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Numerical investigation on the influence of atomic defects on the tensile and torsional behavior of hetero-junction carbon nanotubes

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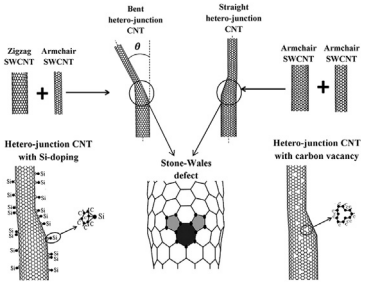
HIGHLIGHTS

- Hetero-junction and homogeneous carbon nanotubes are numerically simulated.
- Two atomic defects i.e. Si-doping and carbon vacancy are introduced to the models.
- Influence of the defects on the Young's and shear moduli of models is quantified.
- Simple relations for the prediction of the influence of the defects are proposed.

GRAPHICAL ABSTRACT



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ABSTRACT

The finite element method was employed for the numerical simulation of hetero-junction carbon nanotubes with all possible connection types and their corresponding fundamental homogeneous tubes. Then, atomically defective hetero-junction carbon nanotubes were modeled by introducing silicon impurities and vacant sites into their structures. Finally, the elastic and shear moduli of all the models were evaluated under tensile and torsional loads, based on the assumption of linear-elastic deformation of these nanomaterials. The results showed that armchair and zigzag carbon nanotubes have the highest Young's and shear moduli respectively, among homogeneous carbon nanotubes. The mechanical tests on the hetero-junction carbon nanotubes revealed that these nanotube types have lower moduli when compared to their fundamental tubes. It was clearly observed that armchair–armchair and zigzag –zigzag hetero-junction carbon nanotubes have the highest Young's modulus among the hetero-junction carbon nanotubes while the shear modulus peaks were seen in zigzag-zigzag models. On the other hand, the lowest values for the Young's and shear moduli of hetero-junction carbon nanotubes were obtained for the models with armchair-zigzag kinks. It was also discovered that the atomic defects in the structure of hetero-junction carbon nanotubes lead to a decrease in their Young's and shear moduli which seems to follow a linear trend and could be expressed by a mathematical relation in terms of the amount of the atomic defect in their structures which could be used for the prediction of the tensile and torsional strength of the atomically defective hetero-junction carbon nanotubes for their proper selection and applications in nanoindustry.

1. Introduction

Since the discovery of carbon nanotubes (CNTs) in 1991 by Iijima

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[1], scholar's attention around the world has been drawn to these nanostructures because of their unique properties and the wide area of their application in the nanoindustry. These nanomaterials demonstrated a high potential to be used as either stand-alone nanomaterials or reinforcements in the structure of composite materials. Strength, lightness and other brilliant mechanical properties of carbon nanotubes have encouraged many scholars to characterize these nanostructures for their application in various nanodevices [2–4]. Since 1991, various approaches have been employed for the mechanical characterization of carbon nanotubes which are generally divided into two groups of experimental and theoretical approaches, all of which yielded a surprisingly high value of about 1 TPa as the Young's modulus of CNTs. Recently, considerable attention has been paid to the finite element method (FEM) which has earned a noticeable popularity among scholars as a material characterization approach [5].

1.1. Literature review: mechanical properties of homogeneous CNTs

In 1997, an experimental investigation was performed by Lu [6] to evaluate the tensile and torsional strength of CNTs. He reported values of 0.97 TPa and 1 TPa as the Young's modulus for single-walled carbon nanotubes (SWCNTs) and for multi-walled carbon nanotubes (MWCNTs), respectively, while a general value of 0.5 TPa was also reported as the shear modulus of CNTs, with consideration of the empirical force constant.

Kalamkarov et al. [7] investigated the mechanical properties of single-walled carbon nanotubes (SWCNTs) by two different approaches of analytical and finite element methods, based on continuum mechanics. According to their analytical calculations, the Young's and shear moduli of SWCNTs were obtained to be about 1.71 TPa and 0.32 TPa, respectively, while their finite element modeling yielded an elastic modulus in the range of 0.9–1.05 TPa for SWCNTs and 1.32 to 1.58 TPa for double-walled carbon nanotubes (DWCNTs). Furthermore, the shear modulus of SWCNTs was found to be in the range of 0.14–0.47 TPa while the range of 0.44–0.47 TPa was reported for three- and four-walled carbon nanotubes. Young's and shear moduli of MWCNTs were also evaluated by Rahmandoust and Öchsner [8] by means of the finite element method. They reported the Young's modulus of MWCNTs to be between 1.32 and 1.58 TPa and their shear modulus to be in the range of 0.37–0.47 TPa.

