Numerical Analysis of the Structural Stability of Ideal (Defect-Free) and Structurally and Morphologically Degenerated Homogeneous, Linearly- and Angle-Adjoined Nanotubes and Cylindrical Fullerenes Under Axial Loading Using Finite Element Method

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We report on the structural stability of ideal (defect-free) and structurally and morphologically degenerate carbon nanotubes and nanotube junction systems under axial loading based on the finite element method. We estimated the values for critical buckling load for uncapped and capped single-walled carbon nanotubes (SWCNTs) and linear and angle-adjoined SWCNT heterojunctions in ideal and structurally degenerate systems containing single-, double-, triple-, pinhole- and pentagon-heptagon (i.e., 5–7) structural defects and also containing a substitutional nitrogen (N) atom inclusion under compressive loading. Absolute atomic vacancy (defect) concentration in studied SWCNTs models

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was assumed to be nil for ideal systems, and was up to 3.0 at.% for structurally and morphologically degenerate systems. It was found that all types of structural defects and the morphological N-defect had reduced the load carrying capacity and mechanical strength in all SWCNT systems studied. The SWCNT models containing physically large vacant sites, such as triple- and pinhole-defects, displayed significantly lower critical load values compared to the systems that contained only a single-, double- or triple-vacancies. In addition, we found that capped SWCNTs performed marginally better in critical load carrying capacity compared to uncapped SWCNT systems. Furthermore, majority of the investigated structures displayed reduced load in SWCNTs with narrower tube widths, proportional to the size and the type of the defect investigated. The effects of chirality, such as zigzag- versus armchair-type, on the structural stability of the investigated SWCNT models were also investigated.

Keywords: Carbon nanostructures; finite element method; mechanical properties; critical buckling load; defects; numerical modeling.

1. Introduction

Following the discovery of carbon nanotubes (CNTs) [Iijima, 1991], significant research effort has been expended to explore the properties and potential applications of these low-dimensional materials. Over the past two decades, it has been found that CNTs display favorable mechanical [Cadek *et al.*, 2002] and opto-electronic properties [Vivien *et al.*, 2002], high chemical inertness [Qureshi *et al.*, 2009], low-thermal degradation [Tian *et al.*, 2004], and can be effectively doped [Suriyasena Liyanage *et al.*, 2014] and processed on a large scale for applied applications as structural fillers [Phang *et al.*, 2006; Imani Yengejeh *et al.*, 2017] or active or passive opto-electronic components [Talin *et al.*, 2001]. In addition, studies exploring the mechanical properties and structural stability of other types of one- and two-dimensional (2D) carbon nanostructures other than those of the single-walled CNTs (SWCNTs), such as fullerenes, nanocones and CNT hetero-junctions, are gradually becoming popular as these explore the potential for construction of rigid molecular templates for applied nano- and macro-molecular engineering applications [Imani Yengejeh *et al.*, 2015]. Investigations concerning the physical properties of CNTs have been formally divided into two major streams of experimental and theoretical studies. The latter employ a large variety of simulation methods including *ab initio* quantum mechanical (QM) approaches to investigate the electronic structure (i.e., the ground state) of complex many-body molecular systems which include QM/molecular mechanical, density functional theory (DFT) methods and other methods to accurately model the exchange and correlation interactions. Despite offering high computational accuracy for modeling electronic properties of relatively small molecular systems, applications of QM methods to large molecular systems ($>1.0 \times 10^2$ atoms) demand extensive computational power and long computational time [Toomsalu *et al.*, 2013]. By employing the QM approaches the mechanical properties of complex molecular systems, including those of single- and multi-walled CNT models, can be effectively estimated by analyzing force field data and the potential energy of a system [Condon and Morse, 1931; Ferguson and Kollman, 1991]. Recent studies have shown that the use of the crystal-based finite element analysis

method (FEM) for modeling of exclusively mechanical properties of small and very large single-body and multi-body ($>1.0 \times 10^5$ atoms) structural models is becoming popular as the FEM approach offers significantly reduced computational time and lowers the demand for resources while rendering highly plausible simulation results. Crystal-based FEM is a versatile continuum mechanics approach used for predicting mechanical properties and deformation-induced crystallographic structures, and it can be applied to solving both elastic-plastic and purely elastic problems of multi-body systems [Ma *et al.*, 2008] and complex CNT model structures [Wang *et al.*, 2009, 2016; Faria *et al.*, 2016; Litak, 2017; Robinson and Adali, 2017; Bocko and Lengvarský, 2017; Timesli *et al.*, 2017; Hosseini-Hashemi and Ilkhani, 2017; Nishimura *et al.*, 2017]. Investigation concerning the mechanical response and structural stability of these quasi-molecular systems is important, as such studies enable researchers to design and imitate the potential behavior of low-dimensional structures that bear close structural resemblance to nanostructured materials found in nature. The paragraph below presents some of the most recent findings on simulated mechanical properties of SWCNT structural systems.

