



Review

On the mechanics of single-walled carbon nanotubes

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ABSTRACT

This review paper discusses some basics in using continuum mechanics and molecular dynamics to characterize the deformation of single-walled carbon nanotubes (SWCNTs). It identifies that the van der Waals force between SWCNTs in a bundle distributes symmetrically and influences the bundle formation, and that to avoid misleading results from a molecular dynamics simulation, the interaction potential, thermostat scheme and simulation parameters must be carefully selected. The paper then points out that when the necessary condition proposed by Vodenitcharova and Zhang and a compatibility condition for elastic constants are satisfied, the intersect of the bending and in-plane stiffness curves in the modulus-thickness plane can determine a unique effective wall thickness of an SWCNT and hence its Young's modulus.

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1. Introduction

Since the discovery of carbon nanotubes, extensive investigations have been carried out on both single-walled and multi-walled nanotubes. A research focus in the field has been to characterize precisely the mechanical properties of nanotubes using various methods including continuum mechanics and molecular dynamics modelling, and to understand the chemical reactivity of nanotubes with a class of matrix materials for stronger interface stress transfer capabilities. Developing efficient techniques for fabricating ceramic-based (Arsecularatne and Zhang, 2007) and polymer-based (Mylvaganam and Zhang, 2007) nanocomposites with tailored microstructures has also been emphasized recently.

There are some basic mechanics issues that have not been clarified and have caused confusions in the research community, such as the determination of wall thickness of nanotubes, their mechanical property assessment, and the reliable application of molecular dynamics.

This review paper will discuss these mechanics issues of single-walled carbon nanotubes (SWCNTs).

2. Mechanics modelling of SWCNTs

Under external loading, a carbon nanotube has been found to deform like a continuum structure and has both membrane and bending capacities. Hence, it will be beneficial if equivalent continuum theories can be established for analysing their mechanical behaviour. This has led to extensive studies on the equivalent or effective properties and geometrical dimensions of a carbon nanotube.

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2.1. Effective wall thickness and Young's modulus

To characterize the mechanical properties of a carbon nanotube, one often directly uses the mechanics quantities defined by continuum mechanics, such as Young's modulus. However, a carbon nanotube has a discrete molecular structure and its 'wall' comprises of only a number of atoms, and hence does not have continuous spatial distribution. Nevertheless, to calculate the Young's modulus of a carbon nanotube, one needs to know the wall thickness of the tube. For example, in a simple tensile loading, the Young's modulus E of a single-walled carbon nanotube is defined as $E = \sigma/\varepsilon$ where ε is the strain, and σ is the axial stress applied on the tube calculated by $F/(2\pi Rh)$ in which R is the radius of the mid-surface of the tube, h is the tube thickness and F is the axial force applied. Although R may be reasonably defined as the imagined surface radius of a nanotube through the theoretical centers of the atoms, h does not exist because a nanotube does not have a continuous wall. In the literature, mechanics modelling has been based on unreasonable assumptions of h . For example, some researchers treated a carbon nanotube as a solid beam (Wong et al., 1997), or a solid cylinder (Govindjee and Sackman, 1999), and some others simply let h be the inter-planar spacing of two graphite layers ($\approx 3.4 \text{ \AA}$) (Yu et al., 2000; Krishnan et al., 1998). As a result, the Young modulus of a carbon nanotube calculated with different h values varies in a wide range.

Vodenitcharova and Zhang (2003) introduced a concept of an effective wall thickness under the umbrella of continuum mechanics. Based on the consideration of force equilibrium and equivalence, they proposed a necessary condition that the effective wall thickness must be smaller than the theoretical diameter of a carbon atom ($\sim 0.142 \text{ nm}$). Their argument is that a cross-section of a nanotube contains only a number of atoms and the forces in the tube are transmitted through these atoms; but in a continuum mechanics model the same forces are transmitted through a continuous wall. Because of this, the effective wall thickness cannot be greater than or equal to the theoretical diameter of a carbon atom; as otherwise, the tube equilibrium cannot be maintained. Vodenitcharova and Zhang (2003) then proposed, using an elastic ring theory and the results from molecular dynamics analysis by Tang et al. (2000), that the effective thickness of a single-walled carbon nanotube should be $h \approx 0.617 \text{ \AA}$, which is about 44% of the theoretical diameter of a carbon atom, and that the effective Young's modulus E of the tube is $\sim 4.88 \text{ TPa}$.

