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Review

Advances in mechanical analysis of structurally and atomically modified carbon nanotubes and degenerated nanostructures: A review

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ABSTRACT

In the past few years, numerous research activities concerning the mechanical behavior of defected and imperfect carbon nanotubes have been conducted. It is reported that the superlative mechanical properties of these nano-structures, i.e. high stiffness, high strength and vibrational response, would be affected by existing or introducing defects and impurities in the structure of the nanotubes. Such defects may results from manufacturing routes or introduced on purpose to tailor certain physical properties. This review attempts to categorize and highlight the advanced breakthroughs and recent studies employed to investigate the mechanical properties, e.g. stiffness, buckling behavior and vibrational response of structural and atomically modified carbon nanotubes. The presented studies cover the mechanical behavior of nanotubes, both theoretically and experimentally which allowed a realistic prediction of the mechanical behavior of defected tubes in a closer form to those found in reality. It was concluded that any type of imperfection, either atomic or structural modification, influences the mechanical behavior of nanotubes and reduces the stiffness and structural stability, as well as vibrational response of these nano-structures. The present review includes: (i) a brief introduction to atomic and structural modification of nanotubes; (ii) a review of mechanical analysis of atomically and structurally modified models in two separate sections; and (iii) a detailed conclusion on the discussed studies and present the potential progress.

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1. Introduction

The industrialized world requires novel and sophisticated technologies, for example, from nano-science to aerospace. Such new technologies desire new devices constructed from new materials. Over the past few decades, carbon nanotubes have generated huge interest from many areas of science and engineering. This is mainly due to their outstanding physical, mechanical and chemical properties, such as high strength, good conductivity, high stiffness, and high aspect ratio but very low density [1–9]. Carbon nanotubes (CNTs) are hollow cylinders, constructed by hexagonal unit cells, shaped by carbon atoms which were found by Iijima in 1991 [10]. Their important mechanical, electrical and thermal properties made these nanostructures distinctive and consequently made them very interesting for a large number of advanced applications as either stand-alone nanomaterials or reinforced composite materials. Numerous investigations have been conducted on obtaining and improving the properties of CNTs. Prediction of Young's modulus (of about 1 TPa) and tensile strength (of up to 63 GPa) for CNTs were of the most important objectives of these studies [11]. These investigations can be divided into two groups of experimental and computational approaches. Molecular dynamics (MD) and continuum mechanics techniques such as the finite element method (FEM) have been the most predominant computational approaches to evaluate the behavior of CNTs [12–14]. These nanostructures exist in single-walled or multi-walled configurations. The single-walled carbon nanotube (SWCNT) [15,16] is formed by rolling a single graphene sheet seamlessly to model a

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cylinder with a diameter of 1 nm and length of order of centimeters. Similar to the basal plane separation in graphite, the multi-walled carbon nanotube (MWCNT) is an array of such cylinders formed concentrically and separated by 0.35 nm with diameters from 2 to 100 nm and lengths of tens of microns.

There are quite a lot of experimental reports on the impurities of CNTs showing the existence of different kinds of imperfections in the structure of CNTs including distortion, bending and twisting along their longitudinal axis [17–19]. Nevertheless, most of researchers considered the perfect form of CNTs in their computational and theoretical investigations and very less attention has been paid to the mechanical behavior of imperfect, impure, curved, and hetero-junction CNTs. The following investigations allow a more realistic prediction of the mechanical properties of structural and atomically modified CNTs in a closer configuration to those found in reality which can be of use and importance in nano-engineering and nano-material production. This review is organized as follows: Section 2 provides a brief introduction to atomic and structural imperfection of CNTs. Section 3 and 4 present a review of mechanical analysis of atomically and structurally modified CNTs including axial and torsional stiffness, buckling behavior and vibrational response of the CNTs, respectively. The last section concludes the mentioned study and provides an overview on the recent advances of modified CNTs.

2. Defective CNT structures

Basically, the defects in the structure of CNTs are divided into two major categories, i.e. atomic and structural modification.

