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Consistent Computational Modeling of Mechanical Properties of Carbon and Boron Nitride Nanotubes

V. VIJAYARAGHAVAN [1] and LIANGCHI ZHANG[1,2,3]

1.—Laboratory for Precision and Nano Processing Technologies, School of Mechanical and Manufacturing Engineering, The University of New South Wales, Sydney, NSW 2052, Australia. 2.—Department of Mechanics and Aerospace Engineering, Southern University of Science and Technology, Shenzhen, Guangdong Province 518055, China. 3.—e-mail: liangchi.zhang@unsw.edu.au

Computational modeling has emerged as a powerful tool in estimating many of the exciting material properties of low-dimensional systems such as nanotubes. There also exists a variation in the reported strength data of nanotubes using different computational techniques. This issue is attributed to the uncertainty in determining the correct thickness of the nanotubes, a fundamental parameter to estimate any mechanics-related properties. The present study establishes a consistent approach in determining the mechanical properties of nanotubes using molecular dynamics (MD) simulation. It was found that the nanotube wall thickness varies with the nanotube radius, which subsequently affects the estimated elastic modulus of the nanotube. There exists a threshold nanotube radius beyond which the elastic modulus remains fairly constant. The results predicted by MD simulation are also consistent with findings from first-principle methods. The findings from this study can be applied for a range of nanomaterials to determine their effective mechanical properties.

INTRODUCTION

Advances in high-performance computing and novel computational techniques have led to a surge in the design and characterization of nanoscale and low-dimensional material structures. Since their discovery in the 1990s,[1] carbon nanotubes (CNTs) have caught the attention of researchers specializing in the field of nanomaterials. The CNT structure is formed by rolling up a layer of graphene to form a one-dimensional structure, and is a representative of a low-dimensional homogenous material structure. Similar to CNTs, research in nanomaterials has focused on the characterization of its heterogeneous counterpart, boron nitride nanotubes (BNNTs). These classes of nanomaterials have today been forayed into a wide range of emerging fields, such as nanosensors, nanocomposites, new materials design, and nanoelectromechanical systems. Computational modeling of nanomaterials has since evolved as a powerful tool in determining the mechanical response of nanotubes in diverse operating conditions. However, the mechanical properties predicted by numerical analysis present ambiguous and scattered strength data for the same nanomaterial. This study focuses on some critical issues in accurately predicting the mechanical properties of nanotubes using molecular dynamics analysis.

Several studies have been undertaken in the past to investigate the mechanical characteristics of carbon and BNNTs. The mechanical characterization of nanotubes using a computational approach is popular, owing to the complexity in determining the strength of low-dimensional nanotubes using experimentation techniques. These computational approaches involve a range of techniques, such as quantum computing, molecular dynamics (MD) simulation, continuum modeling and finite element analysis (FEA). The vast majority of computer-based research is based on MD simulation, due to its speed and cost-effective nature in solving large-scale atomic systems. These studies have been used to report the elastic modulus of nanotubes by systematically considering variations in nanotube diameter,[2–7] lattice defects,[8–11] temperature,[12–14] etc. In addition to MD simulation, the quantum

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computing approach such as ab initio or density functional theory have also been used to study the mechanical properties of nanotubes from their atomic and sub-atomic structure.[15–17] These studies mainly focus on investigating the elastic properties of nanotubes by analyzing their electronic structure. Some studies have also focused on the elastic properties of nanotubes using continuum mechanics-based FEA approach.[18–20] A summary of the mechanical properties of CNTs and BNNTs as reported in past literature studies are tabulated in Tables I and II, respectively.

From the summary of literature studies presented above, it is evident that the elastic modulus of nanotubes varies widely depending on the adopted computational technique. Earlier studies by Vodenitcharova and Zhang[32] and Wang and Zhang[37] attributed this variation to inconsistent wall thicknesses of the nanotubes being adopted in computational modeling. By devising a set of criteria, they formulated a methodology and the necessary and sufficient conditions[38,39] for the rational determination of the effective wall thickness and elastic modulus of carbon nanotubes. With research in BNNTs also gaining traction in recent years, estimating the fundamental mechanics quantities of BNNTs will be significant in the design of BN-based nanomaterials.[40–42] It is also important to adopt a reliable computational scheme with regards to strain rate, relaxation steps, etc. for predicting mechanical characteristics of nanotubes using MD studies. Accordingly, the main objective of the present study involves the computation of the effective mechanical properties of different nanotubes using a MD simulation approach by following the well-established Vodenitcharova-Zhang[32] and Wang-Zhang[37] criteria. The fundamental mechanics quantities of different nanotubes with varying nanotube radii is computed by using a reliable computational scheme which has been established from the corresponding author's research group in Ref. 14 A systematic study of the mechanics quantities of nanotubes with varying nanotube radii presents a clear analysis on the effect of nanotube geometry on the computed mechanics quantities. It is anticipated that the findings reported in this study could provide useful guidelines and improve the reliability in characterizing the mechanical properties of nanotubes using MD simulation.

