Chapter 2
Literature Review

2.1 Axial Stiffness

The stiffness of an object is the rigidity of it in response to an applied load, as shown schematically in Fig. 2.1. The original length L is increased to $L + \Delta L$ under the influence of the external force F.

By applying Hooke's law, the Young's modulus of the CNTs can be calculated by the following equations:

$$\sigma = \text{stress} = F/A \tag{2.1}$$

$$\varepsilon = \text{strain} = \Delta L/L \tag{2.2}$$

$$E = \text{Young}'\text{s modulus} = \sigma/\varepsilon \tag{2.3}$$

The following paragraph presents the results of several investigations on the evaluation of CNTs tensile properties.

Natsuki et al. [7] developed an analytical method for modeling the elastic properties of SWCNTs based on a link between molecular and solid mechanics. In their investigation, a SWCNT is regarded as a continuum-shell structure which is compared to the discrete molecular configuration linked by the C–C bond. They studied the elastic properties of SWCNTs as a function of the nanotube size. Liew et al. [8] examined the elastic and plastic properties of CNTs under axial tension applying the molecular dynamics (MD) approach. They obtained the stress-strain responses to describe the elastic and plastic behavior of single and multi-walled CNTs in their investigations. Moreover, they took the brittle fracture under consideration due to the bond breaking. Consequently, their MD simulations revealed the fact that the outermost layer is the main spot of the fracture damage of CNTs. Later in 2006, Meo and Rossi [9] proposed a finite element (FE) model, based on the molecular dynamics theory so that they would investigate the fracture progress in armchair and zigzag CNTs with defects under uniaxial tensile stress. Their examinations revealed the complete load-displacement relationships for a (5,5) and a (9,0) CNT up to the complete fracture. Based on their findings, they

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concluded that the effect of chirality on the mechanical properties and failure mode of CNTs was quite significant. A year later, Tserpes and Papanikos [10] examined the effect of Stone-Wales defects on the tensile behavior and fracture of different types of SWCNTs, using an atomistic-based progressive fracture model. They predicted a particular reduction in failure stress and failure strain in armchair SWCNTs, contrary to zigzag ones; ranging from 18 to 41 %, respectively. Afterwards, Xiao et al. [11] conducted a computational study on the investigation of the tensile behavior of SWCNTs, using a self developed nano-mechanical testing device. They also studied the tensile strength of SWCNT bundles. They concluded that the tensile strength distribution of CNTs can be adequately described by a two-parameter Weibull model. They finally proposed a method in order to determine the tensile strength distribution of individual CNTs. In 2009, Kuang and He [12] conducted a study to investigate the effect of chemical functionalization on the axial Young's moduli of SWCNTs based on molecular mechanics simulation. They concluded that the Young's moduli depend strongly on the chirality of the CNTs. In addition, molecular mechanics revealed that the functionalization

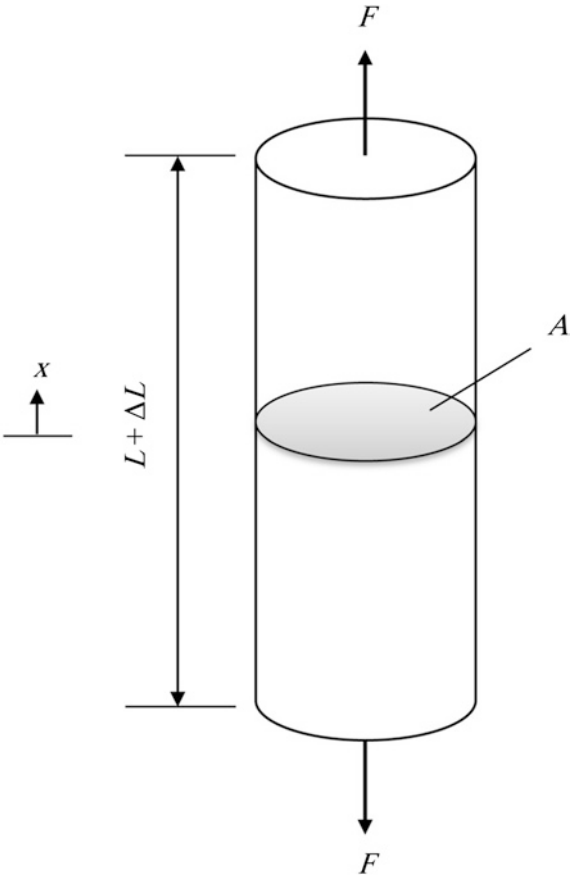

Fig. 2.1 A simple schematic illustration of a tensile test to determine the material stiffness

