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Defects in Nanostructures

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Synonyms

Carbon; Defects; Finite element modelling; Mechanical properties

Definitions

Carbon nanotubes (CNTs) and their derivatives are allotropes of carbon that display outstanding physical properties including excellent thermal and mechanical properties, chemical inertness, and tuneable opto-electronic properties. Owing to these properties, CNTs are considered as an important research subject for scientists. Many investigations have been conducted to explore the properties of carbon nanostructures. The possible introduced defects applied to the structure of the CNTs include carbon vacancies, substitute dopant (e.g., silicon, boron, nitrogen), Stone-Wales pair defects, and so on. Structural are known to greatly affect the mechanical properties of CNTs and CNT-derived materials by reducing mechanical strength and structural stability of these structures. This chapter discusses the most recent studies concerning the mechanical properties of CNTs and CNT derivatives which are defect-free and those containing various types of defects.

Introduction

In recent years, extensive numerical and experimental studies have been conducted to explore opto-electronic and mechanical properties of carbon nanostructures, while studies concerned with estimation of the mechanical properties of other types of one- and two-dimensional nanostructures are gaining popularity as they explore the potential for construction of rigid molecular templates for applied nano- and macromolecular engineering applications. Carbon nanotubes (CNTs) display outstanding physical, thermal, and mechanical properties (Espejel-Morales et al. 2013; Imani Yengejeh et al. 2014a, 2015a; Ruoff and Lorents 1995). These low-dimensional carbon structures are commonly

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used in the field of nano-science and engineering. Nanocones, for instance, have been recently applied in the field of electrical and chemical science, specifically in ultrafine gold needles (Cano-Marquez et al. 2015). Similarly, fullerenes are used especially in bio-medical science (Wolff et al. 2000). As an example, such buckyballs are extensively applied in designing of high-performance magnetic resonance imaging (MRI) contrast agents, X-ray imaging contrast agents, and photodynamic therapy (Lalwani and Sitharaman 2013). CNTs, in both single- and multiwalled structures, are widely applied in industry, from bio-medical to aerospace engineering (Abarrategi et al. 2008; Jakubinek et al. 2015). Such nanostructures are currently used in composite fibers in polymers to improve the mechanical, electrical, and thermal properties of the bulk product. These reinforced composites are applied in aircraft structures (DeLuca et al. 2016). CNTs and CNT-derived materials often deviate from their original defect-free structure and are often affected by structural and topological defects including introduced impurity atoms and vacancies or can also be affected by large-scale deformations such as twisting and bending deformations (Faria et al. 2016; Imani Yengejeh and Öchsner 2014; Imani Yengejeh et al. 2015b). It is therefore important to understand how mechanical properties of CNTs are affected by these defects and be able to predict the extent by which the properties of CNTs become affected. This chapter gives an introduction to different types of CNTs and their derived structures and categorizes some of the most common structural and topological imperfections (Imani Yengejeh et al. 2016); in addition, a review some of the most recent studies describing how atomic defects influence on the mechanical properties of CNTs models is also provided.