DESCRIPTION OF COMPUTATIONAL SCHEME

The present study deals with computational modeling of carbon and BNNTs under tensile loading conditions using MD simulation. The second-generation reactive empirical bond order (REBO)

Table I. Mechanical properties of CNTs reported using computational techniques

Technique	Temperature	Diameter (Å)	Elastic modulus (TPa)
Ab initio method5	NA	6.8–15.67	1.29–1.35
Ab initio method6	NA	6.0–14.0	0.5–0.82
Ab initio method16	NA	6.9	0.83–0.92
Ab initio method17	NA	8.0–20.0	0.8–1.22
Ab initio method10	NA	6.80	0.83–3.02
Atomistic -continuum21	NA	6.8–7.8	1.7–6.9
EAM potential22	300–900 K	4.0–34.0	0.97–1.20
FEA modeling23	NA	0.4–2.7	0.912
Molecular mechanics20	NA	5.0–40.0	0.17–1.44
Molecular mechanics24	NA	12.526	2.56
Morse potential25	0 K, 300 K	16.0	NA
Quasi-continuum26	NA	13.6–14.1	0.79–1.0
REBO potential4	NA	6.9–13.6	NA
REBO potential7	50 K	9.48	NA
REBO potential27	< 0.005 K	24.0–33.0	0.4–0.8
REBO potential28	0 K	4.0–22.0	0.5
Continuum FEA18	NA	4.0–16.0	0.4–0.5
Structural mechanics12	100–2000 K	6.8–13.6	0.62–0.72
Tersoff potential29	300 K	4.0–22.0	1.0
Tight binding30	NA	13.0	0.98
Tight binding15	NA	13.6	0.311
Tight binding31	NA	6.8–14.1	0.4
Tersoff–Brenner14	300 K	13.6	4.88
Shell theory32	NA	13.6	3.5

EAM Embedded-atom method, *FEA* finite element analysis, *REBO* reactive empirical bond order

Table II. Mechanical properties of BNNTs reported using computational techniques

Technique	Temperature	Diameter (Å)	Elastic modulus (TPa)
Ab initio[3]	NA	4.2–19.65	2.901
DFT calculation[2]	NA	4.86–14.04	0.700–0.830
C–L model[19]	NA	NA	0.900–1.000
T–B scheme[33]	NA	8.42–21.06	0.837–0.912
Modified T–B[34]	NA	14.04	0.982–1.113
Tersoff potential[35]	300 K	4.86–8.42	0.730–0.890
MM–DFT model[36]	NA	7.02–24.31	0.83

DFT Density functional theory, *C–L* continuum–lattice, *T–B* Tersoff–Brenner, *MM* molecular mechanical

potential[43] is used to describe interactions between carbon atoms in CNTs. The REBO potential is computationally efficient for modeling covalent bond breaking and forming in large carbon atom systems, while also maintaining the accuracies of the ab initio technique. In addition, the REBO potential also includes a torsional term for describing dihedral angle preferences in a hydrocarbon system, which makes it an ideal potential for modeling CNTs. The interactions between boron and nitrogen atoms in BNNTs is described using a modified Tersoff potential[44] with interaction parameters defined in Ref. 45 The Tersoff potential has been widely used for modeling boron nitride nanostructures with accuracies comparable to experimental observations and first-principle models. CNTs and BNNTs with radii ranging from 0.32 nm to 1.05 nm are considered in this study. To standardize the geometry, a constant length-to-diameter ratio of 7.37 has been adopted across all the nanotubes considered in this study. In an earlier study,[14] the corresponding author presented an extensive analysis on an appropriate computational scheme to be used for accurately and efficiently determining the tensile loading properties of nanotubes using MD simulation. Accordingly, the present study adopts the scheme from Ref. 14 which is described as follows. The first two layers of atoms at either end of the nanotube are rigidly fixed and the remaining atoms are treated as thermostat atoms. Before the application of tensile loading, the nanotubes were thermally relaxed at the required simulation temperature for 2500 fs. The rigid ends of the nanotube were then pulled along axial directions with a strain of 0.0005 to simulate tensile loading. After each fixed displacement, the nanotube structure is then relaxed for 25 fs, following which the required data are extracted. Periodic boundary conditions are applied across axial directions of the nanotube. The simulations are conducted at a temperature of 300 K. All MD simulations described in this work were performed using the open source large-scale atomic/molecular massively parallel simulator package.[46]

RESULTS AND DISCUSSION

Measurement of Nanotube Thickness from Its Unwrapped Nanosheet Counterpart

The fundamental parameter necessary to determine the mechanical properties of nanotubes is their wall thickness. If the wall thickness of the nanotubes can be well defined, then the existing continuum and numerical models can be readily applied to determine their mechanical strength and elastic modulus. While some past studies have reported varying wall thickness data for CNTs ranging from 0.62 Å to 6.5 Å, to the best of the authors' knowledge, no reliable data exist for the case of BNNTs. This inconsistency in wall thickness has led to a scatter of elastic modulus data for nanotubes.