of SWCNTs results in a decrease of the Young's moduli of the corresponding SWCNT composites. Later in 2011, Mohammadpour and Awang [13] developed a FE model based on the molecular mechanics approach for evaluating the tensile properties of SWCNTs. In their investigation, individual CNTs were simulated as a frame-like configuration and the primary bonds between two nearest-neighboring atoms were treated as beam elements. A computational simulation for investigating the mechanical properties of CNTs was conducted by Lu and Hu [14] in 2012. They developed an improved 3D FE model for different types of CNTs. They also investigated the elastic stiffness of graphene as well as the effect of diameters and helicity on the Young's modulus and shear modulus of SWCNTs. Ghavamian et al. [15] investigated the mechanical properties of single- and multi-walled CNTs in their perfect and imperfect form. They introduced some types of imperfections in different amounts to the perfect models. Finally the elastic behavior of the defected CNTs was obtained and compared with those of perfect ones. Their findings indicated that the existence of any kind of imperfection in the perfect models leads to lower stiffness values. Recently in 2013, Kinoshita et al. [16]

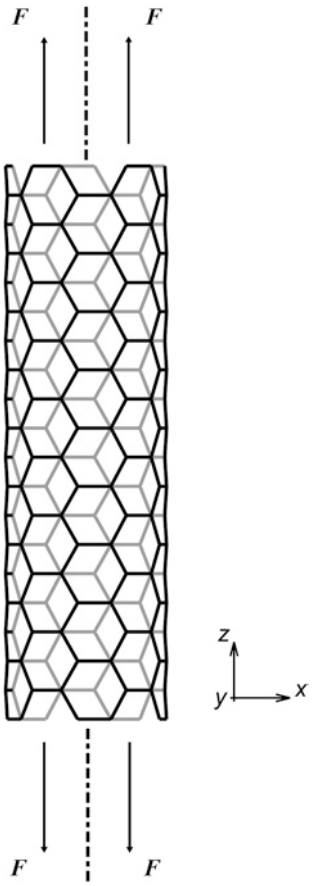

Fig. 2.2 (5,5)-armchair CNT under tensile test

proposed a study in order to investigate the mechanical properties of SWCNTs with one-dimensional intramolecular junctions (IMJs), using first-principle density functional theory calculations. In addition, they examined the effects of pentagon-heptagon defects at a junction on the tensile strength, Young's modulus and breaking strain of CNT-IMJs. The average value of the Young's modulus of CNTs was around 0.9 TPa. They finally found that the tensile strength and breaking strain of CNT-IMJs depend on the position of pentagon-heptagon defects. Figure 2.2 shows a simulated model of a CNT under tensile test.

Figure 2.3 compares the average stiffness of a CNT with other classical engineering materials. The average values for the classical engineering materials were taken from [17–19].