In an attempt to address the continuum-atomic modelling issue, Zhang et al. (2002, 2004) directly linked interatomic potential and atomic structure of an SWCNT with a continuum constitutive model, by equating the strain energy stored in the equivalent constitutive model to that in atomic bonds described by Tersoff–Brenner potential. This method seems to be reasonable because the Tersoff–Brenner potential has been shown to be appropriate for analysing SWCNTs (Mylvaganam and Zhang, 2004). An isotropic constitutive model was therefore derived for SWCNTs subjected to in-plane deformation with two elastic constants, the in-plane stiffness, $K_{in-plane}$, and the in-plane shear stiffness, K_{shear} . Then the following relationship was obtained by comparing the two elastic constants of SWCNTs with their counterparts of three dimensional (3D) thin shells of thickness h :

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

where $G = E/2(1+\nu)$ is shear modulus and ν is Poisson's ratio of SWCNTs which can be obtained from $K_{in-plane}/K_{shear} = (1-\nu)/2$. However, the effective thickness of SWCNTs cannot be determined in this way because only in-plane deformation is considered.

Huang et al. (2006) considered both the in-plane and off-plane deformation of SWCNTs. By using the Tersoff–Brenner

potential, V , and the modified Cauchy–Born rule, they obtained two-dimensional isotropic constitutive relations, where bending stiffness, $D_{bending}$, and off-plane torsion stiffness, $D_{torsion}$, as well as $K_{in-plane}$ and K_{shear} of SWCNTs were calculated as:

$$D_{bending} = \frac{\sqrt{3}}{2} \left(\frac{\partial V}{\partial \cos \theta_{ijk}} \right), \quad D_{torsion} = 0,$$

$$K_{in-plane} = \frac{1}{2\sqrt{3}} \left[\left(\frac{\partial^2 V}{\partial r_{ij}^2} \right)_0 + \frac{A}{8} \right], \quad K_{shear} = \frac{A}{16\sqrt{3}} \quad (2)$$

in which θ_{ijk} ($k \neq i, j$) is the angle between bonds $i-j$ and $i-k$, r_{ij} is the $i-j$ bond length, and A is a function of the first- and second-order derivatives of V with respect to r_{ij} , θ_{ijk} and θ_{ijl} ($l \neq i, j, k$). In this derivation, the bending of SWCNTs was considered as a result of the σ -bond angle change while the off-plane torsion was assumed to be independent of the deformation of the σ -bonds.

However, if we use a three-dimensional continuum thin shell theory, where bending and off-plane torsion are due to the deformation across the wall thickness, we will have a different observation about the deformation mechanics of SWCNTs, because $D_{bending}$ and $D_{torsion}$ of a three-dimensional thin shell are related to the shell thickness h and the in-plane material constants by

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

Combining Eqs. (1) and (3) leads to the following condition:

$$\frac{D_{bending}}{K_{in-plane}} = \frac{D_{torsion}}{K_{shear}} = \frac{h^2}{12} \quad (4)$$

The above derivation indicates that to establish a three-dimensional elastic shell model with a defined effective thickness for SWCNTs, the key is to satisfy condition (4) when the corresponding elastic constants are obtained based on an atomistic potential that accounts for the atomic structure and the deformation mechanisms of SWCNTs. Nevertheless, Eq. (2) was obtained from potential V with $D_{torsion} = 0$, which cannot satisfy condition (4) and hence leads to an ill-defined effective thickness of SWCNTs.