The correct thickness and effective elastic modulus of different nanotubes can be computed using the well-established Vodenitcharova-Zhang[32] and Wang-Zhang[37] criteria. Based on this approach, the axial stiffness (K) and bending stiffness (D) of a nanotube is first obtained from the MD simulations of an unwrapped nanosheet, independent of the disputed elastic modulus (E) and wall thickness (h) values. Accordingly, a single-layer graphene sheet and a boron nitride nanosheet (BNNS) are first considered, representing an unwrapped structure of the corresponding nanotube. The width of the nanosheet should be equal to the circumference of the desired nanotube, which is formed by wrapping the nanosheet perpendicular to the direction of the width. The formation of the nanotube by wrapping up a nanosheet is described in the authors' previous work.[47] As an example, graphene and BNNS of widths 4.26 nm and 4.41 nm are first selected, corresponding to the circumference of a (10,10) CNT and BNNT, respectively. Axial and bending loading are applied separately on the nanosheets to obtain the variation of axial and bending strain energies, as shown in Fig. 1a and b, respectively. The K and D values are then computed from the second derivative of the strain energy polynomial function with respect to the axial and bending strain, respectively. Once these values are

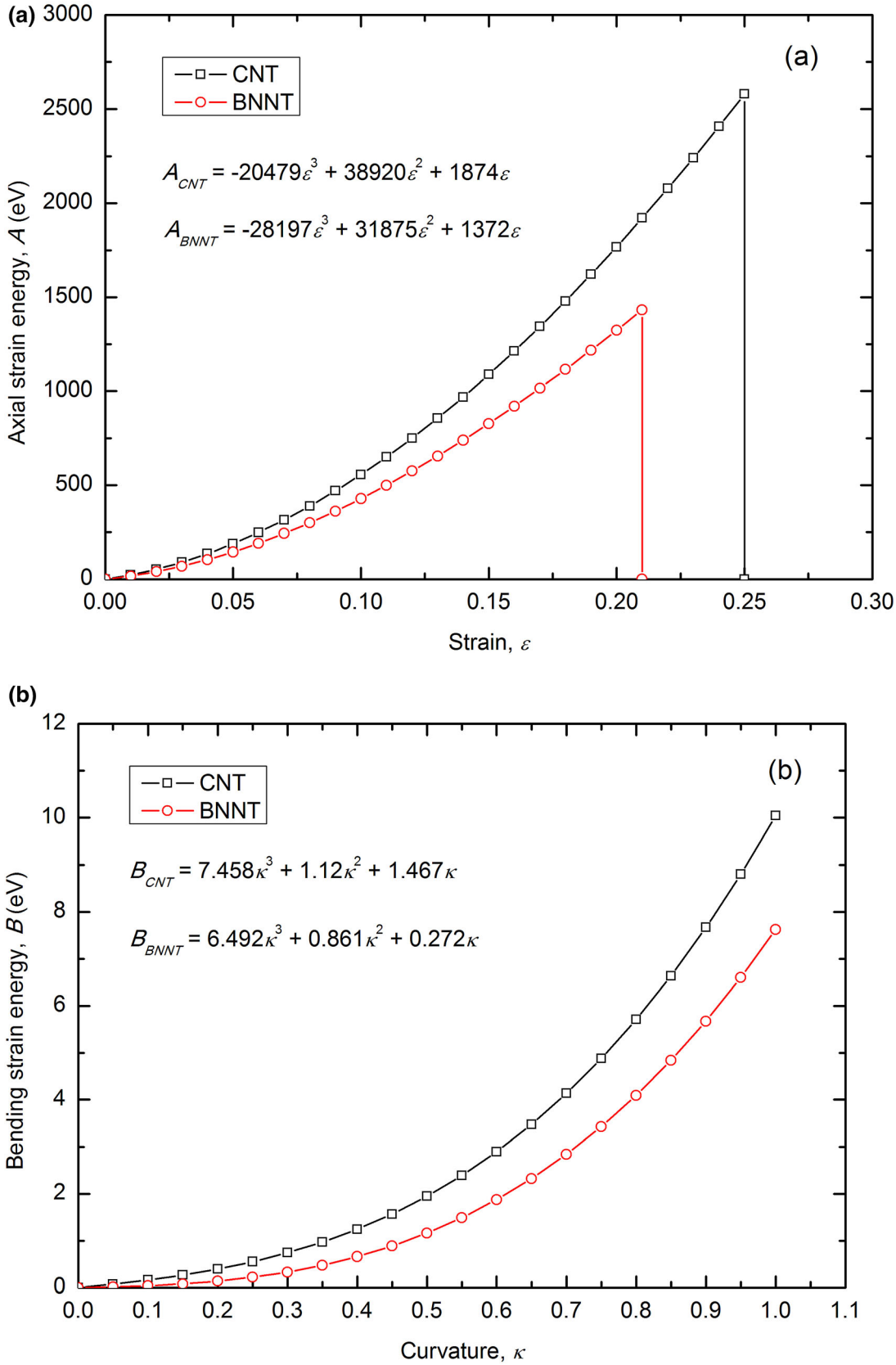

Fig. 1. Strain energy curves of (10,10) nanotubes under (a) axial and (b) bending loading.