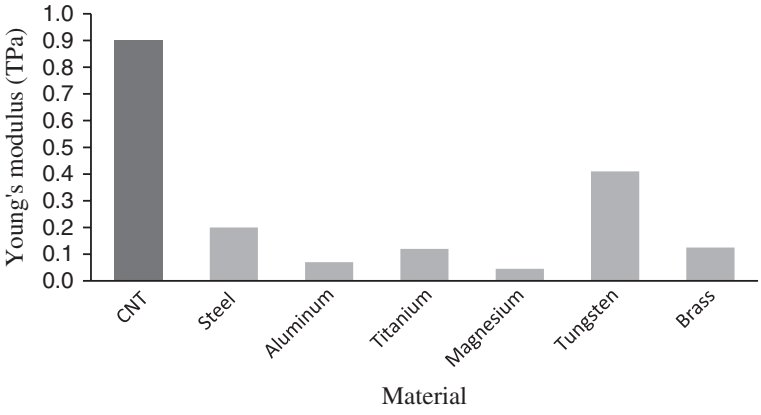

Fig. 2.3 Average Young's modulus values of some classical engineering materials

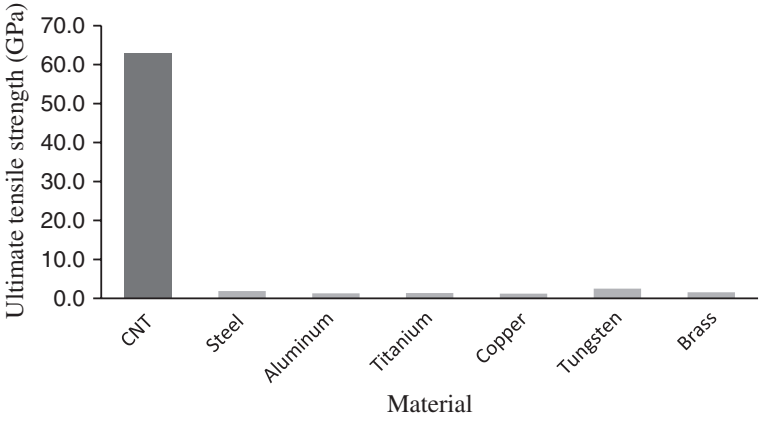

Fig. 2.4 Average ultimate tensile strength values of some classical engineering materials

It can be seen from this figure that the stiffness of a CNT is much higher than that of classical engineering materials, for instance more than four times higher than steel's. The average ultimate tensile strength of a CNT and other classical engineering materials is shown in Fig. 2.4. These average values were taken from [17–19].

As shown in the diagram above, the ultimate tensile strength of CNTs is approximately 70 times larger than steel.

2.2 Torsional Stiffness

In a torsion test, a specimen is twisted by introducing an arbitrary angular rotation θ around their major axis and consequently, the corresponding reaction torque is obtained. Figure 2.5 shows a schematic illustration of a torsion test on a simple cylinder.

For the evaluation of such a torsion test, the shear modulus of the material can be calculated by the following equation [20]:

$$G = {}^{TL}/_{\theta J} \tag{2.4}$$

where θ, T, L and J represent the twisting angle, the torque, the length and the polar moment of inertia, respectively.

The investigation on the torsional stiffness of CNTs is very important for which several studies are presented in the following.

In 2003, Li and Chou [21] investigated the torsional stiffness of MWCNTs. They assumed that the nested individual layers of a MWCNT act as single-walled frame-like structures and simulated by the molecular structured mechanics methods. Their results indicated that the shear moduli and Young's moduli of MWCNTs are in the ranges of 0.4 ± 0.05 and 1.05 ± 0.05 TPa, respectively. In addition, they concluded that the tube diameter, chirality and number of

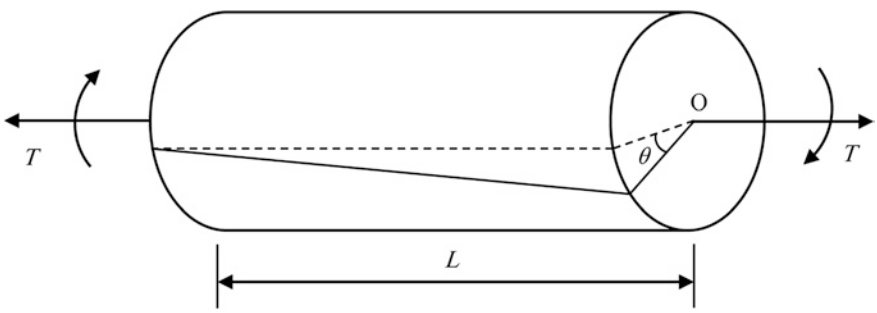

Fig. 2.5 A simple schematic illustration of a torsion test to determine the shear modulus

tube layers have a major effect on the elastic properties of MWCNTs. They also conducted a structural mechanics method for modeling the deformation of CNTs [20]. Their investigations indicated that CNTs are geometrical frame-like structures and the primary bonds between two nearest neighboring atoms act like load bearing beam members. Based on their results, they concluded that by increasing the tube diameter, the Young's moduli of CNTs increase. Later in 2006, Kalamkarov et al. [22] investigated the behavior of CNTs applying different techniques. The first approach models CNTs as an inhomogeneous cylindrical network shell applying the asymptotic homogenization method. Their second approach was based on FE models. Such models were developed for CNTs with different numbers of layers. They could predict the elastic and shear moduli of the CNTs using the deformations from the FE simulations. In addition, they investigated the dependence of the mechanical properties on the number of nanotubes in multi-walled structures. The shear modulus was found to vary from 0.14 to 0.47 TPa for SWCNTs and 0.39–0.62 for double/multi-walled