Agnihotri and Basu [2010] conducted an MD simulation to investigate if a very long SWCNT can be modeled as a Kirchhoff's elastica with a small initial twist. They also indicated that the post-buckling deformation of the low-dimensional structures is strongly affected by the length, diameter and chirality of the nanostructures. Ziaee [2014] applied molecular structural mechanics to investigate the buckling properties of defective armchair and chiral SWCNTs under transverse and axial compression loading. He found that the position of the microscopic impurity in the structure of the low-dimensional material models plays a remarkable role on the change in the value of critical buckling force. Roy Chowdhury *et al.* [2014] performed MD simulations to study the buckling property of single- and multi-walled CNTs with different types of chirality. Their equivalent shell model gave a reasonable estimate of the critical buckling load (CBL)/strain and critical buckling torque with respect to the MD results. Wang *et al.* [2016] investigated the buckling response of SWCNTs under bending loads and found low- and high-strain phases in SWCNT models. The SWCNTs were simulated as thin-wall, circular, crystal systems and the governing equations have been solved by employing a continuation algorithm. Following up on these findings, Faria *et al.* [2016] explored the buckling properties of SWCNTs under combined bending-and-twisting loads. The study examined two chiral types of SWCNT systems, including those of armchair- and zigzag-type and of the same overall length and width. The results were presented in the form of energy diagrams and bending moments plotted against the imposed axial rotations and had shown that the armchair-type SWCNT models exhibited predominantly higher twisting-bending stiffness and strength values relative to the zigzag-type SWCNTs. Litak [2017] simulated mechanical properties of SWCNT under the influence of axial loads, and estimated the critical SWCNT diameter using two different approaches under local shell buckling mode. For the same types of SWCNT models,

Robinson and Adali [2017] applied a nonlocal continuum mechanics approach by implementing constitutive modeling of the tubes with research results obtained for both the uniformly distributed and triangularly distributed axial loads. Bocko and Lengvarský [2017] conducted FEM studies on the buckling response of SWCNT models; they found that the structural stability of SWCNT models can be investigated by modeling these SWCNT systems as beam or shell structures and by applying an analytical shell theory. Hosseini-Hashemi and Ilkhani [2017] studied different types of structural instabilities for a spinning SWCNT models under combined loading by applying the Timoshenko and Euler–Bernoulli nonlocal beam theory [Biot, 1955; Cowper, 1966] in their analysis. Their findings showed that different types of instability modes exist for simply supported SWCNT models. Based on these recent studies, it is clear that additional research efforts are needed to elucidate the effects of structural and topological defects in complex low-dimensional carbon systems, such as SWCNTs, as these systems are more likely to be found in nature.

In this study, we investigate the buckling characteristics in ideal, defect-free, homogeneous, and structurally and morphologically degenerate carbon nanostructures, namely the linearly- and angle-adjointed SWCNT and cylindrical fullerenes models under axial loading, and evaluate the impact of possible structural modifications in these models on their CBL characteristics. The investigated SWCNT and cylindrical fullerene models display significant structural aberrations, that separate them from classical low-dimensional carbon systems investigated in earlier works [Imani Yengejeh *et al.*, 2016]. It is therefore conceivable that the structural stability of such asymmetric models could be greatly influenced by their axial symmetry, relative position of defects in their structure, boundary conditions and other factors. We will illustrate that the mechanical properties of such systems can be effectively studied using the research methodology presented herein.

2. Materials and Methods

2.1. *Spatial geometry of carbon nanostructures*

The majority of known carbon nanostructures, such as spherical and cylindrical fullerenes, linearly- and angle-joined CNT systems, and nanocones can be devised and constructed from pseudo-two-dimensional (2D) single-layer sheets of graphene, as illustrated in Fig. 1.

