Solid State Communications 231-232 (2016) 36–42

Contents lists available at ScienceDirect

Solid State Communications

journal homepage: www.elsevier.com/locate/ssc

A refined finite element analysis on the vibrational properties of ideal and degenerated carbon nanostructures

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ARTICLE INFO

Article history:
Received 4 October 2015
Received in revised form
10 December 2015
Accepted 18 January 2016
Available online 5 February 2016

Keywords:
A. Carbon nanostructures
C. Microscopic modifications
D. Mechanical properties
E. Finite element analysis

ABSTRACT

Different types of degenerated nanostructures were simulated and their eigenfrequencies and corresponding eigenmodes were evaluated by applying the well-established finite element method. In addition, the structural and vibrational stability of these nanoparticles was examined under the influence of microscopic modifications. For this purpose, four common types of atomic defects (i.e. different types of vacancy defects, perturbation, pentagon–heptagon pair defect and chemical doping) were introduced to the finite element models and their vibrational properties were obtained and finally compared to those of perfect, i.e. defect-free, structures. The detailed geometry around a defected area was calculated based on density functional theory and implemented in the finite element model. Based on the results, it was shown that all these structural modifications changes the natural frequency and as a result, reduce the vibrational stability of degenerated nano-materials.

1. Introduction

Carbon nanotubes (CNTs) have been widely perceived as a very promising material for applications in nano-industry due to their superior physical, chemical and electrical properties [1–3]. It has been reported that mechanical properties (e.g. buckling, natural frequency, and Young's modulus) of nanotubes are dependent upon their structural details. This is caused by unavoidably introducing different types of macroscopic and microscopic imperfections during the growth or under electron irradiation, such as the pentagon and heptagon (5–7) pair defect, perturbation and atomic vacancies [4–7]. The investigations on the mechanical properties of CNTs and their modifications are increasing over the past few years in a way that much attention has been paid to the finite element method in order to examine the characteristics of these nanostructures. The results of some investigations on the vibrational characteristics and vibrational behavior of CNTs are presented.

1.1. Research work on perfect nanostructures

The vibrational behavior of single-walled carbon nanotubes (SWCNTs) was investigated by Kahaly and Waghmare [8] in 2008. By obtaining the correlation between eigenmodes of the tube and of the graphene sheet, they found how the rolling of the sheet results in a mixture between modes and changes in the vibrational spectrum of graphene sheets. Their conclusions demonstrated that the radial breathing mode softens with decreasing curvature. In 2009, Hashemnia et al. [9] examined the vibrational response of different types of single-layered graphene sheets and SWCNTs. They performed molecular mechanics simulations for armchair and zigzag CNTs with different boundary conditions. They derived several diagrams indicating the natural frequencies of CNTs and graphene sheets with respect to their aspect ratios. Based on their findings, it was pointed out that the fundamental frequency decreases as the aspect ratio increases. Therefore, it is preferred that these nano-configurations are applied with lower aspect ratios.

1.2. Research work on atomically defected nanostructures

A comprehensive study was conducted by Ebrahim Zadeh et al. [10] to investigate the effect of vacancy defects on the natural frequency of SWCNTs. In addition, the relation between the aspect

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http://dx.doi.org/10.1016/j.ssc.2016.01.015
0038-1098/

ratio and frequency of perfect and imperfect nanotubes, i.e., with removed carbon atoms, was investigated. They also examined the influence of varying the position of one defect along the length of the CNTs on the fundamental frequency of the nanotubes. In 2013, Espejel-Morales et al. [11] studied the vibrational behavior of SWCNTs pristine and doped with B or N. They carried out the electron localization function, electronic partial density of states, charge density, and band structures to investigate the impurity effects on the electronic models. They finally figured out the influence of impurities on the vibrational frequencies by evaluating the radial breathing mode.

Considering the previous studies on the behavior of carbon nanostructures, it should be noted that much more attention should be paid to the mechanical behavior of defected nano-configurations in order to predict the realistic behavior of these nanoparticles in a closer form to those found in reality. In the actual research, different types of microscopic defects (vacancy defects, perturbation) and functionalization (doping) are introduced to several CNTs and degenerated nanostructures and then the eigenfrequencies of these configurations and their corresponding eigenmodes are evaluated. The primary objective of the paper is to understand the influence of topological defects and functionalization modification on the vibrational properties of carbon nanostructures.

