Modal analysis of multi-walled carbon nanocones using molecular dynamics simulation

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Abstract

To design carbon nanocone-based sensing and actuating nanodevices, it is necessary to study their vibrational behavior. For this purpose, modal analysis of multi-walled carbon nanocones are performed using molecular dynamics simulation. Initial closed-tip atomic structures of the carbon nanocones with different apex angles are modeled through a proposed method which is based on the molecular dynamics simulation. The dependency of the resonant frequencies and their corresponding three-dimensional mode shapes on different geometric parameters of multi-walled carbon nanocones are investigated. The results indicate that the order of mode shapes is influenced by the number of layers and apex angle of the multi-walled carbon nanocones. The results also show that the variation of the resonant frequencies with the number of layers depends on the apex angle and shape of the modal displacement. The vibrational behavior of the multi-walled carbon nanocones is also compared with that of the multi-walled carbon nanotubes.

1. Introduction

In modern industry, carbon nanostructures are of great interest because of their potential for structural and electronic applications taking advantage of their novel properties. In particular, cylindrical and conical morphologies of carbon nanostructures are pioneer in this type of applications due to their large surface area and unique shape. Since the discovery of carbon nanotubes (CNTs) [1] and carbon nanocones (CNCs) [2], there has been a great deal of experimental and theoretical researches that focused on their characterization. CNTs and CNCs are good candidates as sensing and actuating elements in nanoscale devices [3–9]. Among these applications, their usage as atomic force microscopy (AFM) tips [3,8] is of particular interest. The proper implementation of CNTs and CNCs as AFM tips, requires comprehensive understanding of their dynamic behavior and a remarkable amount of studies have been performed to investigate the vibrational behavior of these two nanostructures [10–32]. However, the reported works in this field for CNCs are relatively limited as compared with CNTs. Also, the inherent thermal vibration of CNT-based AFM tips, due to the high aspect ratio and small diameter of the nanostructure, reduces imaging quality, but, the sharp tip and less flexibility of CNCs, make them a better candidate to be used as AFM tips [8,33]. So, precise characterization of CNCs is of great importance considering all aspects of this nanostructure.

Due to the technical difficulties associated with the experimental methods for investigating the structures at nanoscale, theoretical and numerical approaches are usually preferred. Continuum mechanics models, molecular mechanics method and molecular dynamics (MD) simulation have been widely used to study and approximate the behaviors of the nanostructures. In the first approach, which is usually based on the nonlocal elasticity theory, CNCs are modeled as beams with varying cross sections [21,30] or as shells [22–24]. The molecular mechanics method is a combination of continuum mechanics models and atomistic approaches. In this method, the bonds between different atoms are represented by structural elements, whereas, the atoms are considered as mass elements and the material constants of the structural elements are obtained by equating the energies of the molecular and structural models. In this way, the nanostructure can be treated as a frame structure and its modal analysis can be performed using the standard finite element method. The vibrational behavior of CNCs, based on this method, has been studied in Refs. [26–28,31].

