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# Influence of combined loading on the structural stability of carbon nanotubes

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## HIGHLIGHTS

- Different geometrical modified carbon nanotubes are numerically simulated.
- The stiffness change is evaluated for different modifications.
- Results are compared to perfect CNTs.
- Combined loadings lead to reduced stiffness values for single- and multi-walled CNTs.
- Twisting is the most critical form of geometrical modifications.

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## ABSTRACT

Numerous armchair and zigzag carbon nanotubes (CNTs) in their perfect and geometrically modified form were simulated and their buckling behavior was investigated through performing computational tests with different boundary conditions. Both computational and analytical results were compared in the case of perfect tubes. Then, three kinds of geometrical modifications, i.e. twisting angle, *z*-distortion along the longitudinal axis, and *xy*-distortion along the radial axis, were introduced to the configuration of perfect CNTs and the buckling behavior of geometrically modified CNTs was numerically evaluated and compared with the behavior of the perfect ones. It was shown that the first critical buckling load of both perfect armchair and zigzag CNTs increases by increasing the chiral number. In addition, it was also concluded that the existence of any type of geometrical modifications in the configuration of CNTs leads to a lower critical load and as a result, lower buckling properties. Finally, it was revealed that by increasing the length of the tubes, the critical buckling load of the CNTs reduces significantly while addition of further walls increases significantly the critical buckling load.



## 1. Introduction

Since the discovery of carbon nanotubes (CNTs) in 1991 [1], these nano-structures have attracted extensive attention due to their significant mechanical and electrical properties. High strength and lightness are two outstanding properties of CNTs which make these nano-particles important to industrial applications. The examinations on CNTs can be divided into two groups of experimental and computational methods. Molecular dynamics (MD) and continuum mechanics approaches such as the finite element method (FEM) have been the most common approaches to study the behavior, e.g. the buckling behavior of CNTs [2]. Real CNTs may be affected by imperfections. On the one hand, so-called atomic imperfections such as vacancies, alien species, and Stone-Wales defects may be distinguished. The second types of imperfections are geometrical modifications of the perfect structure such as curvature, twisting or distortion and are the content of the actual study. In the following, the results of several studies on the evaluation of buckling properties of CNTs are presented.

In 2007, Hao et al. [3] investigated the axial compression of both perfect and atomic defective single-walled carbon nanotube

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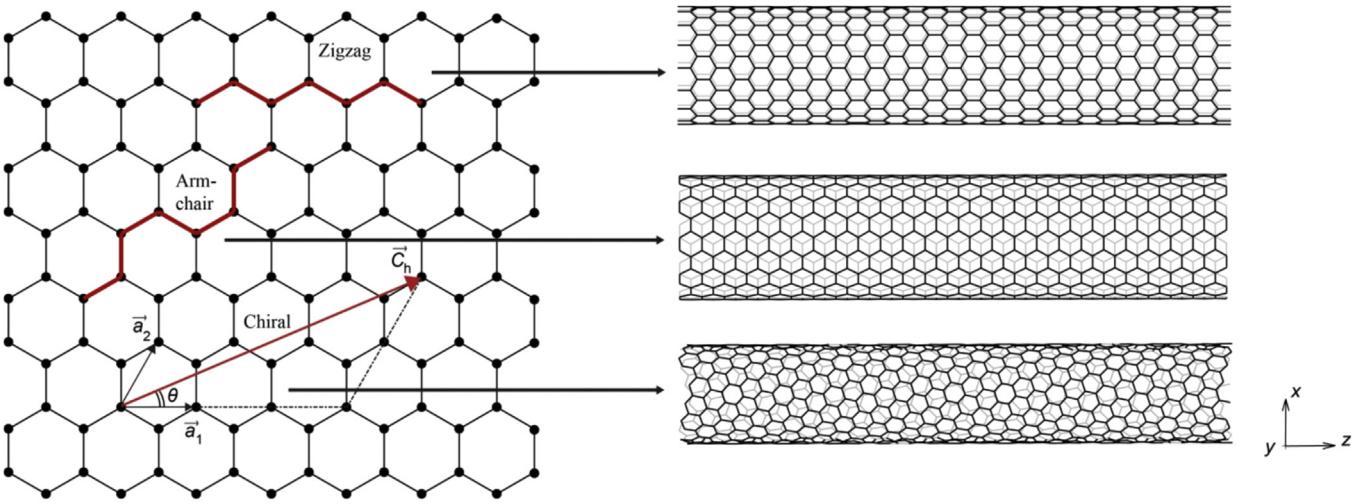


