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On a thickness free expression for the stiffness of carbon nanotubes

Ghasem Ghadyani [a,*], Andreas Öchsner [b,c]

[a] Department of Solid Mechanics and Design, Faculty of Mechanical Engineering, University Technology Malaysia—UTM, 81310 UTM Skudai, Johor, Malaysia
[b] School of Engineering, Griffith University, Gold Coast Campus, Southport 4222, QLD, Australia
[c] School of Engineering, The University of Newcastle, Callaghan 2308, NSW, Australia

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ABSTRACT

A new expression for the stiffness of single-walled carbon nanotubes has been developed in this study. Three general models of single-walled carbon nanotubes (i.e., armchair, zigzag and chiral) have been used to define thickness free expressions of the nanotubes. The best curve fitting function has been obtained to describe the relation between the single-walled carbon nanotubes thickness and its stiffness. The coefficients of all three equations represent the circumferential-specific modulus. Furthermore, the stiffness of single-walled carbon nanotubes which is calculated by substitution of different assumptions for the thickness into the equations is in good agreement with the results of previous studies. The main purpose of this study is to characterize the stiffness of single-walled carbon nanotubes, based on different thickness assumptions. The focus in this study was on single-walled carbon nanotubes. Based on the structures of nanomaterials, this method can be easily applied to other atomic structures. Thickness- free expression which is studied here is in good agreement with quantum/continuum mechanics.

1. Introduction

Over the last decade, carbon nanotubes have gained a lot of interest among researchers mainly because of their exclusive properties. Carbon nanotubes (CNTs) have an extensive variety of capacities for scientific and engineering applications because of their outstanding physical, electrical and mechanical properties and geometrical specifications, such as small diameter and a high aspect ratio. It has been revealed that the dispersion of a few weight fractions of nanotubes in a matrix intensely leads to an increase of electrical, thermal and mechanical properties of composite materials [1–9].

Numerous experimental studies have been performed to determine the mechanical properties of CNTs. However, they show highly different results due to differences in the experimental methods used [1,10–13]. The variety in the reported empirical values is mainly because of the lack of proper direct measuring techniques at the nanometer scale [14].

There are many theoretical (i.e., analytical and numerical) studies employing different methods to investigate and predict the Young's modulus of carbon nanotubes. The theoretical methods can be divided into two major classes: The atomistic methods and the continuum mechanics approaches [8]. The atomistic modeling methods can be categorized into different classes. The first technique used for simulating the behavior of single-walled carbon nanotubes (SWCNTs) is the molecular dynamics (MD) method which is based on inter-atomic potential functions (force fields) to calculate the total energy of a system of particles [15]. The Monte Carlo (MC) simulation method [16], ab initio calculations [17], tight bonding molecular dynamics simulation (TBMD) [18], local density approximation (LD) [19], density functional theory (DFT) [20], Morse potential function model [21,22], and modified Morse potential function model [23,24] are other techniques employed by different scientists. Newton's second law is the main concept of MD and MC simulation methods and the accurate solution of the Schrödinger equation is the major concept of ab-initio methods [25]. In contrast, the MD and MC methods depend on the fact that the forces acting on atoms are acquired by differentiating interatomic potential functions [24].

The size-dependence of elastic properties of SWCNTs has been carefully investigated by different researchers [25–29]. Toshiaki in 2004 developed an algorithm based on an analytical approach and presented formulas for predicting the Young's modulus of SWCNTs. This estimation of stiffness properties agreed logically with the presented experimental and numerical predictions [28]. Chang in 2004 developed closed-form expressions based on an analytical molecular mechanics approach with the concept of the molecular force field and reported size dependent equations of the elastic modulus of carbon nanotubes [25].

* Corresponding author. Tel.: +60 1111605390.
E-mail addresses: g.ghadyani.g@gmail.com (G. Ghadyani), andreas.oechsner@gmail.com (A. Öchsner).

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Guo et al. predicted size-dependent mechanical properties of carbon nanotubes by using the continuum nanoscale theory, including the second order deformation gradient tensor in the kinematic description. Their method can be applicable to other nano-film materials, such as BN and BC3 [30]. Arroyo and Belytschko have employed hyper-elastic membrane models with an extension of the Born rules which leads to a reduction costs of the computational procedures for wide and long nanotubes [31]. Guo and Zhang studied the bending stiffness of SWCNTs by the combination of the deformation mapping method and the molecular mechanics model. Their study shown that the bending stiffness of SWCNTs is almost related to the cube of the tube radius [32].

Wang et al. have been employed a nanoscale quasi-continuum (QC) with utilized higher order Cauchy–Born rule as a linkage between the deformation of the spectrin and the corresponding equivalent continuum [33].