In the third approach, i.e., MD simulation technique, the interaction between different atoms is described by some potential energy functions and the displacement gradient of these functions results in the applied forces on each atom. Then, these forces are used in Newton’s second law to determine the movement of each atom. This method can provide a detailed understanding about dif-
different behaviors of a discrete structure at the nanoscale by taking into account all the effective parameters. The main drawback of this technique is its high computational cost, in comparison with the two other approaches. Aside from being computationally expensive, MD simulations always involve some inevitable errors as a result of their numerical nature and some basic concepts such as cut-off radius, etc. However, MD simulations have some advantages over continuum mechanics models and molecular mechanics method. The main advantage may be its capability in providing direct control over the temperature of the nanostructure. The other advantage of this method is that material properties such as Young’s modulus and Poisson’s ratio are not needed to study the vibrational characteristics of the nanostructures; while, the accuracy of the results obtained using continuum mechanics models depends strongly on such material properties. These material parameters for CNTs and CNCs are proven to be size dependent [34,35] and there is a big scattering in the experimentally reported data. In addition to the material constants, wall thickness of CNTs and CNCs is not a well-defined quantity, which is required in continuum mechanics models. On the other hand, in the molecular mechanics method, the simple harmonic form is usually adopted to describe the energy of bonded interactions under the assumption of small deformation, and also, the nonbonded van der Waals (vdW) interactions are usually neglected. While, in general, MD simulation approach can describe both bonded and nonbonded interactions in a more realistic nonlinear way through different appropriate potential functions. There are a limited number of studies which have utilized MD simulation to investigate the vibrational behavior of CNCs. Firouz-Abadi et al. [29] examined the studies which have utilized MD simulation to investigate the vibrational characteristics of the nanostructures; while, the accuracy of the results obtained using continuum mechanics models depends strongly on such material properties. These material parameters for CNTs and CNCs are proven to be size dependent [34,35] and there is a big scattering in the experimentally reported data. In addition to the material constants, wall thickness of CNTs and CNCs is not a well-defined quantity, which is required in continuum mechanics models. On the other hand, in the molecular mechanics method, the simple harmonic form is usually adopted to describe the energy of bonded interactions under the assumption of small deformation, and also, the nonbonded van der Waals (vdW) interactions are usually neglected. While, in general, MD simulation approach can describe both bonded and nonbonded interactions in a more realistic nonlinear way through different appropriate potential functions. There are a limited number of studies which have utilized MD simulation to investigate the vibrational behavior of CNCs. Firouz-Abadi et al. [29] examined the effect of geometric parameters and temperature on the resonant frequencies of cantilever CNCs using MD simulation. Their results indicate that the resonant frequencies are approximately insensitive to the temperature. Using MD simulation and continuum mechanics beam model, Hu et al. [30] investigated the free transverse vibration of cantilever CNCs and showed that the fundamental frequency of a CNC is higher than an equivalent CNT which has the same length and top radius as CNC. Ansari et al. [31] conducted molecular mechanics and MD simulation methods to study the vibration of CNCs with different lengths, apex angles, and boundary conditions. They proved that the effect of boundary conditions on the natural frequencies is more prominent for CNCs with smaller apex angles. In most of the MD-based vibrational studies, including the ones mentioned above, the desired resonant frequencies of the nanostructure are obtained by applying proper initial deflections similar to the desired mode shapes. This method demands several MD simulations to determine the resonant frequencies of different mode shapes. However, thermal oscillations of atoms during MD simulation of a nanostructure can be used to extract resonant information [20]. Based on this fact, a method was developed in [32] to extract the resonant frequencies and corresponding three-dimensional mode shapes of CNCs using only one MD simulation without imposing any initial deflection on the nanostructure. The effect of the length, apex angle, and boundary conditions on the resonant frequencies and the order of modal displacements were investigated and the results showed that the transverse, torsional, and longitudinal mode shapes shift toward higher mode numbers as the length or apex angle increases. Although, the proposed method was used for CNCs, it can be applied to other types of nanostructures.

CNTs and CNCs can be structurally categorized as single-walled or multi-walled and open-tip or closed-tip nanostructures. Topologically, pentagonal defects are needed to be introduced in the hexagonal graphic network of CNTs and CNCs in order to close their tip. Depending on the number of pentagons at the apex, from one to five, there are five possible CNCs with cone angles of 112.9°, 83.6°, 60°, 38.9°, and 19.2° [36]. A CNT can be regarded as a CNC with apex angle of 0° and six pentagonal rings. In general, most laboratory-grown CNCs are multi-walled carbon nanocoones (MWCNCs) with closed tips. The only single-walled carbon nanocone (SWCNC) that has been produced in large quantities, can be found in particles named carbon nanohorns which are composed of an aggregate of many SWCNCs with apex angle of 19.2° [37].