To obtain a deeper understanding without the influence of the currently debatable wall thickness and Young's modulus, Wang and Zhang (2008a) employed in-plane stiffness $K_{in-plane}$, Poisson's ratio ν , bending stiffness $D_{bending}$ and off-plane torsion stiffness $D_{torsion}$ as independent elastic constants in their mechanics solution to the free vibration of SWCNTs. They found that the off-plane torsion stiffness cannot be zero which is in agreement with molecular dynamics results and experimental measurements in the literature, and that the effective thickness and Young's modulus are about 0.1 nm and 3.55 TPa, respectively, for (10, 10) SWCNTs. Wang and Zhang (2008b) then made an interesting analysis by plotting the diverse values of Young's modulus and wall thickness in the literature on a single diagram, as shown in Fig. 1. They found that those satisfy Vodenitcharova–Zhang's necessary condition (Vodenitcharova and Zhang, 2003) collapse very nicely into the curve of constant in-plane stiffness = 363 J/m^2 . It means that there is something in common in predicting the mechanical properties of SWCNTs when using different methods, although the values of Young's modulus and effective wall thickness still scatter and the experimentally measured properties available correspond to different $K_{in-plane}$ values.

As discussed above, if an SWCNT is modelled as a 3D isotropic shell, the elastic constants of the shell must satisfy $D_{bending}/K_{in-plane} = D_{torsion}/K_{torsion}$, which reflects the bending mechanism of a continuum shell and ensures the existence of an effective thickness. On the other hand, the deformation of SWCNTs in atomistic models is caused by the changes in chemical bonds between neighbouring atoms. Thus, if the $K_{in-plane}$, $K_{torsion}$, $D_{bending}$ and $D_{torsion}$ given by an atomistic theory cannot satisfy the above condition, this

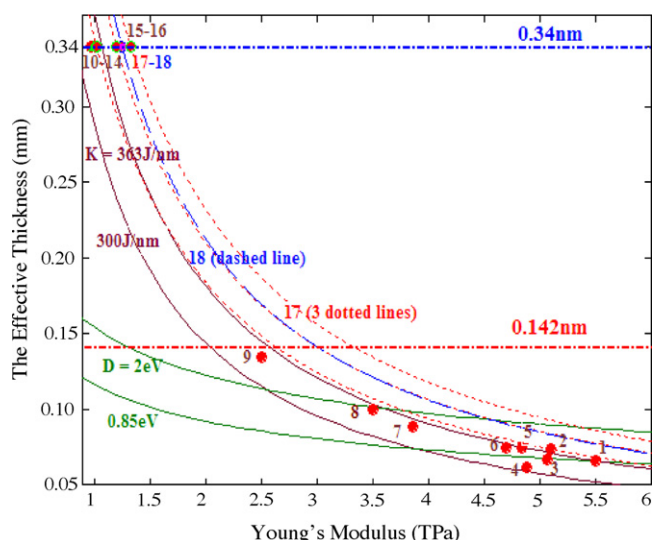


Fig. 1. A comparison of the scattered values of effective wall thickness and Young's modulus of SWCNTs in the literature. Dots numbered are from the papers listed below: 1: Zhang et al. (2002); 2: Zhou et al. (2000); 3: Wang et al. (2005); 4: Vodenitcharova and Zhang (2003); 5: Pantano et al. (2004); 6: Tu and Ou-Yang (2002); 7: Kudin et al. (2001); 8: Wang and Zhang (2008a); 9: Sears and Batra (2004); 10: Lu (1997); 11: Li and Chou (2003); 12: Yao and Lordi (1998); 13: Ozaki et al. (2000); 14: Belytschko et al. (2002); 15: Hernández et al. (1999); 16: Jin and Yuan (2003); 17: Krishnan et al. (1998); 18: Tomblér et al. (2000).