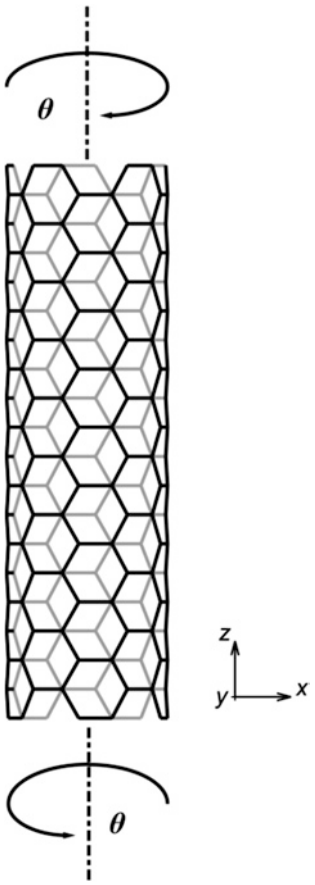

Fig. 2.6 (5,5)-armchair CNT under torsion test

CNTs. After that, To [4] obtained the elastic properties of SWCNTs experimentally and computationally. He mainly investigated the Young's and shear moduli of SWCNTs. He pointed to the fact that the Young's and shear moduli of SWCNTs have been estimated to be constant within the linear domain. In their study, the classical theory of elasticity could be used for the determination of the Young's and shear moduli of SWCNTs. Tsuda et al. [23] evaluated the interface shear strength of CNT-dispersed polymer composites. They pull-out an individual MWCNT from a MWCNT-dispersed/PEEK composite applying a nano-pullout testing system. Moreover, they measured the tensile load using the elastic deformation of an AFM cantilever. In 2012, Viet and Kuo [24] employed both shear lag modeling and finite element analysis (FEA) to analyze the stress distribution in the graphene layers. They also investigated the effect of the aspect ratio on shear transfer efficiency. They evaluated the effective shear modulus of a fractured CNT with respect to the number of broken layers. Their findings revealed that the layered configuration can increase the shear stress concentration. Recently in 2013, Ghavamian et al. [25] obtained the shear modulus of SWCNTs and MWCNTs applying the finite element method (FEM). In order to clarify the most appropriate approach, they determined the shear modulus of CNTs by simulating two basic tests. First, they directly evaluated the modulus by applying a torsion test. Second, they simulated the tensile test in order to obtain the shear modulus. The comparison of both approaches indicates that CNTs behave rather as an anisotropic material. Figure 2.6 illustrates the simulated model of a CNT under torsion test.

2.3 Buckling Behavior

Buckling is understood as a structural instability which results in the sudden failure of a mechanical component. This instability is characterized by the loss of structural stiffness and is susceptible for slender and thin-walled structures as in the case of the considered CNTs. In the basic theory of elasticity, the critical buckling load of a straight elastic beam is presented by Eq. (2.5) as [26]:

$$P_{\mathrm{cr}} = \frac{n^2 \pi^2 EI}{(KL)^2} \tag{2.5}$$

In the above equation, E is the Young's modulus of the material, n represents the buckling mode, K is the effective length constant and I is the structure's second moment of area. As the classical structure of CNTs is mostly presented by a hollow cylinder, Eq. (2.6) can be used to obtain analytical results for straight CNTs as:

$$I = \pi \left[(d+t)^4 - (d-t)^4 \right] / 64 \tag{2.6}$$

where t is the thickness of the tube's shell and d represents the diameter of the pertaining tube.

Figure 2.7 illustrates different possibilities of buckling tests and resultant critical loads that can be acquired theoretically.