Common homogeneous CNTs can be created by rolling a graphene sheet, and categorized as zigzag-, armchair-, or chiral- CNTs, which are defined in terms of their chiral angles, while a linearly-joined CNT molecular system is built by joining two common CNTs together along their axes of symmetry. The latter results in the introduction of Stone–Wales (5–7) defects within the immediate area of their junction. In the situation where the two connecting CNTs display the same chiral angle (i.e., zigzag, armchair, or chiral configuration), the created junction will be

Fig. 1. Single-layer graphene as carbon precursor to common CNT, linearly- and angle-adjointed CNT and cylindrical fullerene.

straight and the 5–7 defects will appear on the same side of the junction. On the other hand, if the CNTs forming the junction are of different chiral angles, the constructed junction will have a bending angle, as illustrated in Fig. 2.

Naturally, cylindrical fullerene structures are constructed from common CNTs those ends are capped, as shown in Fig. 3.

The aim of this study is to simulate mechanical properties of imperfect types of low-dimensional carbon models, which are more likely to be found in nature [Tran and Lambrakos, 2005; Sridhar *et al.*, 2012; Miralles *et al.*, 2012; Bokova-Sirosh *et al.*, 2016]. The planned approach is to explore and predict the buckling response of common SWCNTs and their corresponding degenerated counterparts under the influence of atomic impurities as well as under different boundary conditions.

The atomic and topological defects applied to the structures of this study, are vacant sites (single-, double-, triple- and pinhole- vacancies), 5–7 pair defects, and a nitrogen (N) substitutional defect. Nitrogen atom with its size of 65 pm is

Fig. 2. Jointed CNTs displaying 5-7 pair defects; (a) an angle-adjointed CNT and, (b) a linearly-joined CNT.

Fig. 3. Cylindrical fullerenes, (a) an armchair-type and, (b) a zigzag-type.

approximately 9/10 of the size of a carbon atom and it is assumed to take place of a normally occupied site of carbon atom in the crystal structure of SWCNT or a fullerene model, as shown in Fig. 4 (the position of substitutional N atom is shown as an immobilized, ad-on attachment for clarity).

Fig. 4. Schematic representation of single-, double-, triple- and pinhole-vacancies, Stone–Wales defects and a substitution lattice (i.e., N-atom) defect in the structure of SWCNT and fullerene carbon models.

2.2. Calculation method and experimental design

The simulation technique performed in this study is based on the approach suggested in our earlier work [Li and Chou, 2003], where the low-dimensional carbon systems contain atoms and covalent bonds, with their specific lengths and bond angles are modeled as space-frame structures. When subjected to mechanical loading all of the elements bonded together in these models are assumed to be connecting load-carrying beam members [Li and Chou, 2003; Öchsner, 2018] as shown in Fig. 5.

We attempt to model several types of nanostructures, such as straight and angle-adjointed SWCNT junctions and capped fullerenes and to investigate the CBL in these systems under different boundary conditions. The modeling procedure was the following. In step one, the spatial coordinates of atoms and their bonding vectors for all low-dimensional models were generated using Nanotube Modeler[®] software package (©JCrystalSoft) and imported to a commercial FEM package Marc[®] (MSC Software Corporation, CA, USA), and the CBL of defect-free and ideal SWCNT models was acquired. The overall length of homogeneous and capped SWCNTs was set at 15 nm, while the total length for straight and bending hybrid bonds was varied from 45 to 60 nm and from 35 to 40 nm, respectively. The values of bond strength, E , for an sp²-hybridised single carbon–carbon C–C, $EC-C = 5.484 \times 10^{-6} \text{ N/nm}^2$ and single carbon–nitrogen C–N, $EC-N = 4.806 \times 10^{-6} \text{ N/nm}^2$ were imported to the FE software for processing [Song *et al.*, 2006; Ganesan *et al.*, 2010]. Considering the fact that the C–C bond dissociation energy is approximately 345 kJ/mol compared to the C–N bond of 305 kJ/mol, the inclusion of nitrogen atom into the SWCNT lattice is a weakening factor, which overall reduces the stability of the doped structures

Fig. 5. Simulation of a linearly-joined SWCNT junction as a space-frame model (adopted from Lee and Lee [2012]).

studied [Armentrout, 1990]. The theory of elasticity [Sokolnikoff, 1956] describes the critical buckling response of a system as

$$P_{cr} = \frac{n^2 \pi^2 EI}{(KL)^2}, \quad (1)$$

where P_{cr} is the CBL of the system, K is the effective length constant, E is the Young's modulus of the low-dimensional particle, L is the total length of the structure, n is the buckling mode and I is the second moment of area. The critical buckling response of a system naturally depends on the overall geometry, boundary condition and basic configuration of the system, and during the first step, these variables are defined in the calculations. In our calculations, the values of I have been empirically estimated for the ideal and degenerated SWCNT systems containing (up to 900 atoms), with $K = 2$ used for the cantilever-type systems and an n of 1 used for the initial simulation of the first buckling mode.