atomistic model cannot give rise to a consistent effective thickness and an effective Young's modulus. Based on this Zhang and Wang (in press) concluded that if condition $D_{bending}/K_{in-plane} = D_{torsion}/K_{torsion}$ and the Vodenitcharova–Zhang's necessary condition are satisfied at the same time, the intersect of the $D_{bending}$ and $K_{in-plane}$ curves in the $E-h$ plane determines a unique h and a corresponding E . They therefore proposed the following sufficient condition for determining the effective thickness h of an SWCNT: "The h and E values can be determined by the intersect of the $D_{bending}$ and $K_{in-plane}$ curves in the $E-h$ plane by a continuum or an atomistic model, when condition $D_{bending}/K_{in-plane} = D_{torsion}/K_{torsion}$ and the Vodenitcharova–Zhang's necessary condition are satisfied at the same time".

2.2. Mechanics of bundle formation

A clear understanding of the CNT bundle formation is of importance to the fabrication of CNT ropes or fibres. Lopez et al. (2001), Charlier et al. (1996) and Tersoff and Ruoff (1994) have shown that individual SWCNTs in a bundle are already deformed in an externally unstressed state due to the intertubular van der Waals forces. The SWCNTs are flattened, the lattice constant decreases and the distance between the SWCNTs, called equilibrium distance d , becomes smaller than the equilibrium distance between two graphite layers (3.42 \AA). At a distance equal to d , the resultant forces of interaction between the neighbouring SWCNTs are zero; at a distance larger than d the nanotubes attract each other; and at a distance smaller than d the intertubular interaction becomes repulsive. Tersoff and Ruoff (1994) found that the faceting of the SWCNTs in a bundle is radius-dependent: the cross-sectional distortion of SWCNTs becomes noticeable when their radii are large. Since the bundle polygonization is caused by van der Waals forces, it would be interesting to know their magnitude, distribution and their dependence on the SWCNT radius.

Vodenitcharova and Zhang (2004) analysed a zigzag SWCNT bundle by combining molecular dynamics and continuum mechanics. They consider the deformation of the central SWCNT in a long bundle under the van der Waals forces $p(\theta)$, as illustrated in Fig. 2.

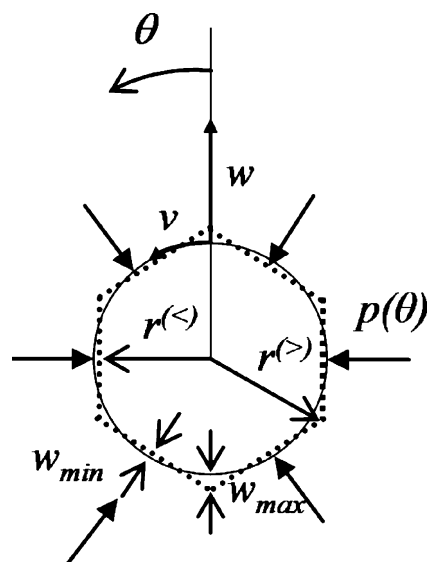


Fig. 2. The central SWCNT in a bundle and the notations used in the continuum mechanics model.

According to the thin shell theory, a point on the mid-surface of the nanotube can undergo displacements in the longitudinal, circumferential and radial directions, i.e., u , v and w , measured from the undeformed geometry. Zero displacements correspond to an isolated SWCNT with no forces acting on it. Since the length of an SWCNT in a bundle is much greater than its diameter and the van der Waals forces along the SWCNT axis can be considered uniform, the SWCNT can be modelled as a ring of unit length under plane-strain deformation with the longitudinal displacement u neglected. The remaining displacements are the radial displacement w (positive outward) and the tangential displacement v (positive in the direction of positive θ , Fig. 2). Using the ring theory of continuum mechanics, Vodenitcharova and Zhang (2004) obtained an analytical solution which shows the following deformation features of an SWCNT in a bundle.