Fan et al. [9] also investigated the mechanical properties of MWCNTs by the finite element method. Eventually, they acquired the Young's modulus of MWCNTs to be about 1 TPa while the obtained shear modulus oscillated between 0.35 and 0.45 TPa. They also discovered that the aspect ratio of DWCNTs is correlated to their critical buckling loads.

Song et al. [10] investigated the elastic properties of perfect and Si-doped CNTs. Finally, they discovered that Si-doping in the structure of CNTs leads to lower tensile strength. Ghavamian et al. [11,12] also developed a numerical simulation, based on the finite element method, to probe the tensile and torsional properties of perfect and atomically defective MWCNTs. Their results showed that CNTs have anisotropic behavior and the atomic defects in the structure of CNTs result in a decrease in their elastic and shear strength. They also presented mathematical relations for predictions of the elastic properties of defective CNTs in terms of the amount of atomic defects.

1.2. Literature review: mechanical properties of hetero-junction CNTs

Apart from the mechanical properties of individual homogenous CNTs, it has experimentally been observed that it is also possible that two CNTs with different chiralities connect together by a heptagon–pentagon kink and construct a hetero-junction or composite CNT. Some particular properties of hetero-junction CNTs, namely, metal/semiconductor or semiconductor/semiconductor behavior provided these nanostructures with a potential to be used as fully carbon made building blocks of nanoscale electronic devices. Furthermore, hetero-junction CNTs which have inherited outstanding properties of CNTs, i.e. flexibility, high stiffness, ultra-high light absorption ability and high electrical conductivity, also offer high mobility, excellent air stability and high conductivity which has made them widely applicable and demanded as solar cells with considerably better efficiencies [13–16]. However, such kinks in the structure of hetero-junction CNTs which are considered as structural defects seem to considerably influence their mechanical properties. Therefore, the necessity of investigations on these particular types of CNT became highlighted and it has recently encouraged some scholars to devote their research to the modeling and characterization of these nanomaterials.

An efficient solar cell with an efficiency of 13.8% was produced by Jia et al. by combining hetero-junction carbon nanotubes and silicon, doped with diluted HNO_3. They discovered that acid infiltration of nanotube networks reduces the internal resistance which leads to a substantial increase in the efficiency of silicon-carbon nanotube hetero-junction solar cells. They also pointed out that their presented fabrication process is significantly simplified, compared with the conventional silicon cells [16].

Meunier et al. [17] created several hetero-junction CNTs by connecting different homogeneous CNTs by insertion of pentagon–heptagon cells in the connection places. It was observed in their hetero-junction CNT creation that the kink, in the place of connection, causes a bending in the structure of hetero-junction CNTs. They also calculated and compared the energy of a pentagon–heptagon defect in the junction location (about 6 eV) with each of the corresponding individual tubes. Saito et al. [18] also employed pentagon and heptagon pairs to construct a three-dimensional model of hetero-junction CNTs through a projection method. According to their model, a three-dimensional dihedral angle was introduced by the kink in the connection place. They also discovered from the value of tunneling conductance for a metal–metal CN junction and a metal-semiconducting CN junction that the kinks in the hetero-junction CNT structure could function as the smallest semiconductor devices.

Xosrovashvili and Gorji [19] used the AMPS-1D device simulation tool to present a numerical simulation of a hybrid hetero-junction SWCNT and a GaAs solar cell by which they analyzed the physics and performances of their models with junction parameters. Eventually, they found that the electrical parameters of the system decreases by the increase in the concentration of a discrete defect density in the absorber layer.

Dunlap [20] connected different carbon tubules through two different connection approaches to create hetero-junction CNTs. First, he assumed different tubules with different helicities to be created by rolling a graphene ribbon with infinite length but finite width into an infinite set of tubes. Then, he connected every two CNTs by locating the obtained CNTs one after each other by translation and rotation to model hetero-junction CNTs. On the other hand, he modeled different hetero-junction tubules by connecting perfect infinite tubule halves by adding one pentagon and one heptagon pair in the connection places. It was revealed from the comparison among his models that the best way to model hetero-junction CNTs is to use pentagon–heptagon connections between sets of tubules in a pair-wise way which causes a bending angle in the kink location with an ideal bending angle of 30°.

Five three-dimensional models of straight hetero-junction CNTs