2.1. Atomic modification

There are some specific types of defects, e.g. doping, carbon vacancy and perturbation which can impure the configuration of CNTs.

2.1.1. Doping

This random imperfection corresponds to the case where a finite number of carbon atoms were replaced by silicon, nitrogen, boron, etc. [20–22].

2.1.2. Carbon vacancies

In such cases, a finite number of carbon atoms are missing in the structure of CNTs.

2.1.3. Perturbation

In this condition, all carbon atoms of the CNT are misplaced for a random length.

2.2. Structural modifications

Apart from atomic modifications in the structure of CNTs, there are other types of macroscopic defect, e.g. hetero-junction, curved tubes, twisted CNTs, spiral deformation, which affect the mechanical behavior of these carbon nano-structures.

2.2.1. Straight hetero-junction

It is possible to connect two different homogeneous CNTs by introducing a pair of pentagon and heptagon defects in the otherwise perfect hexagonal graphite lattice [23]. Hetero-junction CNTs are categorized based on the structures of their two initial homogeneous CNTs. The connecting region of these nano-structures is categorized into three different classifications, i.e. large angle, small angle, and straight connections. Depending on the type of the fundamental CNTs of hetero-junctions, these specific configurations are classified as straight structures and bending models, i.e. if the constituent CNTs of a hetero-junction are in the same type (either armchair, zigzag and chiral), the configuration of the hetero-junction is considered as a straight model and the homogeneous CNTs will be connected with parallel longitudinal axis.

2.2.2. Kink hetero-junction

On the other hand, if the initial homogeneous CNTs of a hetero-junction are not in the same type, the hetero-junction will be created with a bending angle. This type of structure is called a kink hetero-junction. As it is noticeable, the pentagon–heptagon pair defects of straight hetero-junctions both appear in one side of the CNT. In contrast, the pentagon–heptagon pair defects of kink hetero-junctions with bending angles are placed separated in opposite sides of these specific nano-structures [24].

2.2.3. Curvature

Curvature is a very important macroscopic defect in the configuration of CNTs which has a significant influence on the mechanical behavior of these nano-particles. According to experimental and modeling results, one of the key aspects of CNTs which should be properly addressed is initial curvature [23]. Several experiments revealed that the structure of nanotubes will be deformed due to external forces [25].

2.2.4. Twisting

CNTs might be deformed by introducing a twisting angle to the configuration of the tube. This specific modification affects the mechanical properties of CNTs [26]. Some experimental investigations revealed the twisted structure of these nanotubes.

2.2.5. Spiral deformation

This type of deformation occurs when the tube is twisted, like a spring, along its longitudinal axis [27]. Based on this spiral angle, several CNTs can be created with different configuration.

Fig. 1 illustrates a few instances of the mentioned structural and atomic modifications.

3. Research work on atomic modification

The following sections provide a review on the mechanical behavior of atomically modified CNTs.

3.1. Axial stiffness

In 2004, Liew et al. [28] examined the elastic and plastic properties of CNTs under axial tension using the MD simulation. They also modeled the interaction force between atoms applying the second-generation of reactive empirical bond-order potential coupled with the Lennard–Jones potential. They obtained the stress–strain response to describe the elastic and plastic behavior of SWCNTs and MWCNTs. In addition, they discussed and presented the plastic deformation due to the formation of the Stones–Wales defects and the brittle fracture due to the bond breaking. Their simulation revealed that the fracture damage of MWCNTs initially takes place in the outer most layer, and subsequently occurring in the inner layer. Lau et al. [29] presented a critical review on the prediction of mechanical properties of CNTs. They discussed the use of finite element modeling combined with MD simulation for evaluating the mechanical properties of nanostructures. They pointed out that the value of Young's modulus cannot be directly used to estimate the mechanical properties of MWCNTs due to the discontinuous stress transfer inside the nanotubes. Then, in 2006, Meo and Rossi [30] proposed a FE model to investigate the fracture progress in armchair and zigzag CNTs with defects under uniaxial

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