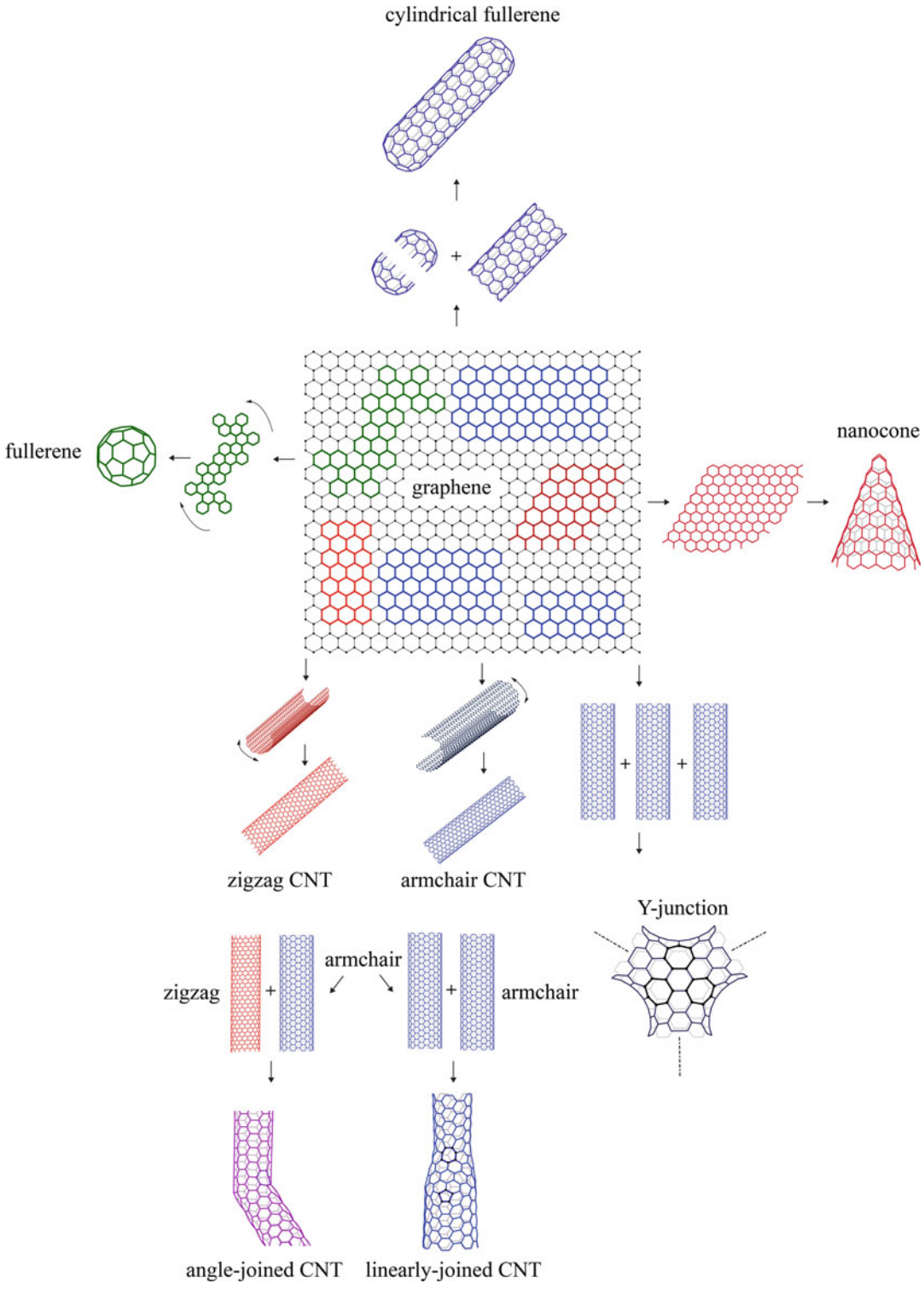
Carbon Nanotubes and Their Derivatives

Most types of carbon nanostructures, including homogeneous zigzag and armchair-type CNTs, cylindrical fullerene, nanocone, Y-junction CNTs, fullerenes, linearly and angle-adjoined CNTs, can be visualized as being constructed from a graphene sheet, as shown in Fig. 1.

