 16–24, 30, 47–49]. Thus the good agreement between the present 2D shell mode with the existing discrete [49, 56] and continuum models [51] for beam-like bending modes of SWCNTs and with all the others [49–52, 54, 55] on the general vibration spectra for a (10, 10) SWCNT implies that the equivalent end conditions of a (10, 10) SWCNT considered in these studies are similar and close to those used in the present work for SWCNTs, although these end conditions were not explicitly specified before [49–52, 54, 55]. Hence, the off-plane rigidity values given by the present study can be considered to be independent of the specific boundary conditions imposed on SWCNTs.

### 3. Conclusions

In summary, the present study found that SWCNTs can be modeled as 2D elastic shells with their deformation governed by four independent elastic constants, i.e., bending rigidity, off-plane torsion rigidity, in-plane rigidity and Poisson ratio (or in-plane shear rigidity), and that the off-plane torsion rigidity of SWCNTs cannot be zero. Moreover, the validity of a 3D isotropic shell model for SWCNTs with well-defined

effective thickness, e.g., 0.1 nm for (10, 10) SWCNTs, can be justified by the fact that the four independent elastic constants of SWCNTs can approximately satisfy the condition imposed on their counterparts of 3D elastic thin shells.

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