The following paragraph summarizes several related studies where the buckling behavior of CNTs was investigated.

Wang et al. [28] conducted a computational study in order to simulate the compression deformation of SWCNTs, using the Tersoff-Brenner potential to depict the interactions of atoms in CNTs. They found that by increasing the radius of CNTs, the Young's modulus of the tubes decreases. In addition, they indicated that there are two different buckling modes for SWCNTs. Kang et al. [29] conducted a study to investigate the buckling behavior of intramolecular junctions (IMJs) under axial compression, using both MD and finite element (FE) analysis. According to their results, it was proven that the critical compressive strain is dependent on the length and radial dimensions of the IMJ. However, it is insensitive to the chirality of the IMJ. An investigation in the mechanical properties of the CNTs under various loading conditions, including compression, tension, torsion, bending and hydrostatic pressure was performed by Motevalli et al. [30]. Their results indicated that the buckling deformations and the critical loads are highly dependent on the ratio of rotational and axial displacement rates. Moreover, they proposed a relationship between the normal and shear stresses which can be established for finding the stress limits when designing practical CNT-based systems in which combined load might be used. The main focus of Poelma et al. [31] in their research was mainly to investigate the buckling behavior of fixed-fixed, both SWCNTs and MWCNTs under axial compressive load, using analytical continuum theory and MD. In addition, in order to apply the boundary conditions

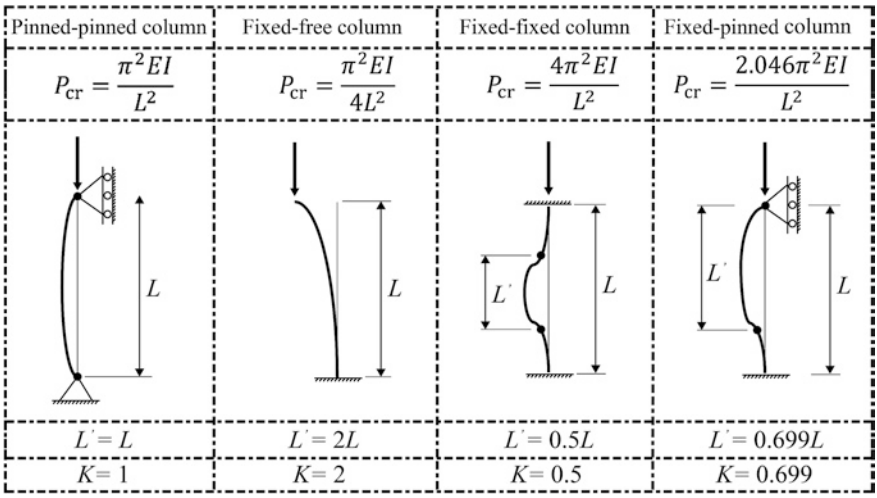

Fig. 2.7 Different conditions of the buckling test, adopted from [27]

and extract the reaction forces during the MD simulation, they used an approach based on the tethering of atoms. The results of their simulation revealed the defects at the ends of the CNT. As a result, the influence of vacancy defects on the critical buckling load and strain was proven to be small at room temperature. Ansari and Rouhi [32] developed an atomistic FE model to study the buckling behavior of CNTs with different boundary conditions. Based to their model, they obtained and then compared the critical compressive forces of SWCNTs with different boundary conditions. They concluded that at low aspect ratios, the critical buckling load of nanotubes decreases considerably with increasing aspect ratio; while at higher aspect ratios, buckling load slightly decreases as the aspect ratio increases. Finally, they found out that increasing the aspect ratio at a given radius results in a convergence of buckling envelops associated with armchair and zigzag CNTs. Xin et al. [33] performed MD simulations for the axial compression of both perfect and defective SWCNTs. Based on their findings, it was proven that any change in length, the chirality, and the initial structural defects of the tube would be effective on the buckling and axially compressive properties of SWCNTs. The investigation on the dependence of the mechanical characteristics of SWCNTs on their length, radius, and chirality was conducted by Talukdar et al. [34]. Their findings revealed the fact that the tensile properties of zigzag and armchair CNTs are not dependent