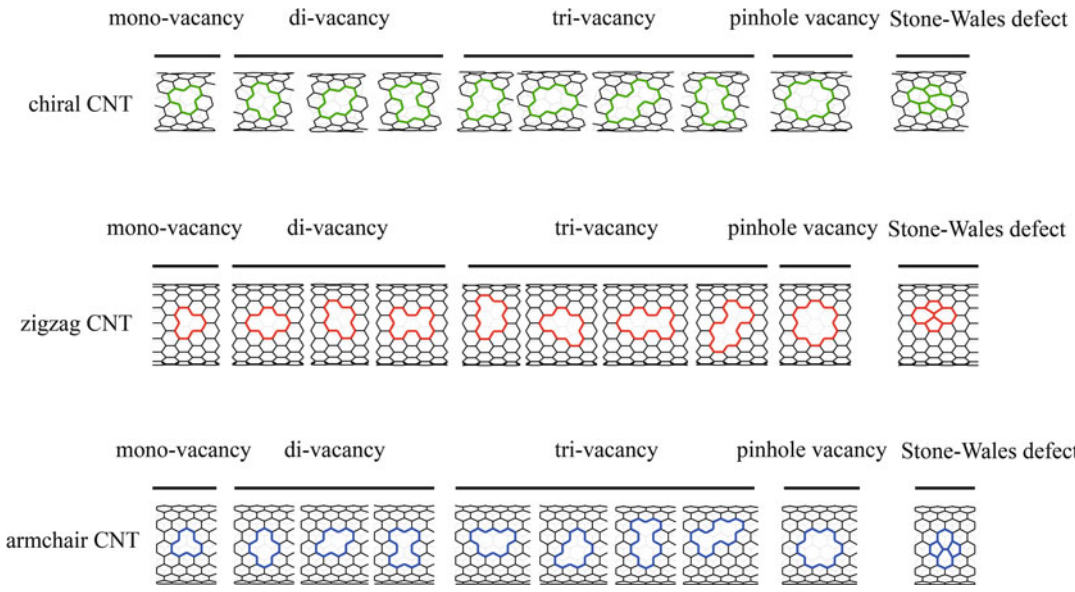
A homogeneous CNT can be visualized as a rolled sheet of graphene, while linearly and angle-adjoined CNTs can be constructed by connecting structurally similar and dissimilar homogeneous CNTs, respectively. The Stone-Wales defects occur to the structures of CNT junction hybrids in various quantities. For linearly-joined CNTs, there are two distinct configuration styles: in the case of parallel longitudinal axes, a pair of Stone-Wales defect is introduced to the structure, while in the case of concentric longitudinal axes, more pentagon-heptagon (5-7) pair defects occur to the low-dimensional system. In the case of angle-adjoined CNTs, 5-7 pair defects are introduced to the system, and pentagon and heptagon defects are separately located at both sides of the connecting region. Y-junction CNTs can be created by connecting three branches of CNTs and the introduction of heptagon defects into the structure of the models. Based on Fig. 1, a Y-junction contains three branches and the connecting region is not arbitrary; that is, the heptagon defects position might not be predictable.

Structural Defects

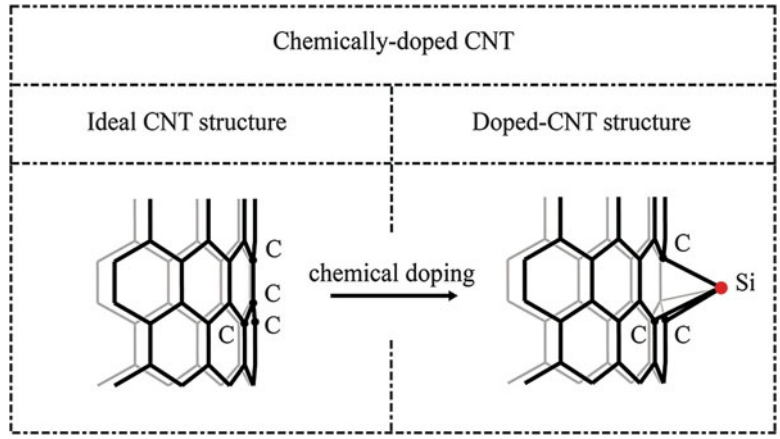
As discussed earlier, carbon nanostructures commonly contain some atomic defects and impurities including, vacant sites, doping agents, 5-7 pair defects, and so on. These small-scale defects are illustrated in Fig. 2, where the chiral, zigzag, and armchair-type CNTs are affected by mono-, di-, tri-, and pinhole vacancies as well as Stone-Wales pair defects. As shown in Fig. 3, dopants such as silicon (Si), nitrogen (N), boron (B), and chromium (Cr) are able to substitute a number of carbon atoms in the crystalline structure thus modifying molecular structure of the CNT. The following studies were conducted into investigating the mechanical, physical, and electronic behavior of defective low-dimensional systems based on the specific types of atomic modification.



Defects in Nanostructures, Fig. 1 Schematic representation of various types of CNT-derived material models constructed from a sheet of graphene



Defects in Nanostructures, Fig. 2 Simulated chiral, zigzag, and armchair CNTs containing structural defects



Defects in Nanostructures, Fig. 3 Substitutional vacancy of CNT

Vacant Sites

Depending on the number of extracted adjacent atoms, vacancy defects are mainly categorized as containing mono-, di-, tri-, and pinhole vacancies. Yamada et al. (2014) observed and demonstrated the presence of defects in the structure of graphene, using a high-resolution transmission electron microscopy (HR-TEM). It was suggested that the presence of such defects imparted significant variations to mechanical, electrical, and thermal properties of graphene. In 2009, Parvaneh et al. (2009) carried out a structural mechanics approach to explore the critical buckling load and structural stability of CNTs under the influence of vacancy defects. Within their study, a nonlinear connector and spring were considered for modeling of the torsional and stretching, and angle variation interactions, respectively. Different types of armchair and zigzag-type CNTs with small and large aspect ratios were simulated, and the different vacancy defects at various regions were investigated; as a consequence, the authors compared their results with those evaluated by molecular dynamics (MD) simulation. It was finally found that both results were in good agreement and expressed similar prediction