In fact, modeling of the closed-tip atomic structures of SWCNCs is not simple. However, in this study, a method has been proposed to construct these closed-tip nanostructures with true arrangement of pentagonal defects based on MD simulation. Upon generating the tip models, atomic structures of MWCNCs with any given length can be obtained using a simple algorithm. Although, the vibrational behavior of the generated nanostructures has been investigated in the present work, however, they can be used in analyzing their other properties.

To the best of the authors’ knowledge, only the vibrational behavior of open-tip SWCNCs has been theoretically reported before [21–32]. Therefore, investigating the vibrational behavior of closed-tip MWCNCs, which are more common in practice than open-tip SWCNCs, can provide useful information in designing CNC-based nanodevices. Hence, this work aims to perform three-dimensional modal analysis of closed-tip MWCNCs using MD simulation and to compare them with the multi-walled carbon nanotubes (MWCNTs). In the following sections, after modeling the

![Fig. 1. Symbols and variables used in the transformation from (a) the polar coordinates of the atoms in the plane of the graphene sheet to (b) their Cartesian coordinates in the constructed SWCNC.](Image)
closed-tip structure of CNCs, the effects of different geometric parameters on the resonant frequencies and corresponding mode shapes (which are usually not addressed in the literature) of closed-tip MWCNCs are investigated, in detail.

2. Molecular dynamics simulation and modeling

Considering the sixfold symmetry of a graphene sheet, the five experimentally observed CNCs [36], can be geometrically modeled, first, by cutting sectors from the sheet with angles of 60°, 120°, 180°, 240°, and 300°, which are known as disclination angles, and then, by rolling the remaining sheet and joining the atoms at the edges. This results in five SWCNCs and their apex angles are obtained by [36]

\[
\theta = 2\sin^{-1}\left(1 - \frac{d_0}{360}\right),
\]

in which \(d_0\) is the disclination angle in degrees. Therefore, apex angles will be 112.9°, 83.6°, 60°, 38.9°, and 19.2° corresponding to the five mentioned disclination angles. Mathematically, the following relations can be used to transform the polar coordinates of an individual atom, \(P(\rho, \varphi)\), in the plane of the graphene sheet to the Cartesian coordinates, \(P(x, y, z)\), in the constructed SWCNC [26]:

\[
\begin{align*}
x &= \frac{\rho \varphi}{2\pi} \cos \left(\frac{2\pi}{\varphi}\right) \\
y &= \frac{\rho \varphi}{2\pi} \sin \left(\frac{2\pi}{\varphi}\right) \\
z &= -\rho \sqrt{1 - \left(\frac{\varphi}{2\pi}\right)^2}
\end{align*}
\]

where \(\varphi\) indicates the angle of the remaining sector in radians. Symbols and variables used in this transformation, are shown in Fig. 1. Except the SWCNC with apex angle of 112.9°, the wall structure of the other four SWCNCs can only be modeled by the

![Fig. 2. Initial two-dimensional structures for the modeling of the cap and wall of the SWCNCs with apex angles of (a) 83.6°, (b) 60°, (c) 38.9°, and (d) 19.2°.](image-url)
described procedure and their closed-tip structures cannot be properly constructed. The closure of the cone tip can be achieved by introducing \( p \) number of pentagonal rings, from one to five, in the hexagonal network of the SWCNC corresponding to the disclination angle of \( \frac{p}{C_2} \frac{60}{C_1} \). In contrast to the simple transformation that was expressed in Eq. (2), to construct the wall structure of SWCNCs, there is not any mathematical relation which can be used to model their closed-tip structures. Moreover, depending on the arrangement of the pentagonal rings, there can be a number of configurations for a given SWCNC and the existence of these configurations, which are referred to as isomers, add to the complexity of the problem. However, knowing that only configurations with isolated pentagonal rings can be stable, and by adopting the most favored tip isomers among them [38], in this work, the following method is used to construct the closed tips of SWCNCs by MD simulation. The modeling procedure is separated into two parts: the construction of closed tip or cap of the SWCNC and its wall structure. The initial two-dimensional structures required for modeling these two parts are given in Fig. 2, in which the upper and lower figures relate to the cap and wall of the SWCNCs, respectively. Only atoms in the shaded areas contribute to the cap or wall construction. In order to model the wall structure of the SWCNC with \( p \) number of pentagons, one sector with disclination angle of \( p \times 60^\circ \) is removed from the graphene sheet and Eq. (2) is applied to the remaining atoms in the shaded area. However, \( p \) distinct sectors with angle of 60° are removed from the graphene sheet to construct the cap using MD simulation. The explained wall