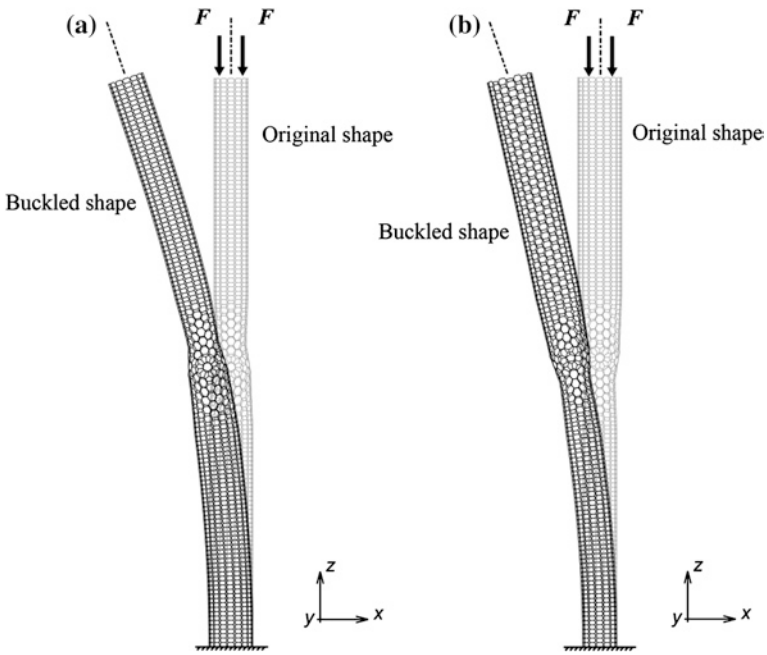

Fig. 2.8 (7,7)–(9,9)-straight hetero-junction CNT's first mode under buckling load in original and buckled form with two different types of cantilevered boundary conditions: **a** wider tube fixed, and **b** thinner tube fixed

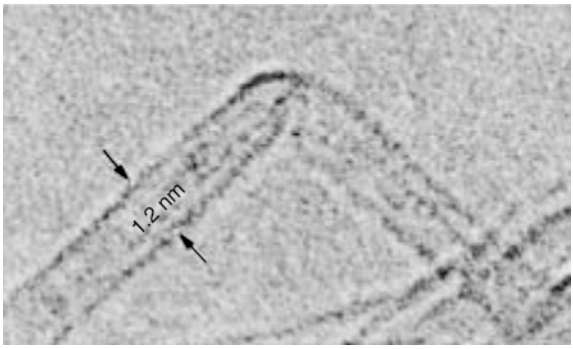

Fig. 2.9 Experimental observation of the buckling behavior of a CNT at nanoscale dimensions [36]

on their length. The fracture patterns showed different modes in each case. In their model, buckling produced wavy structures, kinks, bending, and twisting. Chang et al. [35] obtained analytical solutions for the critical buckling strain of single-walled achiral CNTs under axial compression. They conducted their study based on a molecular mechanics model. According to their findings, it was revealed that zigzag tubes are more stable than armchair tubes with the same diameters. After comparing their results given by continuum mechanics models they found out that the continuum mechanics model underestimates the critical buckling strain for smaller tubes if a Young's modulus for larger tubes is adopted. Moreover, they concluded that the van der Waals interaction has little effect on the critical buckling strain for double-walled carbon nanotubes (DWCNTs). The simulated models of hetero-junctions with original and buckled shape are shown in Fig. 2.8.

Figure 2.9 illustrates experimental observation of the buckling behavior of a CNT.

2.4 Vibrational Behavior

The natural frequency is the frequency of a vibrating system at which the system oscillates at greater amplitude because of the existence of the resonance phenomenon. Geometry, mass, and applied boundary conditions are the factors which influence these quantities. The natural frequency is mainly evaluated to examine the vibrational behavior of structural members. Figure 2.10 illustrates a simple schematic shape of the first mode of vibration of a beam.

The first natural frequency of an Euler-Bernoulli beam element under cantilevered boundary conditions is defined by the following equation [37]:

$$f = (3.5156/2\pi)\sqrt{EI/\overline{m}L^4} \tag{2.7}$$

where E, I, $\overline{m}$ and L are the Young's modulus, the second moment of area, the mass per unit length and the length of the CNT, respectively. The results of several studies on the vibrational characteristics and buckling behavior of CNTs are presented.

