Composites Part B 75 (2015) 73–85

Contents lists available at ScienceDirect

Composites Part B

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

Mechanical characterization of single-walled carbon nanotubes: Numerical simulation study

N.A. Sakharova [a, *], A.F.G. Pereira [a], J.M. Antunes [a, b], C.M.A. Brett [c], J.V. Fernandes [a]

[a] CEMUC – Department of Mechanical Engineering, University of Coimbra, Rua Luís Reis Santos, Pinhal de Marrocos, 3030-788 Coimbra, Portugal
[b] Escola Superior de Tecnologia de Abrantes, Instituto Politécnico de Tomar, Rua 17 de Agosto de 1808, 2200 Abrantes, Portugal
[c] CEMUC – Department of Chemistry, University of Coimbra, Rua Larga, 3004-535 Coimbra, Portugal

ARTICLE INFO

Article history:
Received 18 September 2014
Received in revised form
30 November 2014
Accepted 13 January 2015
Available online 29 January 2015

Keywords:
A. Nano-structures
B. Elasticity
B. Mechanical properties
C. Finite element analysis (FEA)
Young's modulus

ABSTRACT

The mechanical behaviour of non-chiral and chiral single-walled carbon nanotubes under tensile and bending loading conditions is investigated. For this purpose, three-dimensional finite element modelling is used in order to evaluate the tensile and bending rigidities and, subsequently, the Young's moduli. It is shown that the evolution of rigidity, tensile and bending, as a function of diameter can be described by a unique function for non-chiral and chiral single-walled nanotubes, i.e. regardless of the index or angles of chirality. A comprehensive study of the influence of the nanotube wall thickness and diameter on the Young's modulus values is also carried out. It is established that the evolution of the Young's modulus as a function of the inverse of the wall thickness follows a quasi-linear trend for nanotubes with diameters larger than 1.085 nm. The current numerical simulation results are compared with data reported in the literature. This work provides a benchmark in relation to ascertaining the mechanical properties of chiral and non-chiral single-walled carbon nanotubes by nanoscale continuum models.

1. Introduction

Carbon nanotubes (CNTs) are nanostructures attracting research interest due to their extraordinary mechanical, optical, thermal and electrical properties [1]. The CNTs outstanding physical properties such as strength and lightness enable applications in numerous different fields: chemistry, physics, engineering, materials science. From the point of view of structural application, the high stiffness together with low density indicates use of the CNTs as nanoscale fibres for reinforcement of nanocomposite structures (see, for example, [2–4]). This type of application of carbon nanotubes has required the investigation of their mechanical properties, including their deformation behaviour under different loading conditions.

There are two approaches commonly used to study the mechanical properties and deformation behaviour of CNTs: experimental and computational. For single-walled and multi-walled CNTs, methods for measuring Young's modulus based on *in situ* atomic force microscopy (AFM) and transmission electron microscopy (TEM) techniques have been established [5,6]. Although various experimental studies have been carried out to evaluate the mechanical properties of CNTs, there is inconsistency in the experimental results reported in the literature, owing to the complexity of the characterization of nanomaterials at the atomic scale. The common point in the experimental studies is the evidence of the unparallelled mechanical properties of CNTs. Concerning the accuracy of the values of the CNT mechanical properties that are determined, experimental studies still show a wide scatter of their values. From this point of view, computer simulation for predicting the mechanical properties of CNTs has been considered as a powerful tool, due to the experimental difficulties.

The theoretical approaches for the modelling and characterization of the CNTs behaviour can be divided into three main categories: the atomistic approach, the continuum approach and the nanoscale continuum approach. A comprehensive critical review concerning the modelling of the mechanical behaviour of carbon nanotubes has been undertaken by Rafiee and Moghadam [7]. Hereinafter, a brief assessment of main modelling methodologies is carried out.

Atomistic modelling, used solely during the first years of theoretical studies on CNTs, calculates the positions of atoms based on their interactive forces and boundary conditions (see, for example [8]). Atomistic modelling comprises an *ab initio* approach [9] and

* Corresponding author. Tel.: +351 239790747.
E-mail address: nataliya.sakharova@dem.uc.pt (N.A. Sakharova).

http://dx.doi.org/10.1016/j.compositesb.2015.01.014
1359-8368/

molecular dynamics (MD) [10–14]. After this, other atomistic modelling methods, such as tight-binding molecular dynamics (TBMD) [15,16] were developed.

Generally, *ab initio* methods give more accurate results than MD, but they are computationally expensive and only possible to use for a small number of molecules or atoms. Molecular dynamics can be used in large systems and provide good predictions of CNT mechanical properties under different loading conditions, but it is still limited owing to its being very time consuming, especially when long or multi-walled CNTs are simulated. In recent years, the atomistic approaches, due to their big computation cost, have been gradually replaced by continuum approaches, which are at the moment the most indicated for effective computational simulation of large systems.

