Composites Part B 89 (2016) 155–168

Contents lists available at ScienceDirect

Composites Part B

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

Numerical simulation study of the elastic properties of single-walled carbon nanotubes containing vacancy defects

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ARTICLE INFO

Article history:
Received 17 July 2015
Received in revised form
21 October 2015
Accepted 4 November 2015
Available online 30 November 2015

Keywords:
A. Nano-structures
B. Defects
B. Mechanical properties
C. Finite element analysis (FEA)

ABSTRACT

The mechanical behaviour of non-chiral and chiral single-walled carbon nanotubes containing different percentage (up to 10%) and types of vacancy defects is studied under tensile, bending and torsional loading. A three-dimensional finite element model is used in order to evaluate the corresponding rigidities and, subsequently, Young's and shear moduli and Poisson's ratio. The three rigidities decrease with the increase of the percentage of vacancies. Also, the Young's and shear moduli and the Poisson's ratio of single-walled carbon nanotubes are sensitive to the presence of vacancy defects in nanotube: elastic moduli decrease and the Poisson's ratio increases with increasing of the percentage of vacancies. The moduli of single-walled carbon nanotubes with 10.0% of vacancy defects, when compared with the values obtained for perfect nanotubes, are of about 43% for the Young's modulus and of about 33% for the shear modulus. On the contrary, the Poisson's ratio increases of about 4 times, compared with that obtained for the perfect nanotube.

1. Introduction

Carbon nanotubes (CNTs) have attracted great research interest, because of their unparalleled mechanical, optical and thermal properties [1]. In spite of various experimental studies which have been carried out to evaluate the mechanical properties of CNTs, there is a scattering in the experimental results reported in the literature. Such inconsistency is due to complexity of the characterization of nanomaterials at the atomic scale. Another reason of the result's scattering can be associated with the existence of defects in the CNT structure: it is almost impossible to produce carbon nanotubes with a perfect structure because of the manufacturing constraints. It should be noted that the perfection of the lattice of the CNTs, used in experimental studies, has a significant influence on the results. Thus, the numerical simulation of the mechanical properties of carbon nanotubes with defects is an important task, providing data that can be compared with experimental results. The defects of CNT structure, such as single and multiple vacancies, show suitable effects for numerous applications of nanotubes, for example concerning the strength of nanocomposites when CNT vacancy defects act as interfacial bonding places, the storage of hydrogen and the transition of nanotubes from one diameter to another in carbon nanotube heterojunctions. The defects in the CNTs can appear mainly due to the chemical synthesis [2], the chemical treatment in the purification process [3], or when the CNTs are subjected to irradiation [4].

There are three main classes of theoretical approaches for the modelling of the CNTs mechanical behaviour: atomistic, continuum and nanoscale continuum approaches [5]. The atomistic approaches (for example, ab initio [6] and classical molecular dynamics (MD) [7,8]) have big computation costs. In consequence, they have been progressively replaced by the continuum mechanics-based approach (CM) where the real atomic CNT structure is replaced by a continuum medium (see, for example [9,10]). Such replacement of the whole CNT structure allows effective simulation, greatly reducing the computational effort, but does not provide sufficient accuracy in the evaluation of the CNT mechanical properties. Finally, the nanoscale continuum modelling (NCM) approach, where the carbon–carbon (C–C) bond is replaced by a continuum element (as truss, spring and beam) has led to accurate results, overcoming the disadvantages of the MD and CM approaches (see, for example [11–14]). Since Li and Chou [13] have

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http://dx.doi.org/10.1016/j.compositesb.2015.11.029
1359-8368/

linked the interatomic potential energies to the strain energies of an equivalent beam element and established a direct relationship between sectional stiffness parameters and the force field constants, the NCM approach using beam elements has been successfully used to simulate the mechanical behaviour of CNT [14–17].

In recent years, numerical studies regarding the effect of the defects on the CNT mechanical properties have been carried out. For example, concerning the elastic behaviour, Scarpa et al. [18], Parvaneh and Shariati [19], Parvaneh et al. [20], Rahmandoust and Ochsner [21], Ghavamian et al. [22], Ghavamian and Ochsner [23,24] and Poelma et al. [25] simulate the vacancy defects by removing the carbon atoms without reconstruction of the C–C bonds. The studies of Scarpa et al. [18], Parvaneh and Shariati [19] and Parvaneh et al. [20] relate to a few specific types of nanotubes and vacancies, and also relatively small percentages of defects (less than 2.5%). Reduction of the Young's modulus was observed in nanotubes with defects, although it is insignificant in some cases. The studies of Rahmandoust and Ochsner [21], Ghavamian et al. [22] and Ghavamian and Ochsner [23,24] showed that the presence of 0.5 and 1.0% of the vacancy defects in the armchair and zigzag single-walled and multi-walled CNTs leads to the significant decrease of the CNT Young's modulus [21,22], natural frequency [23] and critical buckling load [24] with an approximately linear trend. Poelma et al. [25] found that the position of the single vacancy defect significantly influences the critical buckling load of the single-walled carbon nanotubes at the low temperatures. For studying the fracture behaviour, some authors [26,27] have chosen to rebuild the C–C bonds around the removed atoms. Among their findings, it should be pointed a substantial reducing of the nanotube strength. In summary, with regard to parameters such as rigidity, elastic modulus and Poisson's ratio, only the influence of vacancy defects on the elastic modulus has received main analysis so far, although limited to a few types of single-walled carbon nanotubes.