Since, homogeneous CNTs can be viewed as a hollow cylinder, therefore, the following equation can be used to define the second moment of area:

$$I = \pi[(d+t)^4 - (d-t)^4]/64, \quad (2)$$

where d and t are the diameter of the CNT and the thickness of the CNTs shell, respectively. Here, the t -values of the CNTs and their derivations are the same as the interlayer spacing of graphite (0.34 nm) [Li and Chou, 2003; To, 2006].

In step two, some of the most common atomic defects, including vacant sites, an N-defect, and the 5-7 pair defect were applied to the ideal, defect-free SWCNT

and fullerene models. All of the impurities were introduced and applied using a custom code in MATLAB® (MathWorks, MA, USA) to the original defect-free, ideal models at 1.0, 2.0 and 3.0 at.% to the total number of atoms in the system.

In the final step, the CBL of degenerated SWCNT and fullerene models is obtained and compared to the nondefective ideal configurations. The comparison reference was based on the CBL of the ideal structures. The overall FEM simulation procedure is illustrated in the block diagram shown in Fig. 6.

Fig. 6. Investigation procedure adopted to estimate the structural stability and CBL values in ideal and structurally degenerated SWCNT and fullerene material models.

3. Results and Discussion

3.1. Structural stability of defect-free, ideal SWCNT and fullerene structures

The CBL of defect-free, ideal SWCNT and fullerene models under different boundary conditions is presented in Table 1.

Generally, the FEM results demonstrate that the CBL values vary depending on the structural organization of the low-dimensional systems. More precisely, the stability of the structures depends on the physical height of the constructed models, their axial symmetry, relative position to normal reference plane and their fixation mode. The general observation is that the structural stability of the ideal SWCNT and fullerene models increases by increasing the respective diameter of the tubes.

Table 1. The values for CBL in defect-free, ideal SWCNT and fullerene models used are reference models in this study.

Schematic view	Model	Chirality	Boundary condition	Critical buckling load (nN)
Linearly-joined CNT	(3-3)-(5-5)	Wide-end fixed	0.28
			Narrow-end fixed	0.13
		(5-5)-(10-10)	Wide-end fixed	1.36
			Narrow-end fixed	0.5
		(14-14)-(16-16)	Wide-end fixed	13.58
Angle-adjoined CNT	(3-3)-(8-0)	Zigzag CNT fixed	0.54
			Armchair CNT fixed	0.36
		(5-5)-(10-0)	Zigzag CNT fixed	0.71
			Armchair CNT fixed	0.55
		(7-7)-(16-0)	Zigzag CNT fixed	1.36
Cylindrical fullerene	(5-5) armchair CNT	Top capped capped	0.57
			Bottom-end fixed	0.56
		(6-6) armchair CNT	Top capped capped	0.99
			Bottom-end fixed	0.96
		(10-10) armchair CNT	Top capped capped	4.63
			Bottom-end fixed	4.41
		(9-0) zigzag CNT	Top capped capped	0.59
			Bottom-end fixed	0.58
		(10-0) zigzag CNT	Top capped capped	0.86
			Bottom-end fixed	0.83
Freestanding CNT	(5-5) armchair CNT	—	0.55
		(6-6) armchair CNT	—	0.94
		(10-10) armchair CNT	—	4.31
		(9-0) zigzag CNT	—	0.59
		(10-0) zigzag CNT	—	0.81

Fig. 7. Buckling and deformation characteristics of capped and fixed SWCNTs under compressive load with (a) zigzag-type and (b) armchair-type chiral organizations.

In addition, owing to their straight configuration, linearly-joined SWCNTs display higher resistance for compression loading compared to the angle-adjointed SWCNT models.