for the behavior of defective models. In 2012, Ebrahim Zadeh et al. (2012) investigated the natural frequency of CNTs with single layers under the influence of temperature and vacancy defects based on a well-known structural mechanics approach. The authors mainly introduced atomic defects to their ideal models with single vacant sites and simulated different systems with small and large aspect ratios. It was noted that the presence of vacancy impurities has a significant impact on the natural frequencies of the low-dimensional systems, and by increasing the percentage of imperfections, the natural frequency of the models reduces markedly. It was also pointed out that a significant reduction occurs to the fundamental frequency by increasing the environmental temperature (300 K). Although they investigated various CNTs with different chiralities, the model defects were restricted to single vacancy studies. In 2014, Georgantzinos et al. (2014) applied a structural mechanics method to explore the vibrational behavior of CNTs under the influence of structural defects. Their approach was based on the application of spring elements, and they applied their theory for investigating the vibration characteristics of ideal and defective systems. The introduced defects within this study varied from single to pinhole vacancies, and the influence of such structural defects was explored for different defect regions, tube diameter, and boundary conditions. Based on their acquired results, the natural frequency is directly dependent on the size of the structural defects and the percentage of introduced imperfections. It was also noted that these atomic defects have a significant impact on the vibrational response of single-clamped CNTs in comparison with double-clamped CNTs. In 2015, Brcic et al. (2015) applied the finite element method (FEM) to predict the elastic modulus of straight and waved-form CNTs containing single vacancy defects. The authors pointed out that the characteristics of these low-dimensional systems can be affected by the overall shape of the structures as well as the existence of the atomic defects, and consequently, the mechanical properties of CNTs reduce significantly with the introduction of impurities to their configurations. More specifically, the difference between the longitudinal elastic modulus of straight and waved form CNTs is nearly 90% (from 1069 GPa to 86 GPa) at the largest waviness ratio. Table 1 shows some of the most related studies concerning the investigation of properties of CNT-related systems containing single vacancy defects.

Stone-Wales Defect

As shown in Fig. 1, the Stone-Wales defect occurs by introducing the pentagon and heptagon pair defects in the structure of CNT-related models. Meyer et al. (2008) observed the Stone-Wales defects in graphene membranes which were introduced to the configuration of their carbon nanostructures. These atomic imperfections were the factors that had significant impact on the tensile behavior of graphene sheets and CNTs investigated by Xiao et al. (2010). It was found that the moduli have direct co-relation with the CNT lengths, and additionally, the reduction in the structural stability was suggested to be linearly related to the number of defects per unit surface area, which is defined as the defect density. Applying an atomistic simulation, Lu and Bhattacharya (2005) explored the possible influence of randomly oriented Stone-Wales defects on the ultimate strength, stiffness, and ultimate strain of SWCNTs. Within their study, several types of CNT structures, including armchair and zigzag CNTs with different chirality, were simulated, and a modified Morse potential was considered to model the interatomic forces. The initial results indicated that the presence of the Stone-Wales defects has a pronounced impact on the mechanical properties of the CNTs and reduces the structural stability of the CNT-related systems. In addition, it was noted that the armchair configurations display relatively higher strength in comparison with their zigzag counterparts. In regards to the thermal conductivity of the SWCNTs, the existence of Stone-Wales defects has been suggested to have a measurable effect on such low-dimensional structures. Dai-Li et al. (2013) investigated the influence of such defects on the thermal conductivity of CNTs with single layers using a nonequilibrium MD technique. They categorized their investigations based on various

Defects in Nanostructures, Table 1 Related studies concerning the prediction of mechanical properties of CNTs and CNT-derived materials under the influence of vacancy defects