determined from the MD simulation, they can be used to obtain the important mechanics quantities of wall thickness and elastic modulus, as defined by the following elastic theory equations:

$$K = \frac{Eh}{1-\nu^2} \approx Eh \tag{1}$$

$$D = \frac{Eh^3}{12(1-\nu^2)} \approx \frac{Eh^3}{12} \tag{2}$$

where ν is the Poisson ratio of the nanosheet.

The unique values for E and h for the CNT and BNNT are then determined from the intersection of the K and D curves in the E–h coordinate plane, as shown in Fig. 2a and b, respectively. These unique values of E and h of the CNT and BNNT satisfy the *necessary* condition of the Vodenitcharova-Zhang[32] condition. The *sufficient* criteria according to the Wang-Zhang[37,39] condition states that the computed thickness of the nanotube must not exceed the atomic diameter of the elements comprising the nanotube.

The computed effective thickness and elastic modulus of the different nanotubes, as obtained from the intersection of K and D curves, satisfy both the necessary and the sufficient conditions and are shown in the inset in Fig. 2. The computed effective thickness of both nanotubes is found to be 0.106 nm, which is lower than the elemental atomic diameter of carbon (0.14 nm), boron (0.13 nm), and nitrogen atoms (0.17 nm). It can also be noted that the thickness of the CNT and BNNT are nearly equal to each other. This is expected since, for a given chirality, BNNT and CNT exhibit similar hexagonal lattice structures, and there should not be much variation in the thickness of the cross-section. Also, previous studies have consistently estimated the elastic modulus of CNT to be higher than that of BNNT, regardless of the wall thickness of the hexagonal atomic lattice. As the current approach predicts the elastic modulus of CNT to be higher than the elastic modulus of BNNT, the findings can be validated.