Fig. 3 shows the typical deformation pattern of a (36, 0) SWCNT bundle, where each dot represents a carbon atom on the cross-section of the bundle. It is clear that the central SWCNT has been deformed significantly into a symmetrical faceting shape.

The initial van der Waals interaction energy of the circular tubes in a bundle is very small (2–4 meV/atom). This is in agreement

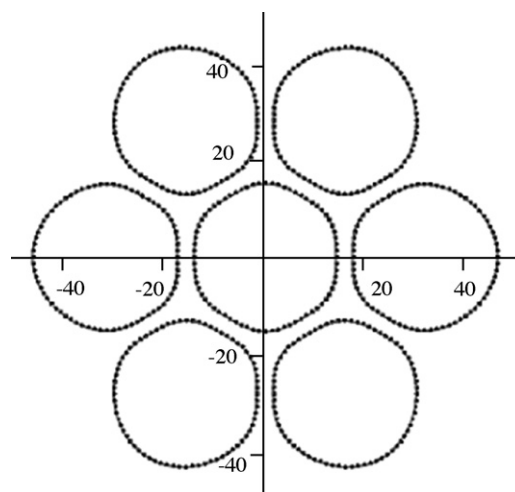


Fig. 3. Cross-sectional view of the deformed (36, 0) SWCNT bundle obtained by the MD simulation. The coordinate unit is Å.

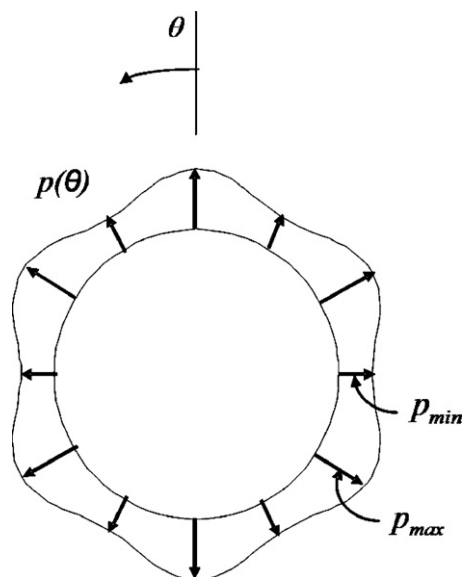


Fig. 4. The van der Waals force distribution on an SWCNT.

with the results reported by Lopez et al. (2001). The strain energy induced during flattening was calculated as the difference in the minimum total energy of the bundle and the total energy of the isolated undeformed nanotubes. It was found that the strain energy varies from 8.3 meV/atom for a nanotube with a radius of 7.05 Å to 7.2 meV/atom for a nanotube with a radius of 14.1 Å. Obviously, the strain energy decreases with the increase in radius, indicating that more energy is required to deform nanotubes of smaller radii. The circumferential displacement v is negligible compared with the radial displacement w , demonstrating that during the bundle formation the nanotube atoms displace predominantly in the radial direction. Furthermore, the van der Waals forces $p(\theta)$ are attractive (negative sign means attraction) and attain their maximum value p_{max} in the channels (see Fig. 4) where the attraction between the neighbouring atoms of adjacent nanotubes is more significant, and their minimum value p_{min} at the points of minimum intertubular distance where the attraction is small. The radial displacement is outward even at the shortest distance between the SWCNTs. For radii greater than 11 Å, the non-uniform inward displacement dominates at the points of minimum intertubular distance. The bundle formation of larger nanotubes is associated with a lower intensity of the attractive van der Waals forces, but the values of both p_{min} and p_{max} are significant. For the nanotube radii considered, p_{max} varies from –6 to –11 GPa and p_{min} varies from –1 to –5 GPa.