The buckling response of capped SWCNT models with different chirality, such as the zigzag- and an armchair-types, under the compressive loading are shown in Fig. 7. Both types of SWCNTs are shown deforming under the compressive load and owing to their structural similarity display very similar buckling and deformation characteristics.

3.2. Validation of the method

The comparison of the FEM results and analytical values obtained from the Eq. (1) indicates the validation of the method. The CBL values of the homogeneous CNTs obtained both computationally and analytically are listed in Table 2.

The analytical results obtained from Eq. (1) provide a comparison between the accuracy of FEM analysis and the analytical calculations, with the relative difference of less than 10%. Although analytical solutions are in good agreement with the computational results, it should be mentioned that the analytical calculation may not be accurate for the evaluation of the CBL in some cases, especially for CNTs with smaller diameters, since it assumes the CNTs as hollow cylinders. However, the nanomaterials are considered here as cylinder-shaped trusses. Therefore, we also compared our FE outcome to the ones evaluated by other numerical approaches.

Table 2. The values of CBL obtained from FEM and analytical equation.

CNT type	chirality (n, m)	diameter (nm)	Length (nm)	Young's modulus (TPa)	Critical buckling load (nN)		Relative difference in%
					FEM results	Analytical solution	
armchair	(5-5)	0.673	15	1.042	0.549	0.595	7.5
armchair	(6-6)	0.808	15	1.042	0.907	0.931	2.58
armchair	(10-10)	1.346	15	1.042	4.312	4.032	6.9
zigzag	(9-0)	0.699	15.4	1.032	0.588	0.643	8.5
zigzag	(10-0)	0.793	15.4	1.035	0.809	0.782	3.45

Our results are to a great extent comparable to the ones obtained by Bocko and Lengvarský [2017] where they applied a shell beam theory and obtained the CBL of an armchair (6, 6) and a zigzag (10, 0) CNT in a very close range compared to our results (with the length of 15 nm).

In addition, our results are also verified with those evaluated by Ansari *et al.* [2011], where MD simulations of nanotubes with chirality types of (8, 8) and (14, 0), respectively, were realized. They incorporated Eringen's nonlocality into the shell theory in order to include the small-scale effects on the axial buckling of SWCNTs with arbitrary boundary conditions. Furthermore, Poelma *et al.* [2012] applied the same MD simulation to evaluate the CBL of different CNTs versus the CNT length to diameter ratio. Within their MD simulation, they applied a spring force identify in the boundary conditions and extracted the reaction forces during the MD simulation. They examined the buckling property of a CNT with the diameter of 0.783 nm, and found the CBL of the CNT with various lengths. Their value of CBL of the CNT with similar aspect ratio was comparable to ours with the relative difference under 10%. Comparing all mentioned numerical simulations, it can be noted that the FE approach is quite reliable compared to MD simulations while the latter one is more restricted to smaller models and is very demanding in regards to computational resources.

3.3. Vertical instability of structurally degenerated SWCNT and fullerene models

In our work, the effects of introducing four different types of vacant sites, a Stone–Waals defect and, an N-substitutional defect, as shown in Fig. 4, at 1.0, 2.0 and 3.0 at.% to the total of carbon atoms in the SWCNT and fullerene models were investigated. Figures 8–13 illustrate that the presence of any type of a vacancy or defect in the structure of the model reduces the values of CBL for all nanostructures models. Furthermore, these figures reveal that all types of structural defects reduce the structural stability of the models. In the case for the angle-adjointed SWCNT junction systems, the change in the CBL values for fixed zigzag-type SWCNT was found to be higher when compared to the armchair-type chiral SWCNT system.

Notably, at 3.0 at.% (i.e., the highest defect concentration), the CBL values of (7-7)–(16-0) angle-adjoined SWCNT in the zigzag-fix boundary condition were found to be reduced by nearly 5.0%, whereas the reduction for the similar fixed SWCNT model with armchair-type chirality was found to be just over 4.0%. The buckling characteristics of linearly-aligned fixed SWCNT junctions, those of wider and narrower diameters, were found comparable with the wider tubes displaying marginally higher structural stability. For instance, in the case of (8,8)–(15,15) linearly-joined SWCNT hybrid system fixed at the wide end, the calculated reduction in the CBL was observed to be nearly 10.0%; this value was lower than the one that was found for the same type of SWCNT hybrid system with fixed at the narrow end.