<table>
<thead>
<tr>
<th>Number of pentagons</th>
<th>( R_1 ) (Å)</th>
<th>( L_{cap} ) (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>8.9523</td>
<td>4.552</td>
</tr>
<tr>
<td>3</td>
<td>11.2259</td>
<td>5.897</td>
</tr>
<tr>
<td>4</td>
<td>15.3468</td>
<td>7.220</td>
</tr>
<tr>
<td>5</td>
<td>25.7220</td>
<td>7.772</td>
</tr>
</tbody>
</table>

Fig. 3. Snapshots from the construction of the cap structures of the SWCNCs with apex angles of (a) 83.6°, (b) 60°, (c) 38.9°, and (d) 19.2° using MD simulation. Side and top views are shown.

Fig. 4. Constructed cap structures of the SWCNCs with apex angles of (a) 83.6°, (b) 60°, (c) 38.9°, and (d) 19.2° using MD simulation. Side and top views are shown and the pentagons are highlighted.

Table 1
Values of \( R_1 \) and \( L_{cap} \) for SWCNCs with different number of pentagons.
construction procedure, generates open-tip SWCNCs, as shown in Fig. 1(b). Eksioglu and Nadarajah [39] argued that the apex angles of the closed-tip SWCNCs and the cone angles of the open-tip SWCNCs, are solely functions of the disclination angle or the number of pentagons in the structure and this means that the open-tip SWCNCs have the same five cone or apex angles of the closed-tip SWCNCs. The only difference is that they lack the hexagons and pentagons that make up the cap of the closed-tip SWCNCs. Regarding this fact and considering Fig. 2, it can be said that the highlighted atoms with solid circles and named by uppercase letters, related to the cap structure, have the same Cartesian coordinates of the corresponding highlighted atoms with solid circles and named by lowercase letters, related to the wall structure, as if they belong to the open-tip SWCNC. So, the three-dimensional model of the cap can be obtained by moving the highlighted atoms in the initial structure toward the position of the corresponding highlighted atoms in the constructed open-tip SWCNC. This procedure can be done based on the following MD simulation steps. MD simulations are performed using LAMMPS software [40] and the adaptive intermolecular reactive empirical bond order (AIREBO) potential [41] is used to describe the interaction between different atoms as

\[ E_{\text{AIREBO}} = E_{\text{REBO}} + E_{\text{b}} + E_{\text{tors}}, \]

where the first term on the right-hand side represents the covalent bonding interactions in carbon and hydrocarbon systems, the second term is the well-known nonbonded Lennard-Jones 12-6 potential, and the third term describes the torsional interaction potential for dihedral angles. The AIREBO potential function, which has the capability of bond breaking and formation, is especially useful in the modeling process of the cap structure.

