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On the characterization of the elastic properties of asymmetric single-walled carbon nanotubes

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ABSTRACT

In order to characterize asymmetric single-walled carbon nanotubes, an algorithm has been developed based on numerical simulation to relate the physical geometry to the elastic properties of asymmetric single-walled carbon nanotubes (SWCNTs). A large number of finite element results for the stiffness of asymmetric SWCNTs has been used to develop a best surface fitting function to define the relationship between the geometry of SWCNTs and their stiffness. However, since the stiffness of asymmetric nanotubes depends upon the configuration parameters, n and m, it was impossible to define any diameter dependency. Based on the maximum reaction force concept and in order to account for the hidden mechanical behavior of asymmetric SWCNTs, the chiral factor (CF) has been employed in this study. The proposed CF converts any asymmetric geometry (n and m) into a value between 0 and 1. A group of the SWCNTs with the same applied boundary condition ($n+m=30$) and different range of the CF was also used for studying of the shear contribution. The chiral factor dependency, which is developed in this study, is applicable for characterising and selecting asymmetric SWCNTs in the design of advanced nanomaterials. Furthermore, the equation which is calculated in this study can be useful for finding the best criteria for selecting asymmetric SWCNTs.

1. Introduction

After the initial report by Ijima in 1991 about the observations of carbon nanotubes, these structures were investigated by researchers from different angles mainly because of some unique properties [1]. There are numerous experimental works reporting various elastic moduli for carbon nanotubes. Empirical methods for estimating the mechanical characteristics of SWCNTs are mostly supported by atomic force microscopy (AFM) and transmission electron microscopy (TEM). Treacy et al. have employed TEM for a variety of multi-walled carbon nanotubes (MWCNTs) in the prediction of thermal vibration and have reported a Young's modulus ranging between 0.4 and 4 TPa. They also found that the stiffness and diameter of MWCNTs have an inverse relation [2]. Krishnan determined the Young's modulus by thermal vibration and reported this modulus to be in the range of 0.8–1.7 TPa [3]. Tensile testing is another experimental method use by Yu et al. who reported Young's modulus in the range of 0.27–0.95 TPa [4]. The cantilever bending method was another method used by Wong reporting large variations of the Young's modulus ranging between 0.68 TPa and 1.88 TPa [5]. Although Lu in 1997, by using an empirical force constant method, has showed that the stiffness and shear modulus increases smoothly with increasing difference between n and m for the chiralities (5,5), (6,4), (7,3), (8,2), (9,1) and (10,0) respectively. Furthermore, he reported an equal Young's modulus (0.972 TPa) and shear modulus (0.457 TPa) for the chiralities (50,50), (100,100) and (200,200) [6].

Size-dependence of the elastic properties of SWCNTs has been carefully investigated by different researchers [7–12]. The numerical approach has been recently accepted to determine the different mechanical properties of SWCNTs in numerous studies. A three-dimensional finite element model has been employed by Tserpes and Papanikos based on the concept that SWCNTs under loading behave like a beam structure. They predicted an average of the Young's modulus and shear modulus of 1.04 TPa and 0.46 TPa, respectively [13]. Ghadyani and Öchsner [14] employed the finite element approach using beam elements to characterize symmetric and asymmetric SWCNTs, based on the sum of the reaction forces. They also introduced a physical factor (CF) which has the

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capability to calculate asymmetric SWCNTs with respect to symmetric SWCNTs with high accuracy. The nonlinear structural response based on the deformation of single and multi-walled carbon nanotubes using a shell theory was predicted by Pantano et al. [15]. Thickness-free expressions have been employed for the stiffness of SWCNTs by Ghadyani and Öchsner [16]. They derived close form equations for predicting the stiffness of SWCNTs with different thickness assumptions which was in good agreement with continuum/quantum mechanics.

Most of the investigations on the mechanical properties of SWCNTs concentrate on continuum models using elasticity theory in order to adjust various practical potentials and simulation results. Despite the variety of theoretical investigations on the macroscopic elastic behavior of SWCNTs, Jin in 2003, inspected in fine detail the elastic behavior of SWCNTs under different deformation modes (using force and energy approach) for armchair nanotubes and determined different values for the same SWCNTs [17]. Cheng in 2009 studied SWCNTs of different radii and two diverse chiralities, including zigzag and armchair with implications for the surface effect by an atomistic-continuum model and distinguished that the Young's modulus of SWCNTs was raised by 17–23% in comparison to experimental data [18]. Ghadyani et al. in 2014, presented the effects of the transverse shear contribution using two different beam elements (i.e., Bernoulli and Timoshenko) to predict the Young's modulus. They also investigated the buckling behavior of carbon nanotubes with different chirality values and predicted values of the Young's modulus around 1 TPa for Bernoulli beam and around 0.8 TPa for Timoshenko beam elements [19].