Comparing the data in Fig. 8 for the linear- and angle-adjoined SWCNTs, it is noted that apart from the tube diameter which directly influences the structural stability of the models, the linearly-joined SWCNTs display higher resistance compared to their angle-adjoined counterparts. Furthermore, the overall formation of junction region of these hybrid systems has a significant impact on their structural stability. More specifically, it is indicated that the structural strength of the systems with parallel longitudinal axes is greater than the ones possessing bending junctions.

The reduction in the structural stability of the double vacancy defected models (all configurations) was higher compared to the SWCNT models containing single vacancy defect. A closer look at Fig. 9, it is indicated that SWCNT with wider diameters are significantly affected by introducing double vacancy defects to their configurations in comparison with the CNT-related systems possessing narrower diameters. Comparing the structural stability of common SWCNTs and cylindrical fullerene (both structures), the highest reduction in the CBL values was observed for the SWCNT systems containing the (10,10) armchair-type chirality, followed by SWCNTs with a zigzag-type chiral organization. The least affected models were SWCNT systems containing the (9,0) and then (5,5) SWCNTs.

According to Fig. 10, the difference between the simulated CBL values of the ideal and triple vacancy defected hybrids was significant, particularly in the case of SWCNTs hybrids containing (7,7)–(16,0) type defects, in which the CBL was recorded at approximately 50% corresponding to 3.0 at.% of triple vacancy defect. While the structural stability of wider hybrid SWCNT systems, such as (7,7)–(16,0) and (8,8)–(16,16) reduced markedly, the thinner two-junction SWCNT systems were found unaffected by these types of structural defects.

As shown in Fig. 11, the pinhole vacancy defect had the most significant impact on the structural stability of the material models, including linearly- and angle-adjoined CNTs, homogenous SWCNTs and cylindrical fullerenes. Such impurity in the structures caused up to a 70% reduction in the CBL in some circumstances. More precisely, in the case of linearly-joined CNTs, the reduction in the CBL of the system with narrow-end fixed was comparatively larger than the one for the systems with wide-end fixed boundary condition. In addition, by increasing the

Fig. 8. Change in the CBL values (abs.%) for (a) degenerated linearly- and angle-adjointed SWCNT hybrid systems with single vacancy defects and fixed armchair- and zigzag-type organizations and (b) degenerated homogeneous SWCNTs and cylindrical fullerenes under axial compressive load.

CNT diameter, the values of CBL of the CNT-related hybrids reduces markedly. The overall response of homogeneous CNTs and cylindrical fullerenes was comparatively similar, apart from the models containing wider diameters, e.g., (10–10) armchair CNT, where the two-end capped cylindrical fullerene had a slight reduction in the value of CBL compared to the other configurations with similar chirality.

Fig. 9. Change in the CBL (in abs.%) for (a) degenerated linearly- and angle-adjointed SWCNT hybrid systems with double vacancy defects and fixed armchair- and zigzag-type organizations and (b) degenerated homogeneous SWCNTs and cylindrical fullerenes under axial compressive load.

Introducing the 5–7 pair defect in the low-dimensional configurations of SWCNT was found to have a minor influence on the buckling load of these structures when compared to the vacant sites, as illustrated in Fig. 12. Overall, the change in the CBL for all models did not exceed 10.0%. With regards to nondefective configurations. The maximum change in the CBL values was found in the linearly-joined SWCNT

Fig. 10. Change in the CBL (in abs.%) for (a) degenerated linearly- and angle-adjointed SWCNT hybrid systems with triple vacancy defects and fixed armchair- and zigzag-type organizations and (b) degenerated homogeneous SWCNTs and cylindrical fullerenes under axial compressive load.

hybrid systems containing (8,8)–(16,16) chirality owing narrow-end fixed boundary condition, by approximately 9.3%.

Followed by 5–7 pair defect, N-doping had the least impact on the buckling response of the low-dimensional structures, as shown in Fig. 13. More specifically, no change was observed in the SWCNT hybrid systems of more than 10.0%, apart from the SWCNT hybrid system containing the (8,8)–(15,15) chirality; the latter was found to contain almost 11.0%.

Fig. 11. Change in the CBL (in abs.%) for (a) degenerated linearly- and angle-adjointed SWCNT hybrid systems with pinhole vacancy defects and fixed armchair- and zigzag-type organizations and (b) degenerated homogeneous SWCNTs and cylindrical fullerenes under axial compressive load.

