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Influence of defects in carbon nanotubes on their buckling behaviour

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Abstract. The paper studies a buckling behaviour of simply-simply supported single-walled carbon nanotubes (SWCNTs) without and with defects. The buckling of carbon nanotubes without and with defects was investigated by the finite element method (FEM). The carbon nanotubes were modelled as beams. The defects were created by removing of randomly determined carbon atoms and beam elements connected to these nodes. The increasing number of defects leads to the decrease of the critical buckling force of SWCNTs. The decrease of the critical buckling force was almost the same for SWCNTs with the same diameter but a different chirality.

Introduction

A nanostructure is a tiny body of size between molecular and microscopic structures. Nanostructures can be divided into several categories of objects: nanobeams, nanowires, nanorings, nanoparticles, nanoribbons, nanoplates, and nanotubes. The discovery of carbon nanotubes (CNTs) in 1991 was a significant breakthrough in the field of nanostructures [1]. Extensive research of CNTs started simultaneously with the discovery of CNTs. It was found that CNTs have extraordinary mechanical, electrical, optical and thermal properties. These properties have been verified by experimental, analytical and numerical methods. The numerical methods include the molecular dynamics simulation (MD), which is a suitable tool for a description of behavior of carbon nanotubes. MD computation has a disadvantage because it puts high demands on computer resources (processors, memory) as well as the computational time. This is a reason why researchers started to use the FEM to describe the behavior of CNTs. The approach was based on the creation of the connection between the MD and the continuum mechanics. This treatment was established by Li and Chou [2] for simulation of graphene sheets and carbon nanotubes. They used a beam element for modelling of interatomic bonds between two adjacent carbon atoms. Then Li and Chou [3] used this approach for a study of elastic moduli of multi-walled carbon nanotubes (MWCNTs), where the van der Waals forces between tubes were represented by nonlinear truss model. The nonlinear behavior of the truss was obtained by the Lennard-Jones potential. Simultaneously with these papers [2, 3] started the investigation of Young's modulus and other material properties of graphene sheets [4] and CNTs by FEM. Hartmann et al. [5] investigated the material properties of graphene by the atomistic simulation approach. They determined

Young's modulus, Poisson's ratio and thickness of graphene from the finite element computations. The beam elements for modelling CNTs were used by Tserpes and Papanikos [6]. The mechanical properties of MWCNTs were also studied in [7], where authors used for modelling CNT beam elements and the van der Waals forces between tubes were modeled by linear spring elements. The stiffnesses of the spring elements were obtained from the equivalent force concept. The same approach for modelling and estimation material properties of CNTs was used in [8, 9]. The researchers used for modelling CNTs the spring elements instead of beam ones. The difference between beams and springs lies in absence of definition of the cross section area as the input parameter for computations. Moreover, different material parameters of Young's modulus, Poisson ration and wall thickness are used in literature so the comparison of inputs and outputs is not easy. Brcic et al. [10] and Sakharova et al. [11] investigated the influence of waviness or vacancy defects on mechanical properties of CNTs. A few years later started an investigation in the area of buckling behavior of CNTs. Researchers have used the experimental, analytical and finite element method with beam, spring, and shell elements. Zhang et al. [12] analyzed buckling of multi-walled carbon nanotubes (MWCNTs) under radial pressure. The molecular structural mechanics approach was used by Hu et al. [13]. The 3D beam elements for modelling interatomic bonds of C-C and rod elements for modelling van der Waals forces were used in this approach. They concluded that their model is adequate for prediction of the buckling load of single- and multi-walled carbon nanotubes with the bigger length. In the paper written by Rahmandoust et al. [14] buckling and natural frequencies of SWCNTs were studied. C-C bonds were represented by an Euler-Bernoulli beam, and they were modelled by the FEM. The results were in good agreement with the analytical solution. The perfect and the geometrically modified CNTs under combined loading were investigated in [15]. The authors concluded that geometric changes reduce the critical load. The buckling behavior of CNTs with junctions were studied in papers [16, 17], where the authors used the MD and FEM simulations. In paper [16] they investigated the influence of strain rate on the magnitude of load force. Xin et al. [18, 19] investigated buckling of defected SWCNTs and DWCNTs by the MD simulation. The CNTs were loaded by axial compression and results were compared with CNTs without defects. They studied the effects of the position of defects on the buckling behavior of CNTs. In [20] the results of investigation of buckling behavior for defected nanotubes can be found. Similar research was accomplished by Ghavamian and Öchsner [21], as well as by Poelma et al. [22]. Torabi et al. [23] investigated the buckling of DWCNTs under three basic load states (tension, bending and torsion) and for perfect and defective nanotubes with the armchair chirality. They used a rigid sphere for modelling carbon atoms, nonlinear springs for modelling C-C bonds and linear springs for the modelling van der Waals forces. The influence of defects in geometry of SWCNTs and MWCNTs on buckling was subject of research that is described in paper [24]. The additional mechanical properties, application areas and behavior of carbon nanotubes are described in publications [25, 26].