**Fig. 1.** Schematic diagram showing zigzag, armchair and chiral CNTs.

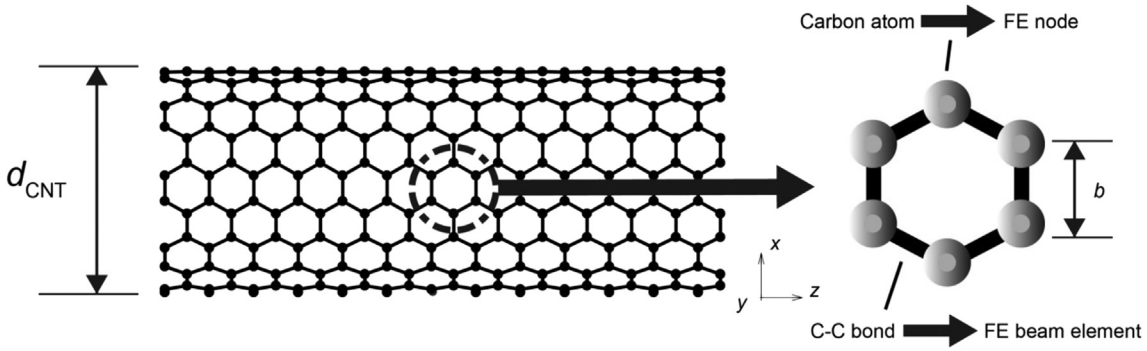


**Fig. 2.** Side view of an armchair CNT as a space-frame structure.

(SWCNTs), applying molecular dynamics simulation. Their findings revealed that any change in the length, chirality, temperature, and the initial structure defects of the CNTs is effective on the buckling and axially compressive properties of SWCNTs. After that, Yao et al. [4] studied the bending buckling behavior of double- (DWCNTs) and multi-walled CNTs (MWCNTs), applying a modified finite element method. They established a relationship between the diameter of CNTs and the critical bending curvature. In addition, they investigated the effect of the number of layers on the buckling load and the critical bending angle of MWCNTs. Then in 2010, Kang et al. [5] conducted a study to investigate the buckling behavior of intramolecular junctions (IMJs) under axial compression. They performed both molecular dynamics simulation and finite element (FE) analysis. The results of both tests indicated that the critical compressive strain is dependent upon the radial dimension and length of the IMJs but independent of the chirality of the IMJs. In 2012, applying the FEM, Ghavamian and Öchsner [6] conducted a study on the investigation of the effect of atomic imperfections on the buckling behavior of MWCNTs. They constructed armchair and zigzag CNTs in their perfect forms. Then, they evaluated the buckling behavior of CNTs by comparing obtained critical buckling loads and analytical calculations. They finally concluded that the existence of any curvature in the structure of CNTs decreases their buckling strength. Recently in 2013, Imani Yengejeh et al. [7] investigated the buckling behavior of straight hetero-junctions and their fundamental armchair and zigzag CNTs, performing a FE approach. They also compared the FE results with the analytical calculations. Their findings revealed that the first critical buckling load of hetero-junctions lies within the value of their constituent homogenous CNTs. In addition, they concluded that the critical buckling load of straight hetero-junctions and their fundamental CNTs increases by increasing the chiral number of both zigzag and armchair CNTs.

Although the previous investigations on the buckling behavior of CNTs have been comprehensive, most of them considered the perfect form of CNTs in their examinations and less concentration has been attracted to study the buckling behavior of imperfect, twisted, and distorted CNTs. The findings of the presented study provide a realistic prediction of the buckling properties of CNTs in a closer form to those found in reality in nano-industry and nano-material production. Within this work, 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 configurations as in the case of the considered CNTs.

## 2. Methodology

### 2.1. Geometric definition

CNTs are assumed to be hollow cylinder shaped structures, as illustrated in Fig. 1, which can be imagined by rolling a graphene sheet into a cylinder with diameters ranging from 1 to 50 nm and