Researcher	Year	Method	Structure	Defect type	Research summary
Poelma et al. (2012)	2012	MD	SWCNTs	Single vacancy	Investigation of the structural stability of CNTs with the presence of single vacant sites; the existence of vacancy defects at the ends and close to the middle of the CNT has the largest impact on the critical buckling load of the systems; the imperfections have smaller influence on the stability of CNT models at room temperature
Amjadipour et al. (2015)	2015	MD and FEM	Curved CNTs	Single vacancy	Prediction of the vibrational response of waved atomically defective CNTs applied in nano-resonators using a combination of MD and FEM; the results show that the tube curvature and vacant sites have significant impact on the vibration properties of SWCNTs; the critical waviness ratio is directly related to the length of SWCNTs
Liao (2015)	2015	MD	Open-tip carbon nanocones	Single vacancy	Exploration of the buckling properties of open-tip carbon nanocones under the influence of single vacancy defects; defining the defective regions and comparing the impact of defects introduced to different regions of the system; the presence of the vacant sites did not change the mode shape of the carbon nanostructures
Liao (2017)	2017	MD	Open-tip carbon nanocones	Single vacancy	Application of MD simulation to predict the effect of atomic defects on the tensile behavior of carbon nanocones; the presence of single vacant sites on the upper region of the nanocones has a major impact on the mechanical properties of the systems and reduces the tensile loads of the models significantly

factors including the length, chirality, diameter of the tube, and the ambient temperature. Based on their findings, it was observed that the thermal conductivity shows an increase while the length of the CNTs grows or in the case of reduction in the diameter. Furthermore, it was indicated that the change in diameter of the CNTs is more highlighted in the case of nondefective models rather than the systems possessing the structural impurities. Table 2 illustrates some of the recent relevant studies concerning the mechanical properties of CNTs and CNT-derived materials under the influence of Stone-Wales defects.

Chemical Doping

CNTs can be chemically doped by the introduction of dopants such as N, Si, B, and Cr and other atoms up to certain percentages under different processing conditions including high pressure and high temperature reactions (Yin et al. 2003), directly during the chemical vapor deposition fabrication process (Kouvetakis et al. 1994), chemical solid-state reaction (Oku and Kawaguchi 2000), and others. Liu et al. (2015) conducted an electro-mechanical examination of doped CNTs in order to prepare Si- and N-doped CNTs and evaluate their electro-catalytic activity as well as their stability by applying the density functional theory (DFT) and stated that such chemically doped materials could be effectively applied as a low-cost catalyst. In addition, the authors expected that their Si-containing carbon materials could be applied as a low-cost, efficient oxygen reduction reaction (ORR) catalyst. Song et al. (2006) conducted a MD investigation to study the influence of Si-doping on the mechanical characteristics of SWCNTs. They mainly concentrated in homogeneous armchair-type CNTs and found that the presence of chemical dopants decreases the Young's modulus of the CNT structures. The study indicated that the nanotube diameter has a slight impact on the Young's modulus of homogeneous armchair SWCNTs. In 2013, Espejel-Morales et al. (2013) presented a comprehensive study on the investigation of the electronic, vibrational, and mechanical properties of B- and N-doped SWCNTs. They simulated several zigzag and armchair CNTs with different chiralities, exploring the behavior of their models under the influence of chemical dopants, and consequently determined the strain energy, the Poisson's ratio, the geometrical structure, and the Young's modulus of their CNT-related systems. A key finding of their investigation was that the zigzag CNTs had larger deformation in comparison with their armchair counterparts, specifically in the case of N-doped configurations. In 2015, El-Barbary et al. (2015) predicted the properties of linearly and angle-adjoined SWCNTs under the influence of B dopants as well as single vacancy defects. They mainly focused on evaluating the formation energy and surface reactivity using DFT and finally concluded that the CNT junctions with bending angles hold the largest surface reactivity. This study indicated that the armchair connected CNTs with parallel longitudinal axes show less resistance in removing carbon atoms from the network of their configuration in comparison with the other types of hybrids. Some of the most related articles concerning the investigation of the mechanical behavior of doped CNTs are presented in Table 3.

Structurally Modified Carbon Nanotubes

Properties of CNTs and CNT-derived low-dimensional materials can be modified significantly by means of manipulation of their physical organization and ordering of these materials by means of axial bending, distortion, twisting, joining, and other manipulations as illustrated in Fig. 4.