The results indicate that the change in the CBL values of material models depends on the type and quantity of the structural defects. More specifically, it is noted that Stone–Wales and substituting dopants defects have minor influence on the structural stability of the models in comparison with the carbon vacancy defects (particularly, pinhole vacancy), which reduce the CBL of the nanostructures up to more than 60%. As previously predicted, it was observed that the CBL of vacancy defective structures reduces as the size of the defect increase. More precisely, the

Fig. 12. Change in the CBL (in abs.%) for (a) degenerated linearly- and angle-adjointed SWCNT hybrid systems with 5–7 pair defects and fixed armchair- and zigzag-type organizations and (b) degenerated homogeneous SWCNTs and cylindrical fullerenes under axial compressive load.

difference between the change in the CBL of the single-vacancy and pinhole vacancy defective linearly-joined CNTs is up to 50% in the case of (8,8)–(15,15). It can be drawn from the computational results that structural modifications could have a significant impact on the mechanical properties of all types of nanostructures including joined CNTs, homogeneous CNTs and cylindrical fullerenes. Such influence leads to a remarkable change in the CBL, and as a consequence, reduction in the structural stability of the low-dimensional material models.

Fig. 13. Change in the CBL in abs.% for N-doped (a) degenerated straight and knee SWCNT hybrid junctions with different chirality and boundary conditions and (b) homogeneous and capped SWCNT under axial compressive load.

4. Summary and Conclusions

Several types of carbon nanostructures including homogeneous, linearly- and angle-adjointed SWCNTs, and cylindrical fullerenes (in both one end capped and two end capped structures) were simulated and their structural stability was investigated through applying a computational approach. Due to the diversity of the investigated material models, an attempt was made to categorize the low-dimensional structures based on their shape and configurations. Following this idea, homogeneous CNTs and cylindrical fullerenes were examined in a same category and

linearly- and angle-adjointed were investigated as they are both hybrid nanostructures. One of the most highlighted features of this study was the application of different CNT models with variable chiralities, as well as boundary conditions. Several material models with different chirality and diameters were examined in order to evaluate the mechanical properties of the degenerated structures. The results indicate that all models of degenerated carbon nano-material models have their own specific critical properties and this is completely dependent on the structural configuration of the low-dimensional structures. More specifically, linearly-joined CNT models display higher stability to external forces in comparison with their angle-adjointed counterparts, due to their straight configurations. In addition, based on the obtained results of homogeneous CNTs and cylindrical fullerenes, it was indicated that these structures display a comparatively similar response to reduction in the CBL, since their overall configurations are similar at large extent. It was also noted that the CBL of nano-material models reduces by introducing microscopic impurities. This reduction leads to lower structural stability of the material models depending on the type and the quantity of the applied defects. These defects were listed as vacancy defects (single-, double-, triple- and pinhole vacancies), substitution dopant (N), and Stone–Wales pair defects. The computational results showed that pinhole vacancy and Stone–Wales pair defects had the most and the least influence on the structural strength of carbon nanostructures, respectively. It was also revealed that the boundary condition had a significant impact on the evaluation of the buckling properties of asymmetric models. For instance, in the case of linearly-joined CNT structures, the change in the CBL of the CNT hybrids in the wide-end fixed was comparatively larger than the one with the narrow-end fixed boundary condition. Similarly to linear CNT hybrids, angle-adjointed CNTs with armchair-type fixed display larger change in the CBL in comparison with those with zigzag-type fixed boundary condition. It was discussed that the buckling properties of structurally identical configurations (such as homogeneous CNTs and cylindrical fullerenes) are comparatively similar. This is probably because that the mechanical properties of the CNT structures are strongly dependent on the shape and configuration of the low-dimensional material models. With regards to the structural defects, it was indicated that the change in the CBL of models with vacancy defect (in its single form) and N-doped conditions is comparatively similar and had a relatively lower influence on the CBL. In contrast, triple and pinhole vacancies had a significant impact on the CBL of the material models and reduce the structural stability of the low-dimensional structures at the largest degree. Apart from the investigation of the mechanical properties of the CNT material models based on FEM and its particular restrictions, other mechanical approaches such as QM and DFT techniques are strongly advised to evaluate the properties of the nanostructures in a more nonrestricted condition, which is currently being investigated by the authors.

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