In the current paper buckling of simply-simply supported single-walled carbon nanotubes under axial load is investigated using FEM. SWCNTs are considered as tubes without and with defects. The commercial program ANSYS Mechanical APDL is used for modelling SWCNTs, where the BEAM4 element with two nodes and with six degrees of freedom at each node is used for modelling the beam. The computations were realized for the nanotubes with 1 %, 5 % and 10 % missing carbon atoms, respectively. The defects were created by removing carbon atoms as nodes and beam elements attached to these nodes. Finally, the critical buckling forces of defected SWCNTs were compared with perfect SWCNTs. The main goal of the paper is to investigate buckling behavior of single-walled carbon nanotubes without and with defects under axial loading. In comparison to the reviewed published papers we have investigated nanotubes with significant higher number of defects. Moreover, we have studied the influence of locations of defects on the magnitude of buckling force.

Theoretical background of carbon nanotubes modelling

The MD approach is usually used for modelling carbon nanotubes. A problem of the method is, as was mentioned above, that at this time also with using supercomputers we can simulate the behavior of carbon nanotubes only with small lengths (several micrometres). Moreover, finding of the solution is an extremely time-consuming process. For this reason, it is better to use the FEM for a description of behavior of carbon nanotubes. The modelling of carbon nanotubes can be realized by different types of finite elements, i.e. bar elements, beam elements, linear and nonlinear spring elements and shell elements. Of course, all models consisting of these different element types lead to different approaches for modelling as well as for defining material properties, boundary conditions and loadings.

The carbon nanotubes are modelled using beam elements, whose properties are obtained by making the connection between the molecular and continuum mechanics. Interatomic interactions in molecular mechanics as bond stretching, bond angle variation, dihedral angle torsion and out-of-plane torsion are replaced by beam elements that represent the load by pure tension, bending and torsion. The following relations between parameters in molecular mechanics k_r, k_θ, k_τ and parameters in continuum mechanics EA, EI, GJ were obtained using this connection [6]:

$$k_r = \frac{EA}{L}, \tag{1}$$

$$k_\theta = \frac{EI}{L}, \tag{2}$$

$$k_\tau = \frac{GJ}{L}, \tag{3}$$

where k_r, k_θ, k_τ are force constants (stiffness) of bond stretching, bond bending and torsional resistance, respectively, and E, G, L, A, I, J are Young's modulus, shear modulus, length of beam, cross-section area, quadratic moment of inertia and polar moment of inertia, respectively [2, 3, 6].

The Eqs. (1) – (3) represent the basic relations for the application of continuum mechanics for solving of carbon nanotubes. By assuming a circular beam section with diameter d and corresponding parameters $A = \pi d^2/4$, $I = \pi d^4/64$ and $J = \pi d^4/32$, then Eqs. (1) – (3) give [6]:

$$d = \sqrt{\frac{k_\theta}{k_r}}, \tag{4}$$

$$E = \frac{{k_r}^2 L}{4\pi k_\theta}, \tag{5}$$

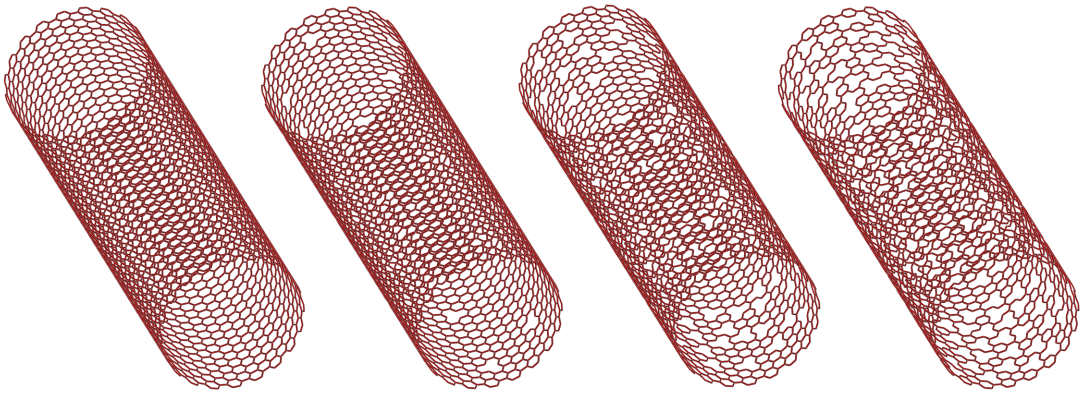
$$G = \frac{{k_r}^2 k_\tau L}{8\pi k_\theta^2}. \tag{6}$$

Here, the parameters are given as [2, 3, 6]: $k_r = 6.52\times10^{-7}$ Nnm^{-1}, $k_\theta = 8.76\times10^{-10}$ Nnmrad^{-2}, $k_\tau = 2.78\times10^{-10}$ Nnmrad^{-2}, $L = a_{C\text{-}C} = 0.1421$ nm. The input data as diameter $d = 0.1466$ nm, Young's modulus $E = 5.488$ TPa and shear modulus $G = 0.871$ TPa are obtained for the beam element modelled using FEM. The simply-simply supported and axially loaded SWCNTs with these properties of the beam elements (BEAM4 – Euler-Bernoulli beam) are modelled in the ANSYS Mechanical APDL. The boundary conditions are applied to the boundary nodes on the beam elements of the SWCNTs. The top level boundary nodes are allowed to move in

the axial direction of the nanotube. The force is distributed to the upper nodes and the total force magnitude is 1 nN. In order to know, at least approximately, number of nodes for modeled nanotubes we can give one representative example with chirality (6, 6) and length 3 nm. Such a model consists of 300 nodes and 438 nanobeams. At the beginning, the static analysis with active prestress effect is performed and then the buckling analysis is performed.

Buckling of carbon nanotubes

The simply-simply supported carbon nanotubes with defects are modelled only using the beam models of CNTs. The defects are modelled by removing of random carbon atoms (nodes) and removing corresponding beam elements attaching to these atoms (nodes). SWCNTs have 0 %, 1 %, 5 % and 10 % removed carbon atoms (nodes) of the total amount (Fig. 1). The defects are made using quasi-random pattern. At the beginning, the defective pattern with 1 %, 5 % and 10 % removed carbon atoms was created for every diameter of nanotube which was copied several times in order to have desired length of whole nanotube. Accordingly, the patterns have certain periodicity. In this section, an axial buckling of simply-simply supported single-walled carbon nanotubes is investigated.



a) b) c) d)

Fig. 1: The armchair carbon nanotubes (20, 20) with defects a) 0 %, b) 1 %, c) 5 % and d) 10 %

Since the location of the defects is a very important factor, their influence to the magnitude of critical force was studied on models divided into 6 parts (Fig. 2(b)). Due to symmetry, the calculations were accomplished only for 4 models – the models had defects in the right bottom part (Fig. 2(c)), whole bottom part (Fig. 2(d)), right middle part (Fig. 2(e)), and whole middle part (Fig. 2(f)). If we want to compute the influence of defect positions we have to remove the same percentage of atoms as before, it means the number that is related to the whole nanotube. In Fig. 3(a) up is given distribution of defects for 1 % of removed atoms. In Fig. 3(a) down is given distribution of defects for 5 % of removed atoms. However, the picture shows that the structure consists of many big gaps so the computations do not have any sense. Accordingly, only computation for 1% defects inside considered part of structure were realized. The results of computations are given in Fig. 4, where the decrease of buckling force in comparison to the nanotube without defects is presented. The semi-logarithmic graph was chosen in order to stress differences between computed values for the whole extent of graph. As the graphs represent decreasing of critical force, the highest values are related to the more danger situations from the point of view of nanotube stability. Accordingly, for the simply-simply supported nanotubes it is more danger to have defects in the middle part of nanotube than on their ends. The concentration of defects on one side lead to smaller critical force as the concentration of defects on the whole part.