The basic assumption of the continuum mechanics-based approach consists of the modelling of CNTs as a continuum structure, concerning the distribution of mass, stiffness, etc., i.e. the real discrete structure of the nanotubes is neglected and replaced by a continuum medium. Some authors have explored continuum shell modelling for studying the mechanical behaviour of CNTs [17–20]. However, the atomic characteristics of carbon nanotubes, such as chirality, are not taken into account in the continuous shell approach, and so their effects on the mechanical behaviour of CNTs cannot be captured. To overcome this obstacle, Chang proposed an anisotropic shell model for SWCNTs [21] that can predict some anisotropic effects related to chirality. Besides shell structures, other continuum structures, such as tubes and plates, are employed in continuum approaches. In the models of Sears and Batra [22], and Gupta and Batra [23] the whole single-walled CNT structure was simulated as an equivalent continuum tube. Wang [24] employed the equivalent elastic plate model. Arash and Wang [25] show the advantages of the continuum theory applied to the modelling of shells and plates. However, whatever the type of the continuum modelling approach, the replacement of the whole CNT structure by a continuum element is not a completely satisfactory method to evaluate CNT properties.

The nanoscale continuum modelling (NCM) consists of replacing the carbon–carbon (C–C) bond by a continuum element. As a result, continuum mechanics theories can be used at the nanoscale, i.e. a linkage between molecular configuration and solid mechanics is recognized. NCM is frequently accomplished by finite element modelling. The main approach in NCM consists of considering different elements, such as rod, truss, spring and beam, well described in elasticity theory, to simulate C–C bonds (see, for example, [26–29]). The first NCM model of CNTs was developed by Odegard et al. [26] and consisted of a continuum truss model. The disadvantage of the truss model is the impossibility of describing the CNT mechanical behaviour under torsional load, because the out-of-plane torsion of the C–C bond cannot be taken into account.

Various FEM models where the C–C bonds are simulated using diverse kinds of elastic spring element, such as linear, non-linear, rotational, torsional, have been recently reported [30–37]. Although the use of spring elements is an effective way for simulation of the bond angle variations, the accuracy of the Young's modulus results depends on the choice of the potential function for the calculation of the force constants.

Since Li and Chou [27] 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, equivalent beam approaches have been successfully used to simulate the mechanical behaviour of CNT, although with different formulations of the inter-atomic molecular potential energies and boundary conditions [28,38–43]. The FE models, which employed beam elements in a three-dimensional (3D) space, developed by Tserpes and Papanikos [26], Papanikos et al. [38] and Avila and Lacerda [39] differ from each other mainly due to the boundary conditions and the method for the Young's modulus calculation. The recent 3D FE model of Lu and Hu [42] used the same formulation for potential energy of covalent system, but considering an elliptical cross-section area of equivalent beam. In another analytical approach developed by Shokrieh and Rafiee [40], the deformations of beam elements were obtained using Castigliano's theorem. In the works of Her [41] and Mohammadpour [43] the modified Morse potential function for the potential energy of the covalent system used to describe non-linear behaviour of C–C bonds was applied. It can be concluded from these studies that nanoscale continuum modelling (NCM) is an adequate modelling technique for predicting CNT mechanical properties and shows results in close agreement with those obtained from MD modelling.

In the present study, the equivalent beam approach is used in order to evaluate the tensile and bending rigidities and, subsequently, Young's modulus of various single-walled carbon nanotubes (SWCNT) structures, as non-chiral (zigzag, $\theta = 0°$, and armchair, $\theta = 30°$) and families of chiral ($\theta = 8.9°; 13.9°; 19.1°$ among others) SWCNTs for a wide range of chiral indices, nanotube length and diameter. A comprehensive study of the influence of the nanotube wall thickness and diameter on the Young's modulus results was carried out. Moreover, the present work provides a benchmark in relation to ascertaining the mechanical properties of chiral and non-chiral SWCNTs by nanoscale continuum models.

2. Materials and methods

2.1. Atomic structure of SWCNTs

A simple way to describe an SWCNT is as a rolled-up graphene sheet giving rise to a hollow cylinder, the surface of which is composed of hexagonal carbon rings (see, for example [44,45]). The hexagonal pattern is repeated periodically, leading to binding of each carbon atom to three neighbouring atoms by covalent bonds. A schematic illustration of an unrolled hexagonal graphene sheet is shown in Fig. 1. The symmetry of the atomic structure of SWCNTs is characterized by the chirality, which is defined by the chiral vector $\boldsymbol{C_h}$:

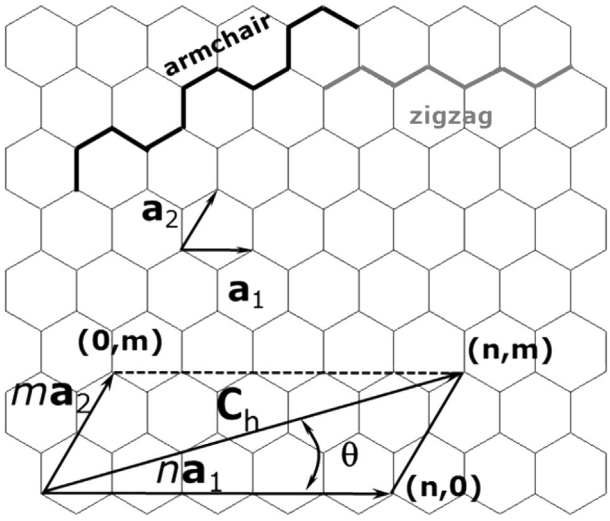

Fig. 1. Schematic illustration of an unrolled hexagonal graphene sheet with definition of chiral vector.