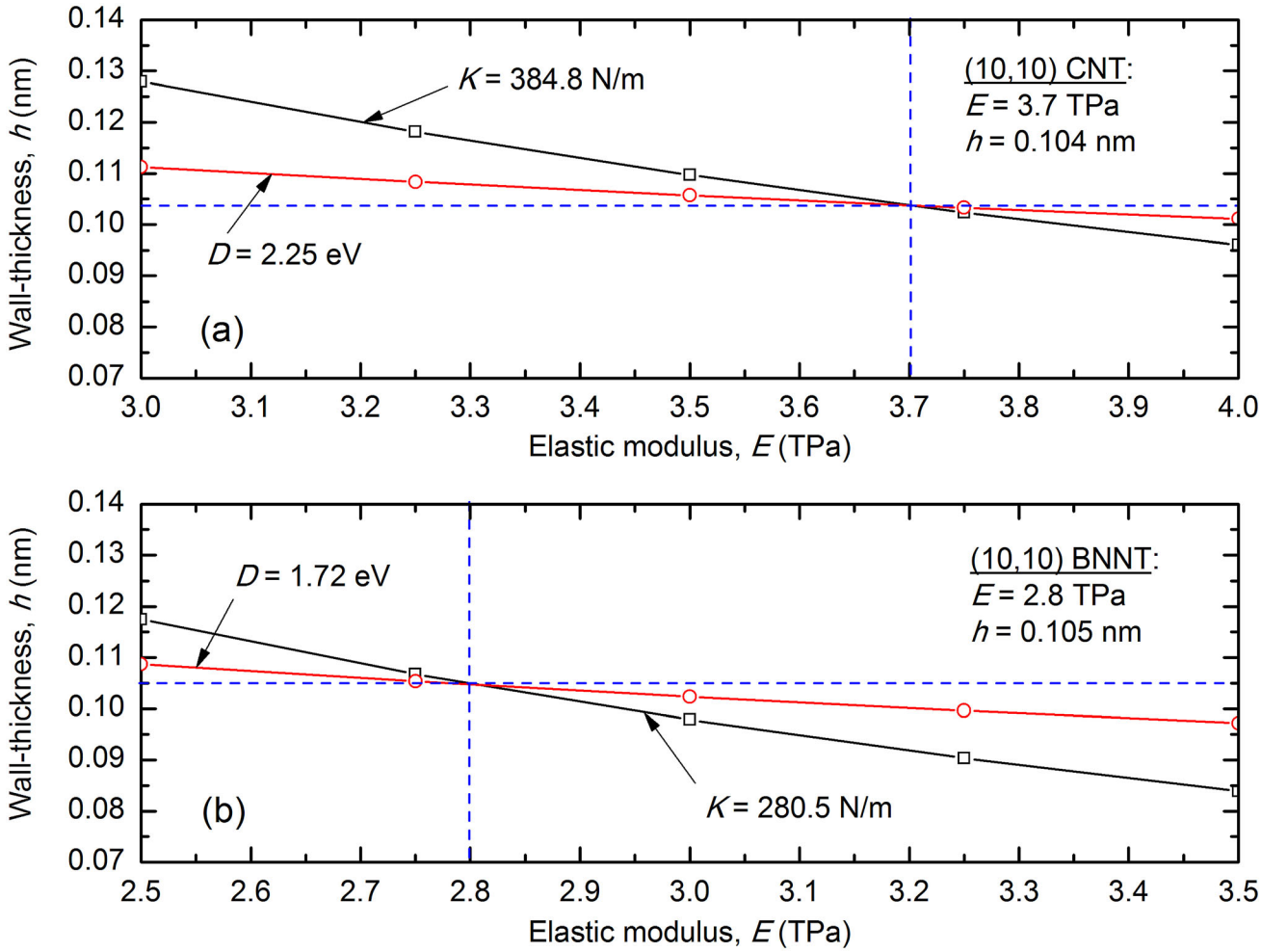

Fig. 2. Computation of wall thickness and elastic modulus of (a) CNT and (b) BNNT by obtaining the intersection points of the K and D curves in the E–h plane.

Effect of Nanotube Radius on Computed Stiffness Parameters of Nanotube

This section will focus on analyzing the effect of nanotube radius on the computed axial and bending stiffness of different nanotubes. As explained in the previous section, the stiffness parameters of different nanotubes of varying nanotube radii can be systematically calculated by using the methodology and set of criteria as established in Refs. 32, 37 Nanosheets of the width equaling the circumference of the nanotubes to be formed and the length corresponding to an aspect ratio of 7.37 are considered. The calculated axial and bending stiffness parameters of different nanotubes are then plotted against varying nanotube radii, R, as shown in Fig. 3a and b, respectively. Regardless of the nanotube type, it can be seen that there exists a *threshold radius*, $R_t \approx 0.6$ nm, after which no appreciable variation of the nanotube stiffness parameters is observed. These trends in the observed variation of nanotube stiffness with the radius of the nanotubes are also in agreement with previous studies.[17,48] The reduced axial stiffness of nanotubes with radii smaller than R_t is attributed to the weaker resistance to tensile loading of the corresponding unwrapped nanosheets with a small width. In contrast, the higher bending stiffness of nanotubes with radii smaller than R_t is attributed to the increase in curvature to which the nanosheets need to be wrapped to form the nanotubes. It follows from the previous section that the thickness and elastic modulus of a nanotube is primarily dependent on its stiffness parameters, which in turn vary according to the radius of the nanotube. This analysis provides an interesting insight into understanding the variations in mechanical properties of nanotubes with different radii, which is described in the next section.

Applicability of Continuum Principles in Estimating Nanomechanical Properties

In estimating the mechanical properties of nanotubes using continuum principles, the thickness of the nanotube in most cases is assumed to be 0.34 nm, which is the inter-layer separation