3. Molecular dynamics modelling

Molecular dynamics simulation has been widely used in characterising the mechanical properties of materials (Zhang, 2006) and in understanding their mechanisms of deformation on the nanometre scale (Zhang and Mylvaganam, 2006). However, the simulations must be done carefully to best represent the reality. First, it is important to select an appropriate interaction potential that can effectively describe the deformation of a nanotube correctly. Secondly, during a loading process, improper treatment of temperature rise can lead to fictitious results. In molecular dynamics, heat conduction is accomplished via the so-called thermostat atoms using a thermostatting method. Adiabatic relaxation method, isokinetic-thermostatting, Andersen stochastic thermostatting and Nose-Hoover feed back thermostatting are

some typical methods for temperature conversion. For small systems, the adiabatic relaxation method can lead to a fluctuation of the vibrational-relaxation rate. In isokinetic-thermostatting, the temperature is maintained in different ways. For example, in the Berendsen thermostat scheme with velocity scaling, the velocities of thermostat atoms are scaled to fix the total kinetic energy. In the Gaussian feedback or Evans-Hoover scheme with force scaling, however, the kinetic energy is monitored and information is fed back into the equations of motion so that the kinetic energy is kept constant to dissipate heat by controlling the thermostatting force. Velocity scaling (Zhang and Tanaka, 1997, 1999) has been widely used because of its simplicity in implementation. For small time steps, the Gaussian isokinetic method and velocity scaling method become identical (Arsecularatne and Zhang, 2007). However, a very small time step will give an unusually high elongation speed. On the other hand, a small displacement step with a small time step will be computationally expensive. The flaw in the isokinetic-thermostatting method is that it is impossible to separate the effects of thermostatting on rate processes. The other two schemes also have this limitation to a certain extent. Thirdly, a system has to be relaxed initially as well as during the simulation so that the velocities of the Newtonian and thermostat atoms reach equilibrium at the specified temperature of simulation; thus appropriate time step and displacement step have to be selected to get a reasonable elongation speed. A natural question is therefore: Which simulation scheme will be appropriate and effective for simulating the deformation of carbon nanotubes? Mylvaganam and Zhang (2004, 2005) have investigated some necessary details that are central to a reliable simulation, such as the selection of potential, number of thermostat atoms, thermostat method, time step, displacement step and the number of relaxation steps.

Consider a single-walled armchair nanotube (10, 10) with 100 repeat units along the axial direction and a zigzag nanotube (17, 0) with 58 repeat units along the axial direction, both having a length of about 245 Å. The interatomic forces will be described by the Tersoff (T) potential and the empirical bond order potential – the Tersoff–Brenner (TB) potential. The simulations will be carried out at 300 K with Berendsen (B) and Evans-Hoover (EH) thermostats and a time step of 0.5 fs. To examine the reliability of the simulations, Mylvaganam and Zhang (2004) carried out the analysis using the following schemes:

- *Scheme 1 (S1)*: In this scheme, the first two layers of atoms on both ends of a carbon nanotube were held rigid. The next four layers were taken as thermostat atoms and the remaining were treated as Newtonian atoms. First, the tubes were annealed at the simulation temperature for 5000 time steps. Then the rigid atoms on both ends were pulled along the axial direction at an increment of 0.05 Å. After each displacement step, 1000 relaxation steps were done to dissipate the effect of preceding displacement step over the entire length of the tube.
- *Scheme 2 (S2)*: In this scheme, all atoms except the boundary ones rigidly held were treated as thermostat atoms. 50 relaxation steps were carried out after each displacement step.

Mylvaganam and Zhang (2004) found that simulation parameters have a remarkable influence on the results. For example, different schemes lead to significantly different stress–strain curves and necking processes, as shown in Figs. 5 and 6. We can therefore conclude that a simulation using Tersoff–Brenner potential and Berendsen thermostat with all atoms as thermostat atoms (except the rigid ones) with 50 relaxation steps after each displacement of 0.008 Å is a reliable and cost effective method.