Most of these larger scale modifications are known to occur in nature owing to variations in fabrication and processing methods used to produce CNTs and related materials. For instance, the linearly and angle-adjoined CNTs are constructed by connecting armchair, zigzag, and chiral SWCNTs and lead to the introduction of pentagon and heptagon pair defects within the structure of these low-dimensional hybrids. Applying the float catalyst approach, Zhu et al. (2002) prepared the growth mechanism of Y-junction SWCNTs and eventually proposed a simple growth model to describe and predict the growth process of the CNT-related junctions. In 2008, Qin et al. (2008) simulated several types of linearly joined SWCNTs and MWCNTs to investigate their mechanical characteristics, based on the MD approach. After examination of the CNT hybrids and observing their failure behavior, it was indicated that the CNT junctions were structurally unstable, specifically in the junction region which is close to that of its thinner constituent CNT. In 2013, Tian and Guo (2013) conducted the same procedure and simulated the failure mechanism of Y-junction SWCNTs to study the effect of heptagon defects in the structure of these CNT-related systems on the SWCNT

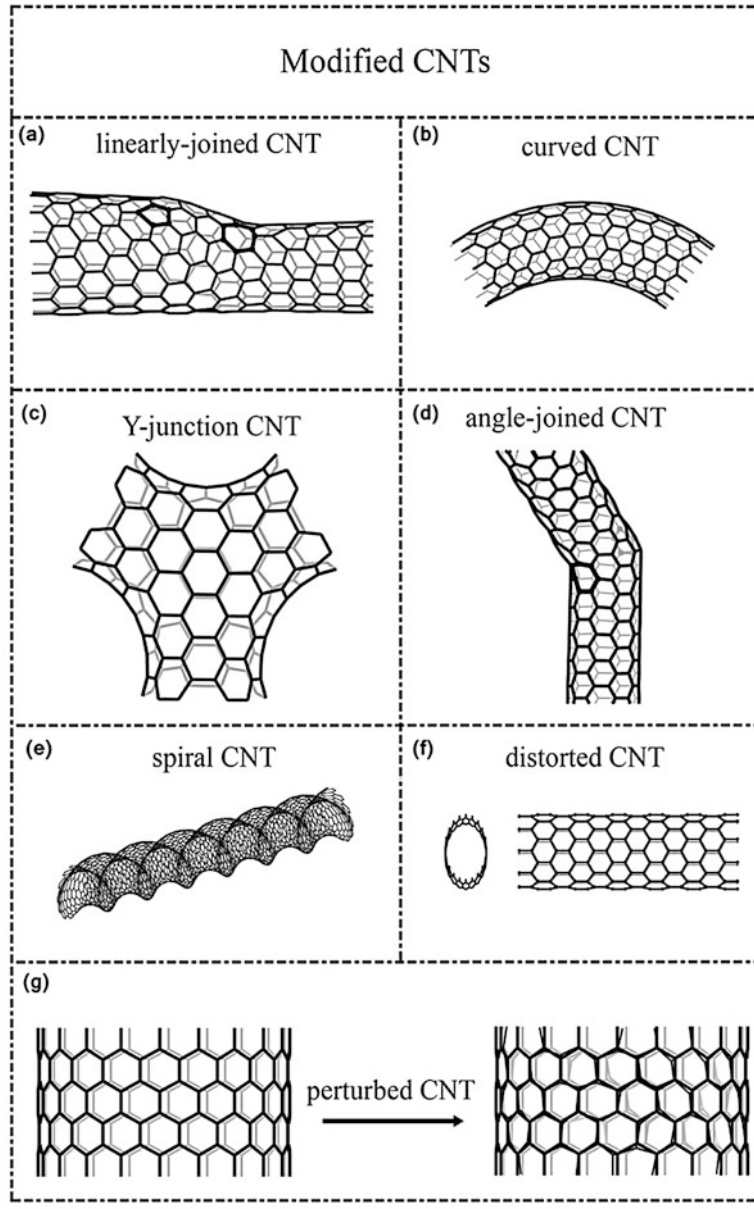
Defects in Nanostructures, Table 2 Related studies concerning the prediction of mechanical properties of CNTs and CNT-derived materials under the influence of vacancy defects