This study aims to contribute towards the study of the mechanical behaviour of single-walled carbon nanotubes (SWCNTs) containing different percentage and type of vacancy defects, using the NCM approach implemented with beam elements. Three dimensional finite element method was used in order to evaluate the tensile, bending and torsional rigidities, and subsequently, Young's and shear moduli and Poisson's ratio of various SWCNTs, as non-chiral (zigzag, $\theta = 0°$, and armchair, $\theta = 30°$) and three families of chiral ($\theta = 8.9°$; $13.9°$; $19.1°$) SWCNTs, for a wide range of chiral indices and diameters. The current systematic study allows improving the information concerning the influence of the presence and density of the vacancy defects on the SWCNTs mechanical properties, in order to better understanding the scattering generally observed in experimental results.

Table 1
Geometrical characteristics of SWCNTs studied and number of nodes and elements of the finite element meshes used (nanotube length 20 nm).

SWCNT type		(n, m)	D_n, nm	$\theta°$	Number of nodes	Number of elements
Non-chiral	Armchair	(5, 5)	0.678	30	1620	2414
		(10, 10)	1.356		3240	4829
		(15, 15)	2.034		4860	7244
		(20, 20)	2.713		7640	11,420
	Zigzag	(5, 0)	0.392	0	930	1384
		(10, 0)	0.783		1860	2769
		(15, 0)	1.175		2790	4154
		(20, 0)	1.566		3720	5539
		(35, 0)	2.740		7420	11,095
Chiral	Family $\theta = 8.9°$	(5, 1)	0.436	8.9	1044	1554
		(10, 2)	0.872		2088	3109
		(15, 3)	1.308		3132	4664
		(20, 4)	1.744		4176	6219
		(25, 5)	2.180		5220	7774
		(30, 6)	2.616		6264	9329
	Family $\theta = 13.9°$	(6, 2)	0.565	13.9	1352	2013
		(9, 3)	0.847		2028	3020
		(12, 4)	1.129		2740	4027
		(15, 5)	1.412		3380	5034
		(18, 6)	1.694		4056	6041
		(21, 7)	1.976		4732	7048
		(24, 8)	2.259		5408	8055
		(27, 9)	2.541		6084	9062
	Family $\theta = 19.1°$	(4, 2)	0.414	19.1	992	1477
		(6, 3)	0.622		1488	2216
		(8, 4)	0.829		1984	2955
		(10, 5)	1.036		2840	3694
		(12, 6)	1.243		2976	4433
		(14, 7)	1.450		3472	5172
		(16, 8)	1.657		3968	5911
		(18, 9)	1.865		4464	6650
		(20, 10)	2.072		4960	7389
		(22, 11)	2.279		5456	8128
		(24, 12)	2.486		6504	9720

2. Materials and methods

2.1. Atomic structure of SWCNTs

The symmetry of the atomic structure of SWCNTs is characterized by the chirality, which is defined by the chiral vector $\boldsymbol{C_h}$ [28]:

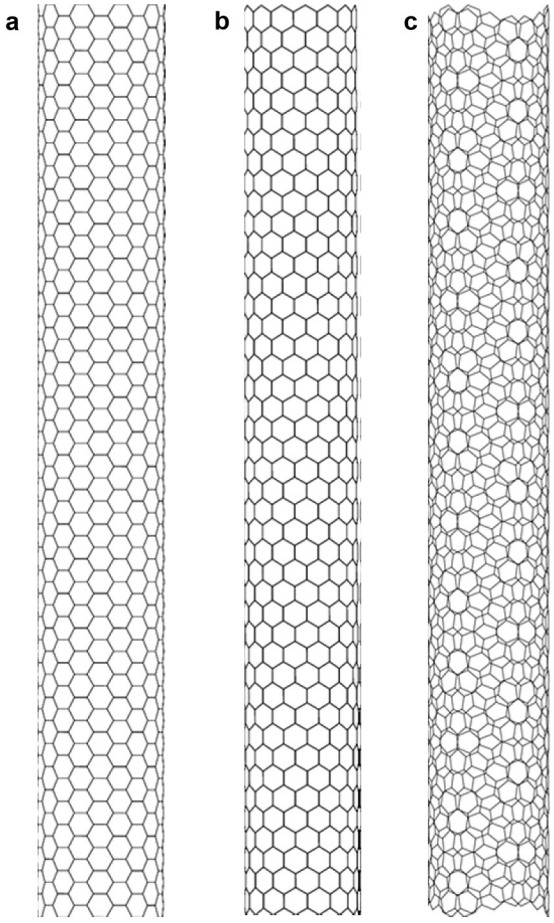

Fig. 1. FE meshes of SWCNTs: (a) armchair (10, 10), (b) zigzag (15, 0) and (c) chiral (15, 3).