In the first step, x, y, and z coordinates of the highlighted atoms in the initial structure of the cap are updated with a slow constant velocity to reach the Cartesian coordinates of the corresponding highlighted atoms in the constructed open-tip SWCNC. This constant velocity for a given coordinate of each atom can be obtained by subtracting the initial coordinate of that atom from the final coordinate and then by dividing the result to the total time of the simulation during this step, which is 1 ns (1,000,000 time steps with time step size of 1 fs). The remaining atoms, i.e., nonhighlighted ones, are equilibrated at 1 K under the canonical ensemble NVT using Nose–Hoover thermostat [42,43]. NVT stands for an ensemble with constant number of atoms, constant volume and temperature. The movement of the highlighted atoms toward their final positions forces other atoms to buckle upward. Once the highlighted atoms reach their final positions, they are fixed. So far, the atoms have taken the approximate shape of the cap, but further steps are needed to put them in proper positions in order to form pentagons or hexagons and construct the desired cap shape. This can be achieved by giving sufficient kinetic energy to the atoms to reach such proper positions and the bond formation capability of the AIREBO potential can form pentagons or hexagons. Thus, in the second step, an NVT equilibration with 200,000 time steps is performed to bring the temperature from 1 K to 2000 K. Then, the temperature is brought from 2000 K back to 1 K in 200 ps, followed by an additional equilibrating process at 1 K running for 100 ps. It is noteworthy that the used temperature of 2000 K, which is especially necessary in the case of the SWCNC with five pentagonal rings, is in agreement with the reported temperature for the nucleation of carbon nanohorn from graphitic patches in [44]. Fig. 3 shows some snapshots from the construction of the cap structures during the explained MD simulation procedure. The final structure of the constructed caps is illustrated in Fig. 4 which highlights the positions of the pentagonal rings. It should be noted that the constructed caps are the most favored tip isomers [38], as stated before, and the construction of the other isomers can be treated in a similar way. Once the cap is generated, it can be used hereafter and mounted on the already constructed wall structure using Eq. (2), to obtain the closed-tip SWCNC with any given length. Considering Fig. 1, in order to model a closed-tip SWCNC with length of L, the R2 radius must be adjusted by the following relation:

\[ R_2 = R_1 + \frac{2\pi(L - L_{\text{cap}})}{\sqrt{4\pi^2 - \varphi^2}} \]

where R1 has a known value for a given SWCNC with p number of pentagonal rings, see Fig. 2, and Lcap can be measured after the construction of the cap. Table 1 summarizes the values of R1 and Lcap for different SWCNCs. In this study, the distance between two neighboring carbon atoms in the plane of the graphene sheet is assumed to be 1.421 Å [26]. The values reported for the Lcap may slightly differ from one MD simulation to another, as a result of using different random numbers at the beginning of the simulation to create the desired temperature. It must be emphasized that the constructed structures so far, are an initial model for closed-tip SWCNCs and are not optimized models with minimum energy. Based on the problem under consideration, standard energy minimization and

![Fig. 5. 3-layer MWCNCs with length of 100 Å and apex angle of (a) 19.2°, (b) 38.9°, and (c) 60°.](image)
equilibration procedures of MD simulation can be performed to eliminate the intrinsic stresses induced during the construction procedure and to reach the specified temperature and equilibrium state.

The generated closed-tip SWCNC structures can be utilized to construct MWCNCs. Modeling of an MWCNC can be accomplished by coaxially locating the second layer inside the first one at a specified distance from the tip and with a length less than the length of the first layer by the same specified distance value, and similarly for the next layers. This distance depends on the apex angle of SWCNCs. Fig. 5 illustrates 3-layer MWCNCs with the length of 100 Å and apex angles of 19.2°, 38.9°, and 60°. The distances between the tips of layers for these MWCNCs are 20.61 Å, 10.37 Å, and 6.92 Å, respectively. These values are adopted from [45] in which the equilibrium locations for nested CNCs have been discussed. However, these values can be considered as a starting
point and the subsequent minimization and relaxation of the MWCNCs, at the specified temperature, will lead to the actual equilibrium distances. Different layers of the MWCNCs are held together by vdW forces and these nonbonded interactions are described by the Lennard-Jones 12-6 part of the AIREBO potential, the second term at the right-hand side of Eq. (3), with the following form [41]:

\[ E_L^J(r) = 4\varepsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right], \]  