Researcher	Year	Method	Structure	Defect type	Research summary
Liew et al. (2004)	2004	MD	SWCNTs and MWCNTs	Stone-Wales defect	Investigation of the elastic and plastic properties of MWCNTs using MD simulation; obtaining Young's modulus, yield stress, Poisson's ratio, etc., of SWCNTs, 2-, 3-, and 4-walled CNTs; the presence of Stone-Wales defects leads to the plastic deformation of the CNT-related structures
Tserpes and Papanikos (2006)	2006	Atomistic-based progressive fracture modelling approach (PFM)	SWCNTs	Stone-Wales defect	Exploration of the tensile behavior of SWCNTs under the effect of pentagon and heptagon pair defects; the presence of topological impurities affects the mechanical properties of CNT-related configurations
Pozrikidis (2009)	2008	MD	SWCNTs	Stone-Wales defect	Prediction of the mechanical behavior of the defective SWCNTs in axial stretch and twist applying the Tersoff-Brenner potential; there is significant difference in the behavior of stretched zigzag and armchair CNTs possessing Stone-Wales defects; twisting the SWCNTs leads to a remarkable deformation in the structures
Ansari et al. (2012)	2012	MD	Single-layered graphene sheets	Stone-Wales and single vacancy defect	Investigation of the mechanical properties of graphene sheets using the Tersoff-Brenner potential function and Nose-Hoover thermostat approach; the introduction of structural defects reduces the failure strain of the graphene sheets significantly, while having a slight impact on the Young's modulus; graphene sheets are noticeably stronger in the armchair direction since the topological impurities have less influence in this direction
He et al. (2014)	2014	MD	Graphene sheets	Stone-Thrower-Wales defect	Exploration of the mechanical characteristics of graphene sheet under the influence of Stone-Thrower-Wales (STW) defects based on MD simulations; in the case of having more than one STW defect, the mechanical response of the structure depends on the tilting angle

Defects in Nanostructures, Table 3 Related studies concerning the prediction of mechanical properties of CNTs and CNT-derived materials under the influence of chemical dopants

Researcher	Year	Method	Structure	Defect type	Research summary
Rahmandoust and Öchsner (2009)	2009	FEM	SWCNTs	Si-dopants and single vacancy	Investigation of the impact of structural and topological defects on the mechanical characteristics of SWCNTs; the structural stiffness of the CNT systems is influenced by the presence of the atomic impurities
Ganesan et al. (2010)	2010	In situ tensile testing	MWCNTs	N-dopants	Prediction of the mechanical response of the MWCNTs by applying quantitative tensile testing; defective and nondefective MWCNTs hold significant load-bearing abilities and it was indicated that the N-doped MWCNTs show a slightly plastic behavior before failure
Cheng et al. (2014)	2014	Thermal annealing method	MWCNTs	B-dopants	Synthesis of B-doped MWCNTs through thermal annealing MWCNTs; using transmission electron microscopy (TEM) used to observe the doping process, indicating that the low-dimensional systems do not catastrophically modify during the doping process
Zhou et al. (2015)	2015	DFT	SWCNTs	Cr-dopants, Stone-Wales, and single vacancy defects	Investigation of the oxygen absorption on atomically and topologically defected SWCNTs; it was indicated that the carbon atoms located at vacant sites are more active; a combination of chemical dopants and defects by absorbing oxygen is potentially effective to improve the properties of CNT-related structures

mechanical properties. They concluded that the failure of their modified CNTs occurs on the main branch under tensile loading, and the other two branches most probably hold their pristine configurations and absorb the energy after the failure of the main branch. Imani Yengejeh and Öchsner (2014) conducted a computational study and simulated several types of spiral armchair, zigzag, and chiral CNTs with different chiralities to explore their mechanical properties. They found that the modified SWCNTs display a comparatively lower Young's modulus in comparison with those with perfect structures. In the case of lineally and angle-adjoined CNTs, the junction region might hold a significant structure based on the type and chirality of the constituent CNTs. In 2016, Mohammadian et al. (2016) conducted a MD simulation to study the influence of the junction region length on the vibrational properties of linearly and angle-adjoined CNTs. Their findings showed that the first and second band of natural frequency oscillations of the CNT-related systems with a longer junction region are relatively larger than those having shorter connecting regions. Notably, the third and fourth natural frequencies of CNT hybrids were found to decrease



Defects in Nanostructures, Fig. 4 Large-scale modifications of CNTs: (**a**) linearly-joined CNT, (**b**) curved CNT, (**c**) Y-junction CNT, (**d**) angle-adjoined CNT, (**e**) spiral CNT, (**f**) distorted CNT, and (**g**) perturbed CNT

with increasing the length of the junction regions. Some of the most recent studies concerning with the investigation of the mechanical properties of modified CNTs are presented in Table 4.