Most of the theoretical research values for the stiffness depend on the thickness assumption. Yakobson et al. by using a molecular dynamics simulation reported 5.5 TPa with a thickness assumption of 0.066 nm [34]. Zhou et al. have employed the tight-binding model and reported a Young's modulus around 5.1 TPa for an effective wall thickness of 0.074 nm which is calculated from strain energies in straight and bent SWCNTs [35]. Kudin et al. by using ab initio computations predicted the stiffness of SWCNTs to be around 3.859 TPa and obtained 0.075 nm as an effective wall thickness [4]. Pantano et al. developed a continuum shell model which predicted the stiffness of 4.48 TPa with a 0.075 nm thickness assumption [36]. Tu and Ou-Yang used a local density approximation model with the same assumption for the effective thickness and predicted the Young's modulus to be around 4.7 TPa [37]. Jalalahmadi and Naghdabadi by using the Morse potential energy predicted a stiffness around 3.4 TPa. Their assumption for the SWCNTs thickness was the cross section of the beam element for the C–C bond which was 0.1296 nm. They also emphasized the need to perform a parametric study for the thickness dependency [38]. The cross section of a beam element for C–C was also used by Tserpes and Papanikos as the effective structure thickness of SWCNTs. They predicted Young's modulus to be around 2.4 TPa with 0.147 nm as an effective thickness [39].

A large number of researchers used the thickness of a graphene sheet (0.34 nm) as the thickness of SWCNTs [40–43]. Lu, by using an experimental force-constant model reported Young's modulus of SWCNTs around 0.97 TPa [1]. His assumption for the effective thickness was 0.34 nm. Rahmandoust and Öchsner by using 0.34 nm as the effective thickness for SWCNTs, investigated the effects of atomic defects (carbon vacancy and doping with Si atoms), and predicted the stiffness in the range of 1.034 to 1.042 TPa [41]. Also, Ghadyani et al. [40], with a thickness of 0.34 nm, presented the effect of the transverse shear contribution using two different beam elements (i.e., Bernoulli and Timoshenko) to predict the Young's modulus. They estimated a stiffness of 1 TPa for the Bernoulli beam and 0.8 TPa for the Timoshenko beam elements [40]. Hernandez et al. with the assumption of 0.34 nm as the effective wall thickness have used the tight binding molecular dynamics method. The Young's modulus was predicted as 1.24 TPa [44]. Jin and Youan in another molecular dynamics simulation, predicted a stiffness of 1.35 TPa for an effective thickness of 0.34 nm [45]. In order to define the effect of the wall thickness on the stiffness, Tserpes and Papanikos [39], have employed 3D elastic beams for estimating the Young's modulus of SWCNTs by using the finite element method and represented the influence of differing wall thickness and chirality on the stiffness. They also predicted the Young's modulus to be between 0.517 TPa and 5.342 TPa based on a thickness in the range of 0.066 nm to 0.69 nm [39].

However, according to the above literature review and based on the approaches of Tserpes and Papanikos [39] and Jalalahmadi and Naghdabadi [38] approaches, the lack of any parametric study for predicting the Young's modulus with different thickness assumptions motivated the authors to start this research. The main aim of this study was to develop for the first time a thickness free expression based on numerical results. The development of a thickness dependent algorithm relating the thickness of SWCNTs and the Young's modulus of zigzag, armchair and chiral nanotubes was another motivation of this study. A further motivation of this study was to

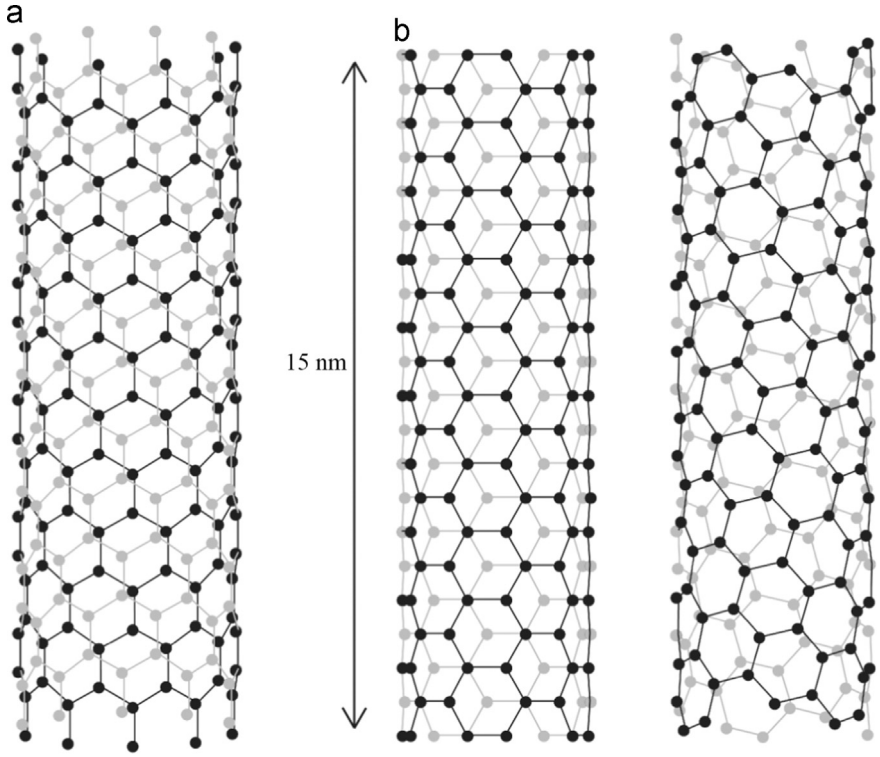

Fig. 1. Atomic structure of the carbon nanotubes with length of 15 nm: (a) armchair (5, 5), zigzag (10, 0), chiral (7, 3).