(5)

where \( r \) is the interatomic distance, and \( \varepsilon \) and \( \sigma \) are the Lennard-Jones parameters. The cut-off radius of 3.0\( \sigma \) is considered in this study to truncate the long-range vdW interactions beyond this distance. Firstly, using the AIREBO potential, initial atomic structures of the generated MWCNCs are energetically minimized to eliminate intrinsic stresses and then they are relaxed for a certain duration, depending on the size of the nanostructures, with time step size of 1 fs at 300 K under NVT ensemble in order to reach the equilibrium states and to obtain accurate interlayer distances. It is important to mention that single-coordinated carbon atoms, i.e., atoms with only one bond, at the large end of the MWCNCs are deleted and the remaining carbon atoms are terminated with hydrogen atoms to prevent bond formation as a result of AIREBO potential implementation. This is necessary because the formation of bonds between carbon atoms of two adjacent layers may hinder their relative axial and/or circumferential movement during the relaxation period. In fact, in real samples of MWCNCs, different layers are connected to each other at the large end [33], however, this is not important here since terminating the end carbon atoms with hydrogen atoms will have negligible or no effect on the vibrational behavior of the equilibrated nanostructure after applying proper boundary conditions at the end region. This procedure will be explained later in more details. Also, it is worth noting that the aforementioned MWCNC structures are different from carbon nanofibers (CNFs) [46] which are made of SWCNTs with cup or lampshade stacked shape. In the study of the structural and elastic properties of CNCs, Wei and Srivastava [47] categorized them into three types: single-shell nanocones, nanocone-stacked structures (CNFs) and multi-shell nanocones. The constructed MWCNCs in the present study can be considered as the third type of this categorization. MWCNTs are the special case of MWCNCs with apex angle of 0°.

MD simulation in conjunction with the spectral analysis is used in this study to extract the resonant characteristics of MWCNCs. Using this method, various resonant frequencies and corresponding three-dimensional mode shapes can be determined through only one MD simulation by recording three coordinates of the thermal vibration of each atom. This simulation method is in contrast with other conventional MD simulations, in which the nanostructure is manually deformed to a shape close to the desired mode shape and then it is allowed to vibrate freely. Based on this method, the relaxed atomistic structures of the MWCNCs obtained using the above mentioned techniques at 300 K under NVT ensemble, are further equilibrated after imposing appropriate boundary conditions to study their vibrational behavior. In this study, cantilever MWCNCs are considered and atoms within 5 Å distance from the large end of the nanostructures are fixed. The length of the MWCNCs refers to their free length. A short NVT equilibration is performed in this step at 300 K and then the ensemble is switched to the microcanonical ensemble NVE (constant number of atoms, volume and energy). Under this ensemble, the MWCNCs are equilibrated for at least 200 ps with time step size of 1 fs. The x, y, and z coordinates of each atom are recorded at every eight time steps. Fast Fourier transformation is applied to the obtained data to transform the time domain into frequency domain. By computing the auto-correlation and cross-correlation of the frequency domain, resonant frequencies and their corresponding mode shapes can be extracted. Further details can be found in [32].

3. Results and discussion

In this section, the vibrational characteristics of the constructed MWCNCs will be presented. The reported resonant frequencies are the average of the results obtained from several MD simulations with different random numbers for generating the specified temperature. This can help to identify the resonant frequency peaks in the power spectrum diagrams and also to obtain more reliable

![Mode shapes corresponding to the first to fifth (from left to right) resonant frequencies of the 100 Å and 38.9° cantilever MWCNCs with (a) 1 layer, (b) 2 layers, (c) 3 layers, and (d) 4 layers.](image-url)
results. Moreover, several MD simulations have been carried out for a given MWCNC, in which the individual layers of the initial structure are randomly located inside each other with different angular orientations. It should be noted that different layers are free to rotate with respect to each other during the first equilibration step of the MD simulation in order to result in a nanostructure with minimum potential energy. The results reveal that the resonant frequencies and their corresponding mode shapes are independent of the angular orientations of different layers with respect to each other.