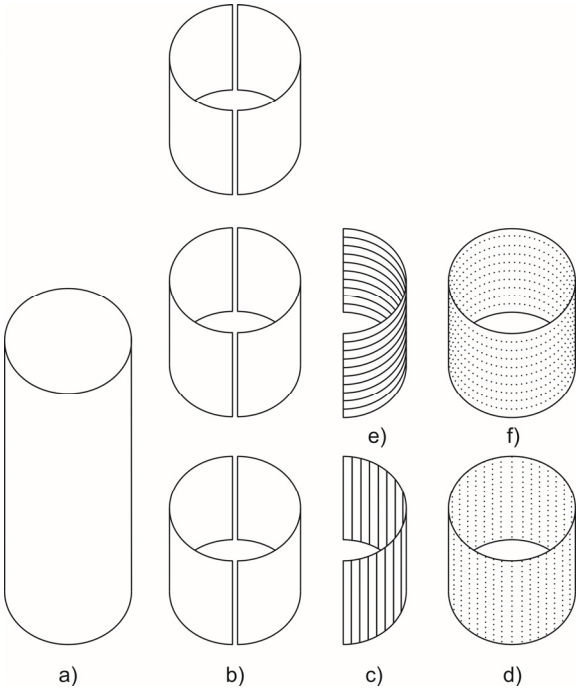


Fig. 2: The scheme of nanotube for description of areas with removed atoms a) whole nanotube b) partitioned nanotube c) bottom right part of nanotube d) whole bottom part of nanotube e) middle right part of nanotube f) whole middle part of nanotube

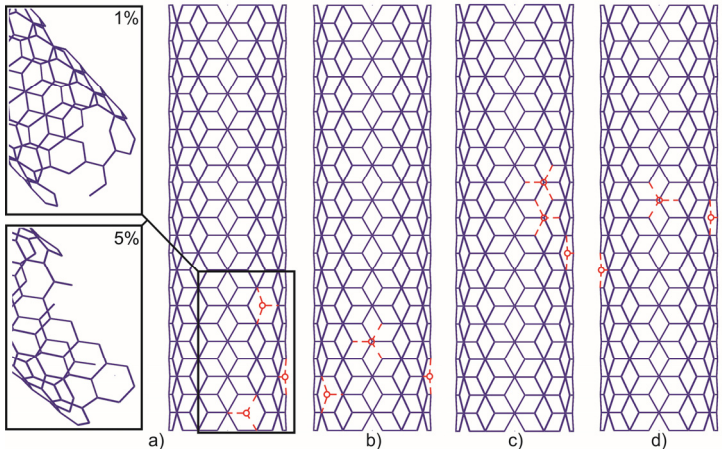


Fig. 3: The scheme of nanotube for description of areas with removed atoms a) whole nanotube b) partitioned nanotube c) bottom right part of nanotube d) whole bottom part of nanotube e) middle right part of nanotube f) whole middle part of nanotube