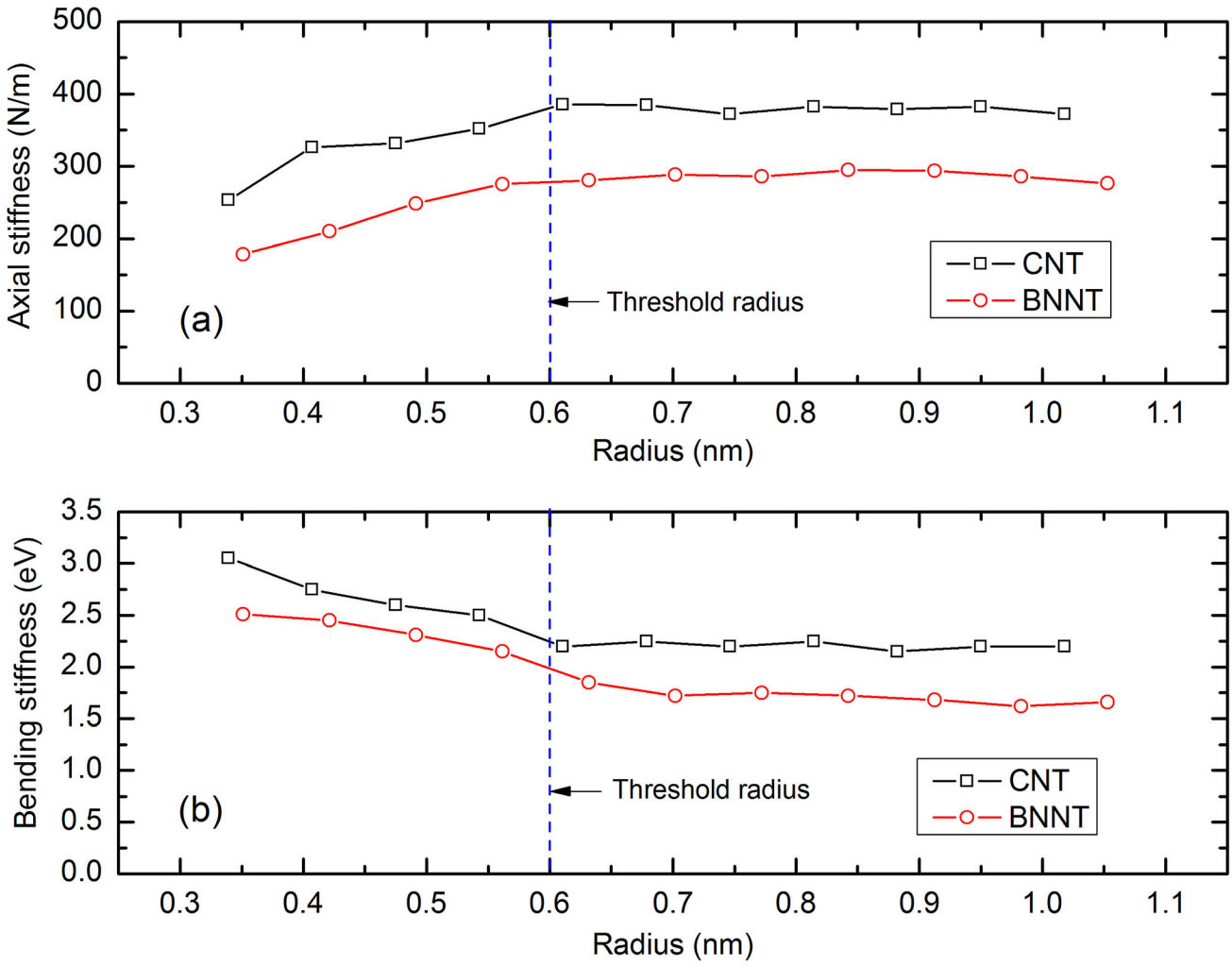

Fig. 3. Plot of (a) axial and (b) bending stiffness of different nanotubes as a function of nanotube radius.