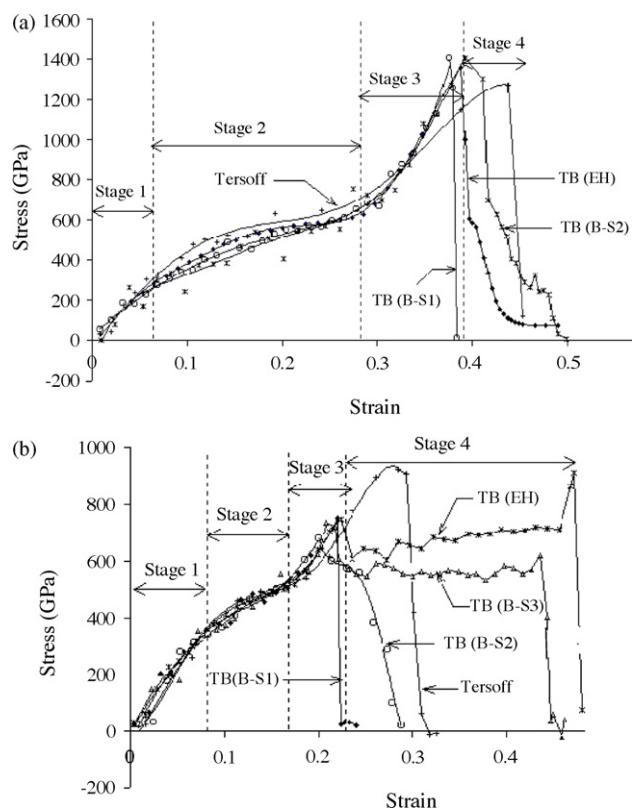


Fig. 5. The stress–strain curves of (a) a (10, 10) armchair SWCNT and (b) a (17, 0) zigzag SWCNT using Tersoff and Tersoff–Brenner potentials. In the figure, TB(B-S1) is the calculation with Berendsen thermostat using Scheme 1, TB(B-S2) is that with Berendsen thermostat using Scheme 2, and TB(B-S3) is that as in TB(B-S2) but with a smaller displacement step of 0.008 Å. TB(EH) is the calculation with the Evans–Hoover thermostat.

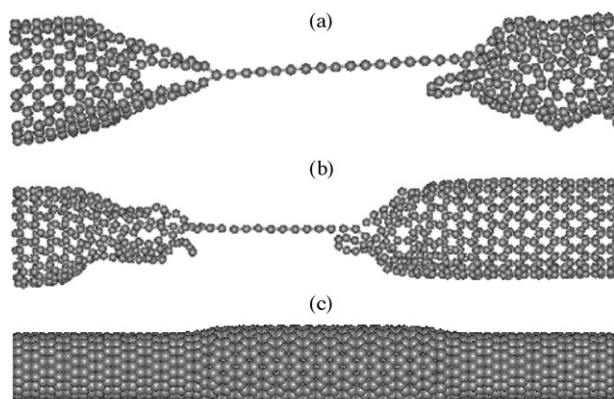


Fig. 6. Deformation of an SWCNT when using Berendsen thermostat: (a) an armchair tube, (b) a zigzag tube and (c) necking that propagates along a zigzag carbon nanotube.

4. Concluding remarks

We have discussed some fundamentals of the mechanics of SWCNTs, including the determination of the effective wall thickness for continuum mechanics modelling, and some basics for reliable molecular dynamics simulations. It is clear that studies along the line are far from sufficient, particularly in the areas of modelling using continuum mechanics, and the coupled approach using both MD and continuum mechanics.

In the literature, there are different views on the mechanical characterisation of CNTs. For instance, some researchers think that there is no need to clarify the effective wall thickness and Young's modulus of CNTs, because one may use other parameters in a specific application, e.g., using bending stiffness. The author believes that the effective wall thickness and Young's modulus are the most fundamental mechanics quantities for modelling using the well-established continuum mechanics theory. Bypassing the basics in case-studies cannot verify, at the grassroots level, the applicability of continuum mechanics theory to nano-analysis.

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