In order to ensure the validity of the obtained numerical results for MWCNCs, the reported results from other approaches and research works are compared to the obtained results using the present method. Table 2 compares the first transverse resonant frequencies of the cantilever (5,5)-(10,10) MWCNTs with different lengths obtained using the proposed method to those obtained by deflecting the nanostructure in the transverse direction, i.e.,

![Fig. 11. Mode shapes corresponding to the first to fifth (from left to right) resonant frequencies of the 100 Å and 60° cantilever MWCNCs with (a) 1 layer, (b) 2 layers, (c) 3 layers, and (d) 4 layers.](image)
It can be inferred that in all cases, the number of layers increases. Considering different mode shapes of the MWCNCs in Figs. 9–11, it is observed that all five resonant frequencies for all apex angles increase as the number of layers increases. However, the amount of the increment depends on the mode number and apex angle of the MWCNCs. Also, the results indicate that for a given number of layers, the resonant frequencies and their range of change from the first mode to the fifth mode decrease as the apex angle increases. An unexpected behavior is observed for the first resonant frequency of the MWCNCs with apex angle of 38.9°, which have higher frequency values than those with apex angle of 19.2° (see Fig. 16 for the case of MWCNCs with three layers). Figs. 9–11 reveal that MWCNCs with apex angle of 19.2° exhibit mostly beam-like mode shapes while those with two other apex angles, especially the apex angle of 60°, have shell-like modal displacements. For the apex angles of 19.2° and 38.9°, beam-like mode shapes are shifted toward the lower mode numbers as the number of layers increases. Considering different mode shapes of the MWCNCs in Figs. 9–11, it can be inferred that in all cases, deformation pattern of the inner layers follows the shape of the outer layers.

In order to investigate the vibrational behavior of MWCNCs, it is also helpful to study the effect of layer numbers on the variation of the resonant frequencies which correspond to a specific mode shape as shown in Figs. 12–14. These diagrams demonstrate that the number of layers has little effect on the variation of the resonant frequencies with transverse modal displacements. However, this effect is more for radial mode shapes. Except the second transverse resonant frequencies of MWCNCs with apex angle of 19.2°, all other resonant frequencies increase as the number of layers increases. The rate of this increase depends on the mode shape and apex angle of the MWCNCs. For example, resonant frequencies corresponding to all five mode shapes for the apex angles of 38.9° and 60° vary almost linearly with the number of layers. In the case of the apex angle of 38.9°, the slope of change of the transverse frequencies is less than that of the radial frequencies. The resonant frequencies for 60° MWCNCs with four-fold and three-fold rotational symmetry, as well as, with six-fold and two-fold rotational symmetry vary almost linearly such that they get closer to each other as the number of layers increases. On the other hand, in the case of the apex angle of 19.2°, only the resonant frequencies corresponding to the radial mode shapes with two-fold (the first one) and three-fold rotational symmetry, increase almost linearly with the number of layers, however, the frequencies which correspond to the second two-fold symmetric and the first transverse mode shapes have different behavior. Considering similar radial mode shapes in Figs. 12–14, it is observed that the slope of change of frequencies increases as the apex angle of MWCNCs decreases. The results also demonstrate that the order of the modal displacements depends on the number of layers and the apex angle.