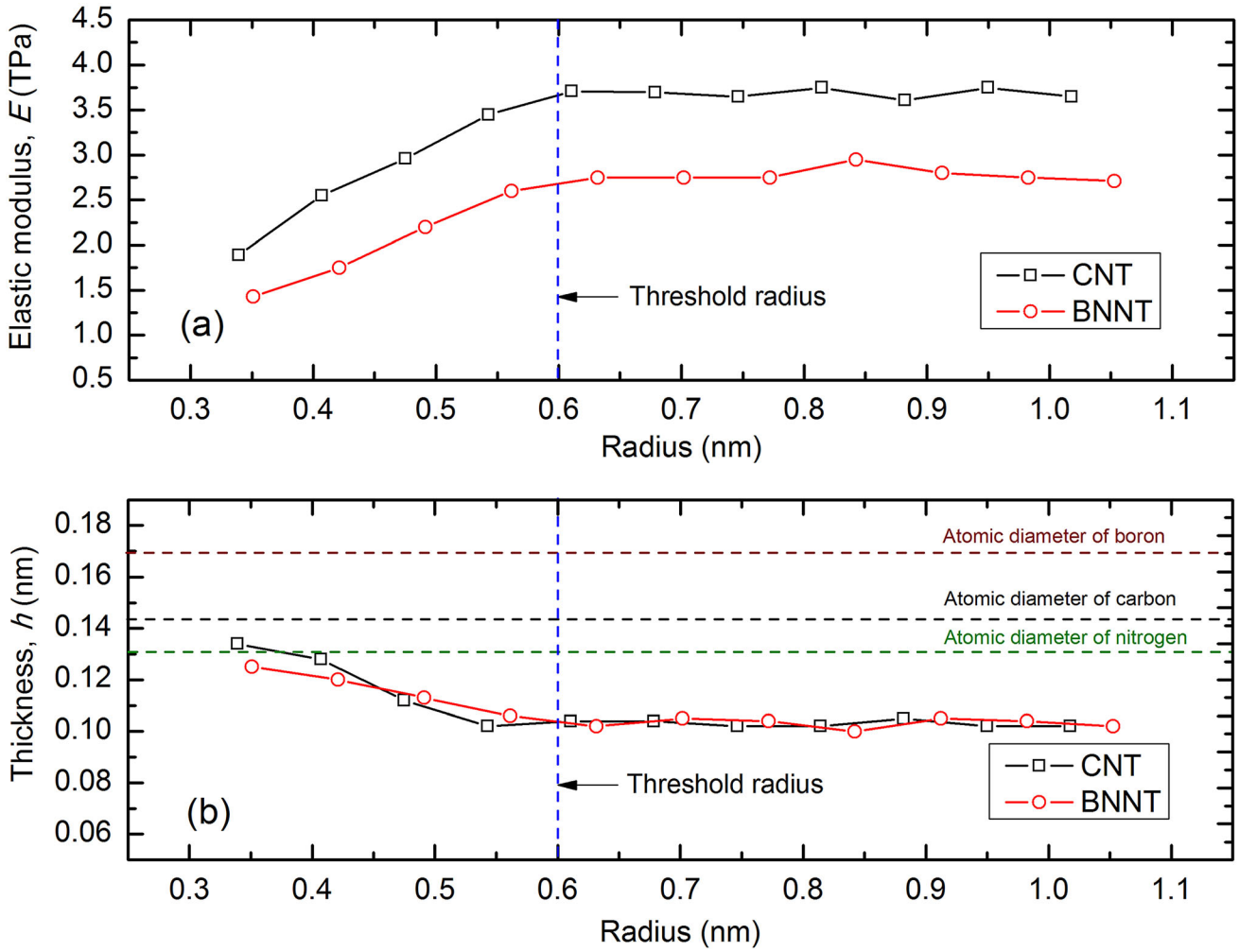

Fig. 4. Measures of (a) elastic modulus and (b) wall thickness of different nanotubes.

distance between adjacent graphene sheets. As highlighted in Refs. 32, 37, the atomic diameters of carbon, boron, or nitrogen atoms are much lower than 0.34 nm, which renders the assumption to be invalid. This uncertainty in the assumption of the exact wall thickness has led to a scatter in the measured elastic moduli of nanotubes. It is also commonly assumed that all nanotubes, regardless of their radius, exhibit equal wall thicknesses. This assumption is also not entirely valid, as it has been shown in previous sections that the wall thickness depends on the nanotube stiffness, which can again vary depending on the nanotube radius. It would be useful to determine the wall thickness and elastic modulus of nanotubes for varying nanotube radii, from which the wall thickness or elastic modulus for nanotubes with any given radius can be readily determined. Using the methodology as described in "Measurement of nanotube thickness from its unwrapped nanosheet counterpart" section, the elastic moduli and wall thicknesses of different nanotubes are computed and plotted as a function of nanotube radius, as shown in Fig. 4a and b, respectively. For smaller nanotubes, the wall thickness tends to approach the diameter of the atomic elements comprising the nanotube. This is expected, since the cross-section of a nanotube with the least possible radius should ideally consist of one or two atoms,and the diameter of the individual atom can be taken as the wall thickness of the nanotube. For nanotubes whose radius exceeds R_t (0.6 nm), the wall thickness does not vary much with the variations in the nanotube radius, and is estimated to be around 0.104 nm. This value of wall thickness can be used in the continuum modeling approach to determine the mechanical characteristics of nanotubes provided the nanotube radius exceeds R_t. Correspondingly, it is also observed that the elastic modulus of nanotubes initially increases, and approaches stable values for the nanotubes once the nanotube radius reaches R_t. This phenomenon is also in agreement with some previous studies which predicted that the elastic modulus of nanotubes with larger diameters approaches the value

