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Analytical prediction of Young's modulus of carbon nanotubes using a variational method

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ABSTRACT

Molecular mechanics and solid mechanics are linked to establish, a nanoscale analytical continuum theory for determination of stiffness and Young's modulus of carbon nanotubes. A space-frame structure consisted of representative unit cells has been introduced to describe the mechanical response of carbon nanotubes to the applied loading. According to this assumption a novel unit cell, given the name mechanical unit cell here is introduced to construct a graphene sheet or the wall of the carbon nanotubes. Incorporating the Morse potential function with the strain energy of the mechanical unit cells in a carbon nanotube is the key point of this study. The structural model of the carbon nanotube is solved to obtain its Young's modulus by using the principle of minimum total potential energy. It was found that the Young's modulus of the zigzag and armchair single-walled carbon nanotubes are 1.42 and 1.30 TPa, respectively. The results indicate sensitivity of the stiffness and Young's modulus of carbon nanotubes to chirality but show no dependence on its diameter. The presented analytical investigation provides a very simple approach to predict the Young's modulus of carbon nanotubes and the obtained results are in good agreement with the existing experimental and theoretical data.

1. Introduction

Following the discovery of carbon nanotubes (CNT) in early 1990s by Iijima [1], CNTs have been the subject of numerous studies due to their very distinct properties. CNTs are recognized to possess extraordinary characteristics and exceptional properties that have drawn great deal of attention in scientific communities. These outstanding properties including high stiffness-to-weight and strength-to-weight ratios, low density, and remarkable electrical and thermal conductivity have stimulated a large number of researches to focus on CNTs and explore their characteristics and potential technological applications [2,3].

Various experimental techniques including atomic force microscopy (AFM), transmission electron microscopy (TEM), scanning electron microscopy (SEM), and Raman spectroscopy have been employed for direct measurement of the Young's modulus of CNTs. In spite of the significant scatter in the reported data, the Young's modulus of CNTs lies on the order of 1 TPa [4–8].

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Nomenclature

m,n	chiral index
L	CNT length
C_h	chiral vector
a_1,a_2	primitive vectors of the Bravais lattice
r_0	C–C bond equilibrium length
d	CNT diameter
Θ	helicity angle
V_r	bond stretching potential
V_Θ	bond angle bending potential
D_e	dissociation energy
β	fitting parameter
k_Θ	bending stiffness
F_r	Morse force
M_Θ	Morse torque
b	hexagon diameter
F_b	internal force of a diagonal bar
A_0	cross sectional area of bar members
σ	stress
ε	strain
E_r	Young's modulus of the side members
E_b	Young's modulus of the diagonal members
U_{MUC}	total strain energy of MUC
e_i	bar extension
n_z	number of MUCs in a zigzag CNT
$U_{Z\text{-}CNT}$	total strain energy of a zigzag CNT
x,y,z	displacement components
X	longitudinal displacement of CNT
V	potential energy of the external force
Π	total potential energy
K_{Zig}	longitudinal stiffness of a zigzag CNT
A_{CNT}	cross sectional area of CNT
t	CNT wall thickness
E_{Zig}	Young's modulus of a zigzag CNT
n_a	number of MUCs in an armchair CNT
$U_{A\text{-}CNT}$	total strain energy of an armchair CNT
E_{Arm}	Young's modulus of an armchair CNT
K_{Arm}	longitudinal stiffness of an armchair CNT

Computational simulation and analytical modeling are other options in nanoscience to prevail the difficulties of experimental methods. Atomistic simulations and molecular methods fall in this category which can be studied based on both classical and quantum mechanics. Jin and Yuan [9] carried out molecular dynamics (MD) simulations to find elastic moduli of many armchair CNTs. Liew et al. [10] used MD simulation to study elastic and plastic behavior of CNTs under axial tension. They also investigated the effect of defect and length-to-diameter ratios on mechanical properties of CNTs. WenXing et al. [11], by employing MD simulations calculated Young's Modulus for many CNTs with different geometries and concluded that the Young's modulus of CNTs are weakly affected by both chirality and diameter. Chandraseker and Mukherjee [12] used a quasicontinuum analysis and ab initio calculations to obtain the Young's modulus of CNTs. The above mentioned predictions of molecular dynamics approaches are presented in Table 1.

Atomistic simulations are essentially restricted by the power and speed of the computers, especially for large systems such as nanocomposites and nanofluids in which the number of atoms and molecules are in the order of Avogadro's number. Another alternative which can eliminate the difficulties of atomistic simulations is continuum modeling and simulation of nanoscale systems. The continuum modeling of CNTs is developed based on the Cauchy–Born rule that relates the energy for an equivalent continuum to that at the atomic scale [3]. This rule states that in a crystalline solid subjected to a small deformation, the position of all atoms within the crystal follow the overall strain of the media and any point in the continuum is a representative of the crystal structure with homogeneous deformation. Some studies on continuum modeling of mechanical properties of CNTs are briefly described below.

Jiang et al. [13] investigated the effect of CNT diameter and chirality on its mechanical properties using a continuum model. They found that although the influence of chirality on mechanical properties is significant, the effect of CNT radius