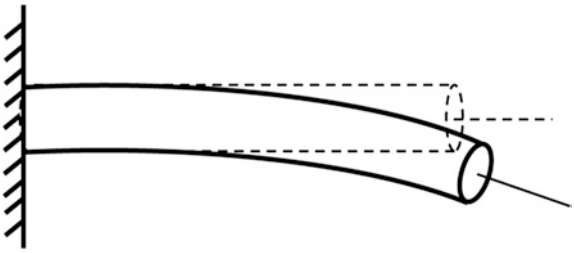

Fig. 2.10 A simple schematic illustration of the first mode of vibration of a beam

Behera and Chakraverty [38] investigated the vibrational behavior of nonlocal nanobeams based on Euler-Bernoulli and Timoshenko beam theories. They established expressions for the free vibration of Euler-Bernoulli and Timoshenko nanobeams within the framework of Eringen's nonlocal elasticity theory. In their study, the numerical results for the free vibration of nanobeams have been presented, applying simple polynomial and orthonormal polynomials in the Rayleigh-Ritz method. In this way, one can easily handle the specified boundary conditions at the edges. They also compared their investigations with the results of the existing literature. Finally they could obtain frequency parameters for different scaling effect parameters and boundary conditions. Their results revealed that small scale effects considerably influence the free vibration of nanobeams. In addition, they concluded that nonlocal frequency parameters of nanobeams are smaller when compared to the corresponding local ones. Through nonlocal elasticity theory, the axial vibration of single-walled CNTs embedded in an elastic medium was investigated by Aydogdu [39]. He also used the nonlocal constitutive equations of Eringen in the formulations. He discussed the effect of various parameters such as stiffness of the elastic medium, boundary conditions, and parameters on the axial vibration of nanotubes. He finally concluded that the axial vibration frequencies of the embedded CNTs are highly overestimated by the classical continuum rod model which ignores the effect of small length scale. After simulating two configurations of homogeneous CNTs (armchair and zigzag) based on the FE method, Ghavamian and Öchsner [40] introduced the three most likely defects to their models in order to represent defective forms of SWCNTs. These defects are Si-doping, carbon vacancy, and perturbation. They finally investigated and compared the vibrational properties of perfect and defective CNTs. Their results showed that SWCNTs have a natural frequency in the range of 18.69 and 24.01 GHz. Furthermore, it was concluded that the existence of any type of irregularities on CNTs leads to a lower value of natural frequency and vibrational stability. Seyyed Fakhrabadi et al. [41] conducted a study investigating the vibrational properties of the two and three junctioned CNTs with different geometries and boundary conditions. They applied a well-known molecular mechanics approach to the modal analysis of the CNTs. Their results covered the natural frequencies and their corresponding mode shapes. They presented the results of the two junctioned CNTs with different lengths and diameters and also with cantilever from right side, left side, and doubly clamped boundary conditions in detail. In addition, they investigated the natural frequencies