Toshiaki in 2004 developed an algorithm based on an analytical approach and presented formulas for predicting the Young's modulus of SWCNTs. This estimation on stiffness properties agreed logically with the present experimental and numerical predictions [20]. Xiaoa et al. have employed an analytical molecular approach model based on the modified Morse potential for the estimation of stiffness of the carbon nanotubes [21]. Chang and Gao, developed closed-form expressions based on an analytical molecular mechanics approach with the concept of the molecular force field and reported size dependence equations of the elastic modulus of carbon nanotubes [7]. With an analytical approach, Popov and Doren have made estimations in their study on the effects of chirality on the mechanical properties of SWCNTs using a dynamic model for 23 asymmetric nanotubes [22]. WengXing et al. employed molecular dynamics simulation by a second generation reactive empirical bond order (REBO) potential and estimated the stiffness to be around 0.9 TPa for all configurations. They predicted a lower value of stiffness for chiral SWCNTs when compared with armchair and zigzag SWCNTs [23]. Fang et al. developed a closed-form expression of armchair tubes based on the criteria $(\cos(30^\circ - \theta))$ to predict the surface Young's moduli for chiral single-walled carbon nanotubes (SWCNTs). They also found that both the diameter and chiral angle can affect the surface Young's moduli of chiral nanotubes [24]. Zhang et al. (2007) developed closed-form expressions for the surface Young's modulus and the Poisson's ratio of achiral and chiral carbon nanotubes. Their results showed that the stiffness of SWCNTs depends on both diameter and chirality [25]. A five independent variables algorithm was introduced by Ye et al. in 2009 for the prediction of the elastic properties of SWCNTs via a molecular mechanics approach. In order to solve some errors, they introduced two modified methods by analysing the features of the final governing equations [26]. A closed-form expression for the stiffness and Sear modulus of symmetric and asymmetric SWCNTs has been predicted by Chang [27]. He reported an average of 0.49 TPa and 1.2 TPa for the Shear modulus and the stiffness.

Hernandez (1998) by using a non-orthogonal tight-binding formalism reported 1.24 TPa for chiral SWCNTs [28]. Popov and Doren (2000), by using Born's perturbation method calculated the stiffness for all the configurations [22]. Meo and Rossi (2004) reported the stiffness of chiral and achiral SWCNTs to be around 0.9 TPa based on the nonlinear and torsional spring elements [29]. Ávila and Lacerda (2008) by using a molecular mechanics approach evaluate the stiffness of SWCNTs for armchair, zigzag and chiral nanotubes [30]. Based on the molecular mechanics approach, Lu and Hu improved a 3D finite element model for armchair, zigzag and chiral single-walled carbon nanotubes (SWNTs) by considering an elliptical cross-section for the beam elements. Their prediction value for chiral SWCNTs was lower than other standard configurations (i.e,. zigzag and armchair) [31]. In the most recent study by Sakharova et al. (2015), an equivalent beam element has been used in order to carry out a systematic evaluation of the tensile and bending rigidities. They reported the stiffness to be in range of 1.07–2 TPa [32].

However, according to the literature and based on the different approaches for the chiral SWCNTs which is studied by Fong (2007), Sakharova (2015) and Chang (2010), both the diameter and chirality (n and m) can effect on the Young's moduli simultaneously. The main aim of this study is to develop a simple factor to characterise and simplify the definition of stiffness for asymmetric SWCNTs. In this study, the stiffness of SWCNTs is obtained from the maximum reaction force which is calculated from Eq. (13). According to this study, the ranges of variation of the stiffness and shear modulus for asymmetric configurations have an average of 1.2 TPa and 0.484 TPa, respectively.

2. Research methodology

2.1. Physical and geometrical structure of carbon nanotubes

In the structural analysis of SWCNTs, a single graphene sheet is rolled along a specific vector to form a cylinder creating the SWCNTs in the range of nanometres. These hollow structures have lengths over 10 mm with diameters ranging from 1 to 50 nm [33]. The physical structure of a general nanotube is described by its diameter (d_t) and chiral angle (θ) as represented in Fig. 1. The chiral vector $\vec{Ch}$ is defined by $\vec{a}_1$ and $\vec{a}_2$ as basic vectors with an angle of 60° between them:

$$\vec{Ch}=n\vec{a}_1+m\vec{a}_2 \tag{1}$$

The angle between $\vec{Ch}$ and the zigzag axes ($\vec{a}_1$) is most commonly known as the chiral angle, θ, and can be computed as follows:

$$\cos(\theta)=\frac{2n+m}{2\sqrt{n^2+m^2+nm}} \tag{2}$$

The length of the chiral vector (L) can be directly defined by (n, m) and related to the diameter (d_t).

$$d_t=\frac{L}{\pi}=\frac{a_0\sqrt{m^2+mn+n^2}}{\pi} \tag{3}$$

where $a_0=\sqrt{3}\,b$ and b = 0.142 nm is known as the length of the C–C bond [14,33].

There are many symmetric equations defining geometrical and physical properties of carbon nanotubes. These equations have mostly been generated by Dresselhaus et al. [33]. According to their work, based on the relation derived for symmetric groups, there are three basic types of carbon nanotubes (i.e., zigzag, armchair and chiral), clearly defined with respect to the chiral vector and chiral angle of the rolled up single graphene sheet. For a general nanotube with a chiral angle in the range of $(0^\circ < \theta < 30^\circ)$