The variation of the first transverse resonant frequencies versus the number of layers for cantilever MWCNCs with different lengths and apex angles of 19.2° and 38.9° is illustrated in Fig. 15. It is observed that for a given length, MWCNCs with wider apex angle have higher frequencies. Also, the resonant frequencies and the rate of their change with respect to the number of layers decrease by increasing the length of MWCNCs for both apex angles. However, in the case of the apex angle of 19.2°, the rate of change of the frequencies reduces rapidly and they tend to reach a constant value as the number of layers increases. It also can be seen that with the apex angle of 38.9°, the frequencies vary almost linearly. For the same number of layers, this fact can be attributed to the further longitudinal distance between two adjacent layers of MWCNCs with the apex angle of 19.2°, see Fig. 5. Considering the first transverse mode shape of the vibration, further distance between two adjacent layers causes the inner layers to get closer to the fixed end, where the atoms of the outer layers have negligible displacement. This behavior is in contrast with the one that was observed in Figs. 12 and 13, in which, the rate of change of the frequencies corresponding to the first two-fold and three-fold symmetric mode shapes, was higher for MWCNCs with the apex angle of 19.2°. This behavior can be explained by the same reason discussed above, i.e., different distances between two adjacent layers for the apex angles of 19.2° and 38.9°, however, in the case of the mentioned radial mode shapes, atoms near the fixed end of the MWCNCs have significant displacement as compared with the first transverse mode shape, considering Figs. 9 and 10.
results also show that the first transverse resonant frequency of MWCNCs increases by increasing the number of layers. This is in contrast with the behavior of MWCNTs in which the first transverse resonant frequency decreases as the number of layers increases [13,19].

In order to further compare the vibrational behavior of MWCNCs and MWCNTs, the first five resonant frequencies of 100 Å cantilever MWCNCs with three layers and a capped (5,5)-(10,10)-(15,15) MWCNT are depicted in Fig. 16. Corresponding mode shapes for the MWCNT are given in Fig. 17. It should be noted that other configurations with different chiralities could be used to construct an MWCNT with three layers, however, a type that possesses small diameter and can be easily capped, is selected here. So, it would be possible to have a relevant comparison between MWCNCs and MWCNTs. It is observed that the range of change of the first five frequencies is more for the MWCNT as compared with the MWCNCs. Moreover, the MWCNT behaves like a beam and its mode shapes are transverse (the first and the second), torsional, longitudinal and radial, respectively. The torsional and the longitudinal mode shapes for MWCNCs reveal themselves at higher mode numbers. The results also show that the first transverse resonant frequency of the MWCNT is too lower than that of the MWCNCs. The frequencies corresponding to this mode shape of the vibration, play an important role in applications such as AFM imaging and mass detecting resonators. A higher transverse resonant frequency implies higher mass sensitivity, more stability and less thermal noise of the nanostructure. This fact, together with the unique conical shape and sharp tip of the MWCNCs, makes them as a more appropriate candidate for such applications which has been previously addressed in some studies [8,33,48].

4. Conclusions

In this paper, the vibrational behavior of MWCNCs was investigated using MD simulation. A method was proposed to construct the initial atomic model of the closed-tip MWCNCs with pentagonal defects by implementing MD simulation. The atomic motions during the equilibrating process of the nanostructure were used to extract the resonant frequencies and their corresponding three-dimensional mode shapes. The effect of the apex angle and
number of layers on the resonant characteristics of the cantilever MWCNCs was examined. It was observed that MWCNCs with apex angle of 19.2° have wider range of change of the first five resonant frequencies and behave more like a beam as compared with MWCNCs with apex angles of 38.9° and 60°. Also, it was shown that the transverse mode shapes shift toward the lower mode numbers as the number of layers increases. The results revealed that the rate of change of the resonant frequencies versus the number of layers, depends on the shape of the modal displacement and apex angle of the MWCNCs, and, in general, frequencies corresponding to the radial mode shapes are more sensitive to the number of layers. It was shown that the order of the mode shapes depends on the number of layers and apex angle of the MWCNCs. The obtained results indicated that the rate of change of the first transverse resonant frequencies with respect to the number of layers decreases as the length of the MWCNCs increases, especially, in the case of the apex angle of 19.2°. The comparison between the vibrational behavior of MWCNCs and MWCNTs revealed that the first transverse resonant frequency of the MWCNCs is higher than that of the MWCNTs. This result, together with the fact that MWCNCs have sharp tips, indicates their higher potential in practical applications such as probe tips in AFM imaging. The results of this study can be helpful in designing MWCNC-based sensing and actuating nanodevices.

References