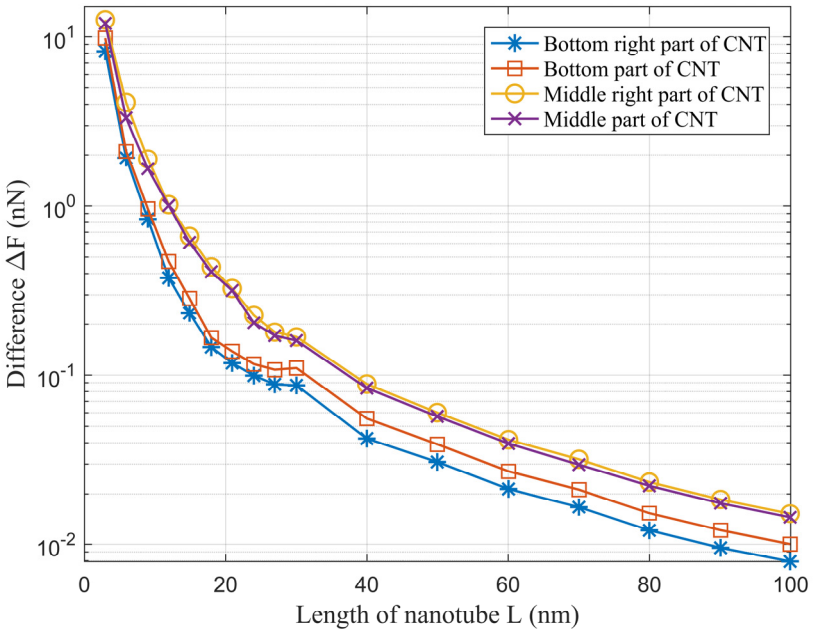


Fig. 4: Differences of critical buckling forces between perfect and defective carbon nanotubes (6, 6) in different parts of nanotube

The critical buckling forces F_{cr} of the single-walled carbon nanotubes (Table 1) under axial loading with vacancies 1 %, 5 % and 10 %, and length from the range L = 3 nm to 100 nm are shown in Fig. 5 – Fig. 6. The tendency of decreasing of the critical buckling force F_{cr} is almost the same in all cases, but a slight deviation can be seen for the curves that represent different levels of vacancies in the structures. The critical buckling force F_{cr} is the same for SWCNTs with the equal diameters, that is, the F_{cr} is independent of used chirality types (armchair, zigzag) of SWCNTs. The graphs show quantitative relations for magnitude of buckling force with respect to the number of vacancies in the nanotube of a given chirality and length. On the right side of the graphs (long nanotubes) we observe the Euler buckling. The shell buckling begins for nanotubes of length approximately 27 nm (at the beginning of plateau part) moving to the left side of graphs. However, on the basis of previous computations we can state that the shell buckling modes are not adequate to corresponding shell modes and accordingly the computed buckling forces are smaller. The graphs show obvious fact that increasing number of vacancies leads to the moving of the Euler buckling to the left side.

Table 1: The modelled carbon nanotubes with basic parameters

Nr.	Armchair SWCNT		Zigzag SWCNT	
	Chirality	Diameter (nm)	Chirality	Diameter (nm)
1.	(6, 6)	0.8142	(10, 0)	0.7834
2.	(10, 10)	1.357	(20, 0)	1.5669
3.	(15, 15)	2.0354	(26, 0)	2.0369
4.	(20, 20)	2.7139	(35, 0)	2.742

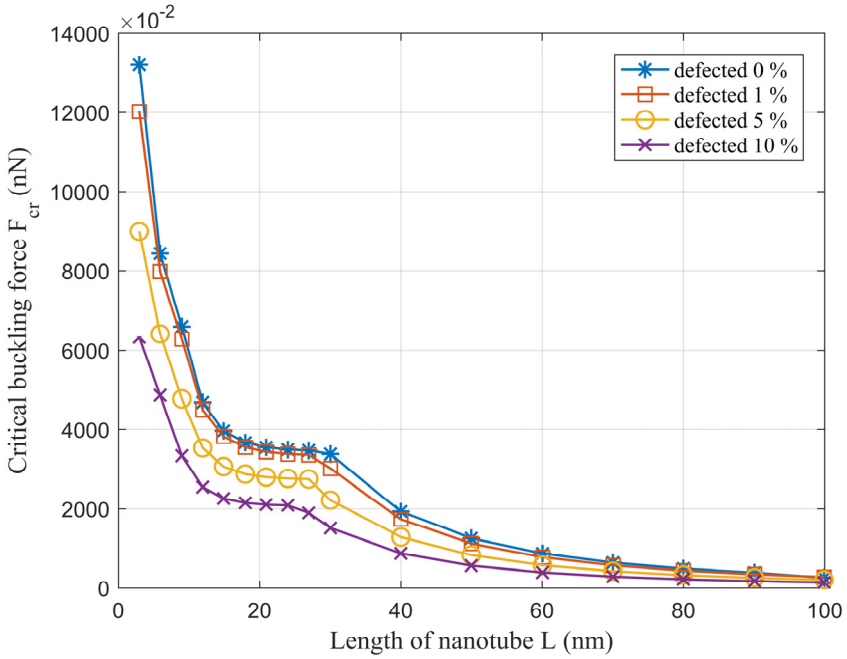


Fig. 5: The critical buckling force F_{cr} of the defected armchair carbon nanotubes (20, 20) with diameter D = 2.7139 nm