Summary and Concluding Remarks

This chapter briefly reviewed key studies concerned with the investigation of the mechanical properties of ideal, defect-free, and defective CNTs and CNT-derived structures containing the most common structural defects listed under two categories, namely, the small-scale defects including atomic and structural defects such as vacancy defects, chemical doping, and the Stone-Wales defect, and, the large-scale defects that include Y-junctions, linearly and angle-adjoined CNTs, structurally perturbed, and distorted CNTs. Based on the

Defects in Nanostructures, Table 4 Related studies concerning the prediction of mechanical behavior of modified CNT structures

Researcher	Year	Method	Structure	Defect type	Research summary
Filiz and Aydogdu (2010)	2010	Nonlocal rod theory	Linearly-joined CNTs	Axial vibration property	Application of nonlocal constitutive equations of Eringen to examine the vibrational behavior of linearly-joined CNTs; it was indicated that the frequency parameter of CNT hybrids can be optimized by modifying the length of the connecting regions
Kang et al. (2010)	2010	MD and FEM CNTs	Linearly joined	Buckling property	Investigation of the buckling behavior of CNT hybrids using the combination of MD and FEM; it indicated that the critical compressive strain is variable based on the change in the length and chirality of the joined CNTs
Seyyed Fakhrabadi et al. (2012)	2012	Molecular mechanics	Two- and three-junction CNTs	Vibration property	Conduction of a modal analysis to evaluate the mode shapes and fundamental frequencies of the modified CNT-related systems; the low-dimensional systems possessing shorter lengths and wider diameters hold greater natural frequencies
Li et al. (2013)	2013	MD	Linearly-joined CNTs	Buckling property	Investigation of the structural stability of linearly joined CNTs at finite temperature; the results revealed that the CNT junctions will significantly deform at a high strain rate; the CNT-related systems possessing a long length will exhibit their mode as shell buckling
Imani Yengejeh et al. (2014b)	2014	FEM	Curved SWCNTs	Vibration property	Investigation of the vibrational response of structurally curved CNTs both analytically and computationally; bending and curvature in the configuration of CNTs reduces their natural frequencies
Mohammadian et al. (2017)	2017	Molecular mechanics	Linearly and angle-adjoined CNTs	Vibration property	Evaluation of the first five natural frequencies of the CNT-related junctions and exploring the effect of changing the location of the connection region on the mechanical properties of the models; predicting structural stability of the low-dimensional systems possessing the atomic and structural defects; a significant reduction occurs with the fundamental frequencies of defective models

gathered data, it was noted that most studies were conducted by applying MD simulations, and much more attention needs to be drawn to other approaches such as FEM and quantum mechanics. In addition, it was revealed that a great deal of publications mainly concentrated on the investigation of homogeneous CNTs, while the mechanical characteristics and properties of other types of low-dimensional structures (e.g., nanocones, cylindrical fullerenes, bucky-balls) need to be explored and investigated. According to the reviewed investigations, CNTs and their modification display outstanding mechanical properties (critical buckling load to up to 100 nN, natural frequencies in the THz domain, Young's modulus of about 1 TPa, and tensile strength of up to 63 GPa) which make these specific materials the main focus of investigations. Nevertheless, not all carbon nanostructures are structurally nondefective and different types of defects may occur to their configurations. It has been reported that the mechanical properties of carbon nanostructures significantly change and their structural stability reduces remarkably. The deviation in the mechanical properties of CNTs and CNT-derived structures depends on the type and size of the defects. The mentioned studies concluded that due to the presence of atomic and structural modifications, the structural stability, and consequently, the structural strength of the CNTs and their modifications reduces significantly with respect to the type and size of the defects. Such defects may reduce the mechanical properties of the CNTs up to 70% in the highest rate. It was concluded that the nondefective CNTs display comparatively higher values of critical buckling load, natural frequency, Young's modulus, and tensile strength. With regards to the vacancy defect, no such categorization was considered and the influence of other types of vacancy defects such as double-, triple-, and pinhole vacancy on the mechanical properties of the nanostructures was not fully addressed. Concerning the chemical doping, the main purpose of controlling the properties of nanostructures needs to be thoroughly investigated. Modulating the electrical properties of CNTs by the intentional introduction of impurities into the carbon nanostructures should be deeply explored, and the investigations concerning the reaction of intercalation with electron donors or acceptors require much more attention. Some of the mentioned studies compared the relationship between the different types of structural defects in the reduction of mechanical properties. Some researcher compared the results of their investigations with the outcomes derived from other approaches. Investigating the mechanical properties of defective and nondefective carbon nanostructures in a combination of MD and FEM seems to be a significant approach to study and predict the characteristics of the nano-configurations.

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