2. Materials and methods

2.1. Geometric definition and atomic defects

As illustrated in Fig. 1, all types of CNTs and degenerated nanostructures, including, CNTs, hetero-junctions, bucky-balls, nanocones and capped tubes are constructed of a graphene sheet. The diameter range of the CNTs is from 1 to 50 nm and lengths of over 10 μm. A homogenous CNT is viewed as a rolled graphene sheet with a specific width, while a hetero-junction CNT, treated as a wrapped graphene sheet with a specific geometry, is constructed by connecting two homogenous CNTs through the introduction of pentagon and heptagon pair defects into the connecting region. By connecting a half bucky-ball with the homogeneous CNTs, capped structures are simulated. Each simulated nanostructure has its specific geometry as well as outstanding mechanical behavior.

In realistic situations, different types of microscopic defects might be introduced to the nanostructures unavoidably. It has been reported that these impurities have a significant effect on the behavior of nano-materials [12–14]. Among all microscopic defects, there are some important impurities including, carbon vacancies, 5–7 pair defect, perturbation and chemical doping. The vacancy defect is categorized into different types including mono-, di-, tri-, and pinhole vacancies. All these topological and microscopic imperfections in the structure of graphene sheet are illustrated in Fig. 2.

2.2. Material parameters and boundary conditions

In the structure of a CNT, carbon atoms are bonded together by covalent bonds which have their particular lengths and angles in a three-dimensional space. It was supposed that CNTs, when subjected to loading, behave like space-frame configurations. Therefore, the bonds between carbon atoms are assumed as connecting load-carrying generalized beam members, while the carbon atoms act as joints of the member [15]. This idea is illustrated in Fig. 3.

The local geometry around a defective area was separately simulated and these refined results of the deformed geometry were implemented in the finite element model. The local areas around several defects in graphenic surfaces were modeled at the density functional theory (DFT) level, using the B3LYP functional and the 6–31G(d) basis set as implemented in Gaussian ® software [17]. The B3LYP/6–31G(d) provides reasonably good accuracy and has been recently applied to model graphene and 2D polymers [18]. Hydrogen-terminated graphene flakes (up to $C_{120}H_{30}$) with corresponding defects (5–7 pair defect, mono-, di-, tri- and pinhole vacancies) were used as the model systems. The highest possible symmetry was applied to each structure, and atoms were free to relax. For $C_{119}H_{30}$ (simulating the mono-vacancy) and $C_{117}H_{30}$ (simulating the tri-vacancy) molecular geometry was calculated for the triplet states which were found to be more stable than the singlets.

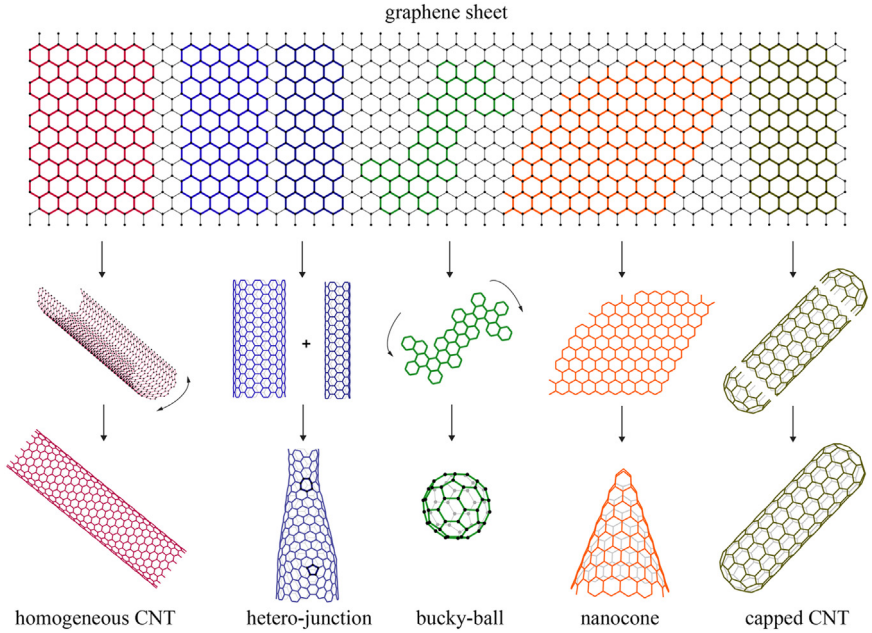

Fig. 1. Schematic of different allotropes of carbon materials. All these nano-configurations are constructed by graphene sheets.