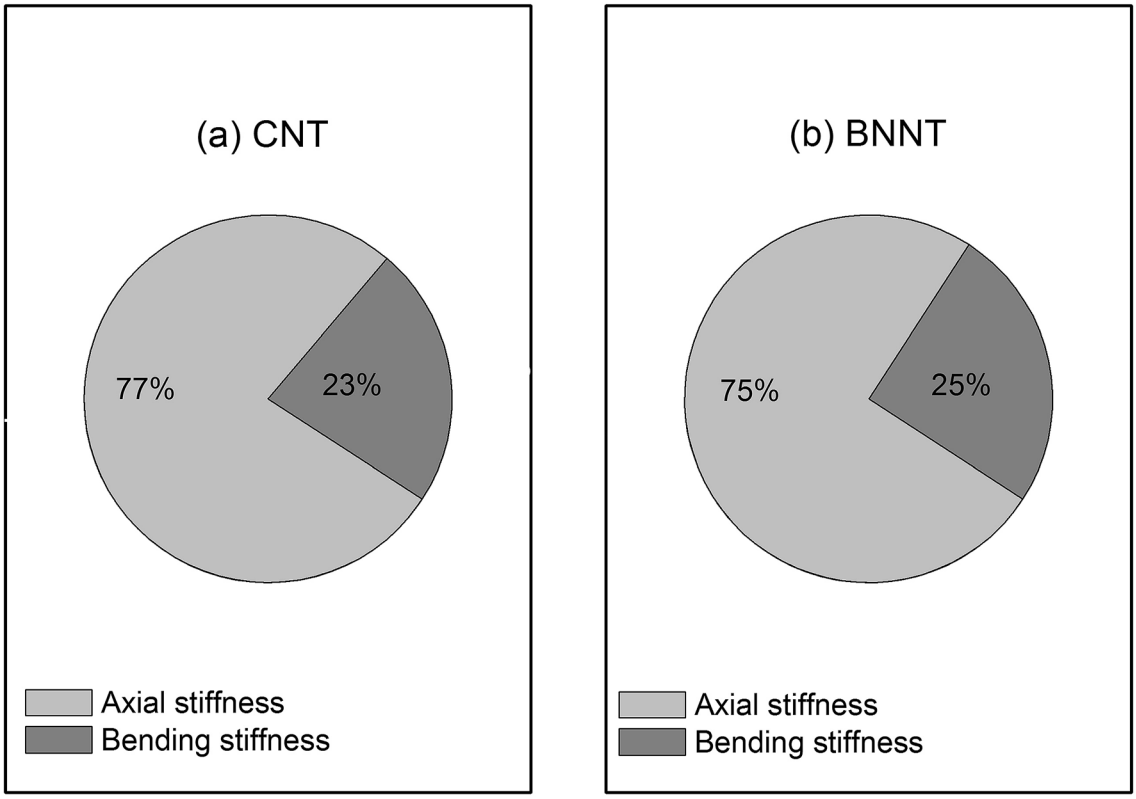

Fig. 5. Sensitivity of the elastic moduli of (a) CNT and (b) BNNT to stiffness parameters.

of a two-dimensional nanosheet due to the decrease in curvature.[49,50] For nanotubes with radii more than R_t, the elastic modulus of CNT and BNNT is found to be around 3.75 TPa and 2.80 Tpa, respectively. These values are found to be in good agreement with the values of the elastic modulus predicted using computationally expensive ab initio techniques[3,10] or molecular mechanics models.[24,32] In concurrence with the conclusions made in Refs. 14, 32, 37, these studies also reinforce the importance of calculating the correct wall thickness of nanotubes in achieving a reliable estimate of their mechanical properties regardless of the computational technique adopted.

Sensitivity Analysis of Axial and Bending Stiffness on Elastic Modulus of Nanotube

It is also useful to predict the sensitivity of the wall thickness and elastic modulus of nanotubes to the calculated axial and bending stiffness values obtained by wrapping up of the nanosheet to form a nanotube. The measure of sensitivity of the elastic modulus (M_{EM}) to the considered stiffness variables (S_i) is given as:

$$\mathrm{Range}_i = \mathrm{EM}_{\max}(S_i) - \mathrm{EM}_{\min}(S_i) \tag{3}$$

$$M_{\mathrm{EM}} = \frac{\mathrm{Range}_i}{\sum_{j=1}^{n} \mathrm{Range}_j} \times 100 \tag{4}$$

where $\mathrm{EM}_{\min}(S_i)$ and $\mathrm{EM}_{\max}(S_i)$ are the minimum and maximum values of the elastic modulus, respectively, measured for the range of a particular stiffness variable considered. The other stiffness variable is maintained at its average value.

In the present study, the computed axial stiffness was found to vary from 253.26 N/m to 372.3 N/m for CNTs and from 178.75 N/m to 276.42 N/m for BNNTs. The bending stiffness was found to vary from 2.2 eV to 3.05 eV for CNTs and from 1.66 eV to 2.51 eV for BNNTs. The elastic modulus of the different nanotubes are then computed for the lowest and highest values for either one of the axial or bending stiffness value ranges, while maintaining the other stiffness variable at the mean value. The percentage influence of each of the stiffness variables on the elastic moduli of CNT and BNNT is depicted in Fig. 5a and b, respectively. It is clear from this figure that the elastic moduli of both CNT and BNNT are significantly influenced by the axial stiffness of the nanotube. This means that the measure of axial stiffness is a good indicator to express the elastic modulus of nanotubes, without the need to measure the wall thickness. This is also evident by comparing Fig. 3 with Fig. 4, where an identical trend is observed in which the axial stiffness and elastic modulus vary for different nanotube radii. Additionally, since the axial stiffness can be measured directly from the atomistic simulations, it can also be used as a metric to

express the strength of nanotubes without the need to compute the actual value of the wall thickness.

CONCLUSIONS

This paper has presented an investigation on the determination of some mechanical properties of nanotubes using MD simulation. The literature data of computational characterization of CNTs and BNNTs are first presented, and show a wide scatter of the elastic moduli of nanotubes. To address this, the effective wall thicknesses of different nanotubes are first computed using the well-established Vodenitcharova-Zhang[32] and Wang-Zhang[37] criteria. The elastic moduli of different nanotubes for a range of varying nanotube radii are then computed. The study shows that there exists a threshold nanotube radius, beyond which nearly uniform wall thickness and elastic modulus values are observed, regardless of any variation in the nanotube radius. For nanotubes with radii smaller than that of the threshold, the wall thickness will vary and will lead to a variation in the measured elastic modulus of the nanotubes. Sensitivity analysis showed that the elastic moduli of nanotubes are predominantly affected by the axial stiffness. It is anticipated that the findings from the present study are expected to further improve the reliability of predicting the mechanical characteristics of a wide range of nanostructures using computational modeling techniques.

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