Mechanical Properties of Single-walled Carbon Nanotubes - A Finite Element Approach

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Keywords: single-walled carbon nanotubes, mechanical properties, finite element model

Abstract: In this paper, the mechanical properties, such as the axial and radial Young’s moduli, shear moduli, buckling loads and natural frequencies, of single-walled carbon nanotubes, are estimated by a finite element approach. Each carbon nanotube is simulated as a frame-like structure and the primary bonds between two nearest-neighboring atoms are treated as isotropic beam members with a uniform circular cross-section. In the modeling work, the BEAM4 element in commercial code ANSYS is selected to simulate the carbon bonds and the atoms are nodes. As to the input parameters of the BEAM4 element, they are determined via the concept of energy equivalence between molecular dynamics and structural mechanics, and represented in terms of the force constants of the carbon bonds found in molecular mechanics. Based on this modeling concept, finite element models of both armchair and zigzag types of carbon nanotubes with different sizes are established and the mechanical properties of these tubes are then effectively predicted. Most of the computed results which can be compared with existing results show good agreement. Moreover, the effects of tube diameter, length etc., on the mechanical properties are also investigated.

Introduction

Extensive research activities have been devoted to carbon nanotubes (CNTs) since their discovery by Iijima in 1991 [1]. Due to the exceptional mechanical properties: small size, low density, high stiffness, high strength etc., CNTs represent a very promising material in many areas of science and industry. However, the understanding of the mechanical properties of CNTs is still insufficient so that the design and optimization of CNTs in nanoengineering is limited.

Researchers have tried to estimate the mechanical properties of multi- and single-walled nanotubes (MWNTs and SWNTs) in many ways, such as experiments, molecular dynamics, and elastic continuum modeling approaches. For example, experimental investigations conducted by Treacy et al. [2], Krishnam et al. [3], Wong et al. [4], who used TEM/AFM to measure the Young’s modulus of CNTs, reported values ranged from 0.90 to 1.80 TPa. Due to the difficulties in experimental investigation of CNTs, theoretical modeling techniques have also been developed to estimate the mechanical properties of CNTs. Among the available modeling techniques, the molecular dynamics (MD) method which is based on the force field and total potential energy related to the interatomic potentials for CNTs in a macroscopic sense has been used most extensively (Iijima et al. [5]; Gau et al. [6]; Zhang et al. [7]; Zhou et al. [8]; Belytschko et al. [9]). In this method, the bonding and nonbonding potentials are represented in terms of the force constants and the distance change among the atomic bonds, and then elastic moduli are determined by applying different small-strain deformation modes. However, MD simulation which has to consider the thermal vibration of atoms is not efficient for long time or static problem. Since it’s time consuming, the analysis of CNTs by MD is limited. The other approach is the continuum/finite element method. Since a nanotube can be well described as a continuum solid beam or shell subject to tension, bending, or torsional forces, it is reasonable to model the nanotube as a frame- or shell-like structure, then the mechanical properties of