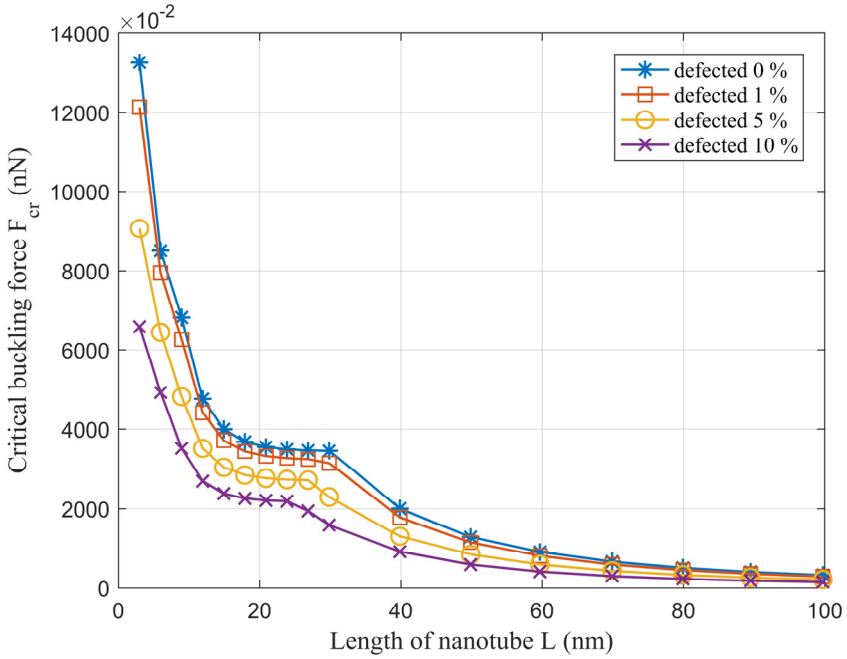


Fig. 6: The critical buckling force F_{cr} of the defected zigzag carbon nanotubes (35, 0) with diameter D = 2.742 nm

The average values of decrease of critical buckling force F_{cr} for the modelled simply-simply supported CNTs are given in Table 2.

Table 2: The decrease of critical buckling force F_{cr} for the defected carbon nanotubes with respect to perfect carbon nanotubes

Carbon nanotube		Decrease of critical buckling force F_{cr} (%)		
Chirality	Diameter (nm)	Defect 1 %	Defect 5 %	Defect 10 %
(6, 6)	0.8142	13.48	41.03	54.49
(10, 10)	1.357	7.57	33.09	56.58
(15, 15)	2.0354	8.72	33.79	55.89
(20, 20)	2.7139	6.96	31.55	53.35
(10, 0)	0.7834	12.25	34.62	74.27
(20, 0)	1.5669	11.77	40.53	65.55
(26, 0)	2.0369	11.66	34.43	53.08
(35, 0)	2.742	9.61	34.01	54.09

Conclusions

The buckling of axially loaded armchair and zigzag single-walled carbon nanotubes without and with defects was investigated. The SWCNTs were modelled by the beam finite elements. The properties of the beam finite element model were determined from the connection of the molecular and continuum mechanics. The critical buckling forces were calculated for four armchair and four zigzag carbon nanotubes with various lengths. The critical buckling forces of these defected SWCNTs were investigated. Defects were realized by removing of random carbon atoms (nodes) and beam finite elements attached to these atoms (nodes). It is apparent that the increasing number of defects leads to the decrease of the critical buckling force of SWCNTs. The decrease of the critical buckling force was almost the same for SWCNTs with the same diameter and different chirality. The small difference was caused by the random location of relatively homogeneously positioned vacancies.

The results show that the buckling of carbon nanotubes can be simulated by beam model. The all computations are not more time consuming. The next step can be the application of Eringen nonlocal theory for considering the small scale effect of CNTs and modeling of carbon nanotubes by springs elements because some authors state that spring models are more useful for carbon nanotubes [8, 9], especially in case of bending.

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