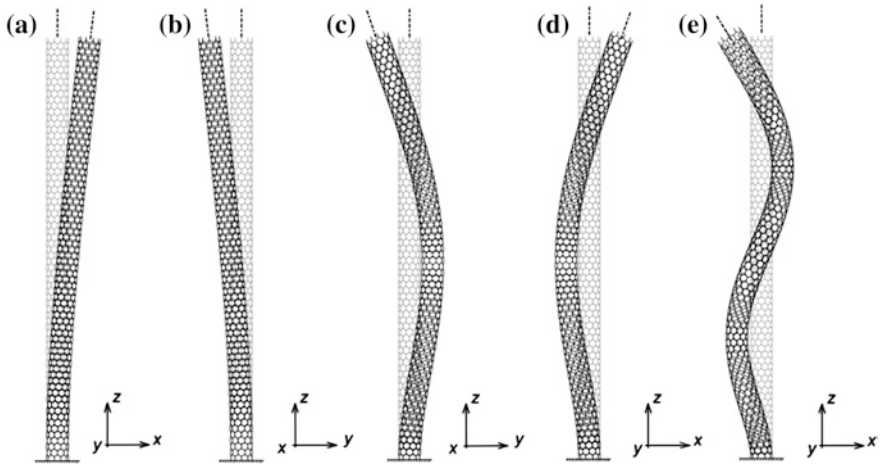

Fig. 2.11 First five eigenmodes of a (10,0)-zigzag CNT

of the three junctioned CNTs with different lengths, diameters, and various boundary conditions. Rahmandoust and Öchsner [27] simulated single-walled carbon nanotubes in their perfect forms applying the finite element method (FEM) in the MSC. Marc software. Afterwards, they investigated the buckling behavior and resonant frequency modes of zigzag and armchair models. Their results indicated that there were similarities between the buckling behaviors of SWCNTs under cantilevered boundary conditions. Nevertheless, it was observed that the value of the first mode of frequency is more accurate than the higher modes. Firouz-Abadi and Hosseinian [42] conducted a study to investigate the free vibrational characteristics of SWCNTs in the vicinity of a fully constructed graphene sheet. They applied a molecular structural mechanics model and considered nonlinear van der Waals interactions in order to obtain the elastic deformation of the nanotube. Their investigation results were in very good agreement with the results in the literature. Consequently, they carried out a survey on the natural frequency of the CNTs beam-like modes in various distances from the graphene sheet. Biao et al. [43] employed an atomic finite element model based on a virtual spring model for armchair and zigzag SWCNTs in order to determine the relation between axial load and frequency shift. They also introduced the Tersoff-Brenner potential so that the interaction between the atoms would be defined as well as the mechanical properties of the springs in the model. By applying finite element theory and techniques, they could obtain the fundamental frequency shifts of transverse and radial vibration modes of SWCNTs. They found out that the fundamental frequencies of the two modes are typically as high as hundreds of gigahertz. In addition, by increasing the stretching load, these frequencies decreased linearly, despite growing with the increase of the compression load. They studied various types of nanotubes with different diameters, chirality, and lengths. Their results revealed the fact that by increasing the length and diameter, both the frequency sensitivities

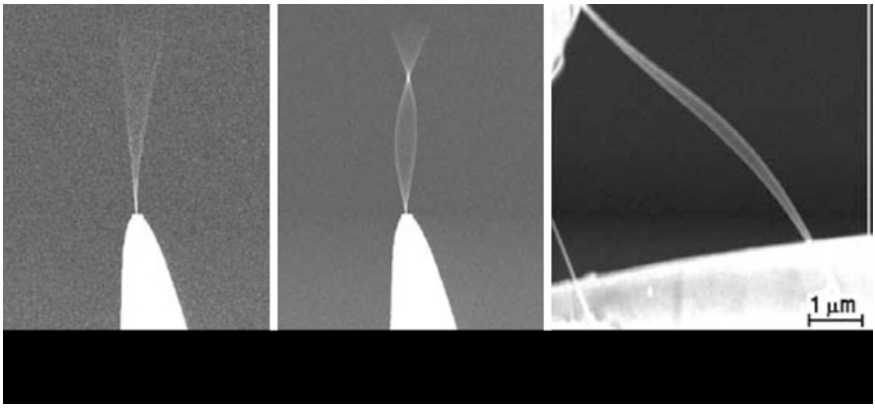

Fig. 2.12 SEM images showing the first harmonic and the second harmonic resonant oscillations of an individual MWCNT, and the resonant oscillation of a MWCNT bounded at both ends [45]

for transverse and radial vibration modes decrease. Nevertheless, they proved that there are some exceptions in nanotubes with small-diameter. Filiz and Aydogdu [44] investigated the axial vibration of CNTs hetero-junctions using a nonlocal rod theory. They applied the nonlocal constitutive equations of Eringen in the formulations. They used various types of hetero-junctions with different lengths, chirality, and diameters. For each case, the effect of nonlocality, length of the CNTs, and length of each segment were investigated. Their results showed that by joining CNTs good vibrational properties are obtained by suitable selection of parameters. Figure 2.11 illustrates the first five eigenmodes of a CNT in the simulation.

The SEM image of resonant oscillations of an individual MWCNT is shown in Fig. 2.12.

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Imani Yengejeh, S.; Kazemi, S.A.; Öchsner, A.

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