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Estimation and Validation of Elastic Modulus of Carbon Nanotubes Using Nano-Scale Tensile and Vibrational Analysis

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Abstract: In this paper, the atomistic-continuum mechanics method (ACM) is applied for carbon nanotube modeling. The atomistic-continuum mechanics is based on the transformation of chemical bonds between atoms in molecular mechanics into appropriate elements in finite element method and continuum mechanics. Spring elements are treated as chemical bonds between carbon atoms in carbon nanotube, whose force-displacement function is determined by the Reactive Empirical Bond Order (REBO) potential model. The advantages and unique feature of ACM method is same analytical model can be used for both tensile and vibration analyses, and most importantly, there are no prior inputs such as Young's Modulus, cross-section area and density will be needed in the frequency analysis of ACM approach. As a result, not only Young's modulus could be obtained but also modal analysis could be achieved with affordable computational time by personal computers. The validity of the results is demonstrated through comparisons to numerical and experimental results provided by other papers. In addition, based on classic structural dynamics, the feasibility of the ACM method has been verified by comparing the results of Young's modulus analysis and modal analysis.

Keywords: Carbon nanotubes, finite element, atomistic-continuum method, Young's modulus, modal analysis, REBO

1 Introduction

The notable material properties of carbon nanotubes (CNTs) with ultrahigh Young's modulus, thermal conductivity, and ballistic electrical transport have made them

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very attractive for microelectronic interconnections, thermal management, and nano-scale device applications. Carbon nanotubes are a new form of carbon material, which was first discovered in 1991 by Iijima S. (1991) in the NEC Laboratory, Japan. Carbon nanotubes could be viewed as sheets of graphite rolled into seamless cylinders. Apart from being in the form of single-walled carbon nanotubes (SWCNTs), nanotubes can also have multi-walled carbon nanotubes (MWCNTs) which contain several coaxial cylinders, with each cylinder being an SWCNT. Carbon nanotubes are chiral structures and the circumference of any carbon nanotube could be expressed in terms of the chiral vector [Dresselhaus, Dresselhaus and Saito (1995)]. The chirality could determine whether a nanotube will conduct in a metallic or semiconducting manner [White and Mintmire (2005)]. Carbon nanotubes possess many unique and remarkable properties. The measured resistivity of metallic carbon nanotubes is in the order of 10^{-4} ohm-cm at 300K [Thess, Lee, Nikolaev, Dai, Petit, Robert, Xu, Lee, Kim, Rinzler, Colbert, Scuseria, Tomànek, Fischer and Smalley (1996)]. The thermal conductivity of single-walled carbon nanotubes at room temperature could be as high as 6600 W/mK [Berber, Kwon and Tomànek (2000)] and 3000 W/mK for multi-walled carbon nanotubes [Kim, Shi, Majumdar and McEuen, (2001)]. Moreover, there has been much effort to take advantage of the combined structural and electronic properties of the carbon nanotubes in the field of nano-electro-mechanical systems (NEMS), such as electromechanical actuators [Roth and Baughman (2002)] and nano- mechanical sensors [Mercuri and Sgamellotti (2007)].

Besides, much interest had also been focused on the notable mechanical properties of carbon nanotubes, particularly in terms of their high Young's moduli. However, a large variation of Young's modulus was also disclosed for single-walled carbon nanotubes (SWCNTs) like 0.32-1.47 TPa [Salvetat, Briggs, Bonard, Bacsa, Kulik, Stöckli, Burnham and Forró, (1999); Yu, Files, Arepalli and Ruoff (2000); Tombler, Zhou, Alexseyev, Kong, Dai, Liu, Jayanthi, Tang and Wu (2000)]. Considering the difficulties in the measurement of mechanical properties of individual carbon nanotube, the computer simulations based on reasonable physical models could provide experimentalists with references. In recent years, there are many works reported in the field of CNT modeling and can be generalized into two main simulation models, including the atomistic-based and the continuum-based models. The anterior models are currently restricted within hundreds of atoms by recent computational technology, such as ab-initio methods [Sanchez-Portal, Artacho and Soler (1999)] and tight-binding methods [Goringe, Bowleryk and Hernandez (1997); Hernandez, Goze, Bernier and Rubio (1998)]. Likewise, several methods are available for the continuum mechanics. To derive an analytical model for the mechanical properties investigation of CNT, Chang and Gao (2003) proposed an

analytical model to relate the elastic properties of SWCNT to its atomic structure. Zhang, Huang, Geubelle, Klein and Hwang (2002) incorporated interatomic potentials into a continuum analysis without any parameter fitting to study the linear elastic modulus of a SWCNT. Based on molecular dynamics (MD), several research works have been reported by considering different loading conditions, such as tension [Chen, Cheng, and Hsu (2007) and Zhou and Shi (2002)], temperature dependent plastic collapse under axial compression [Wei, Srivastaca, and Cho (2002)], buckling [Yakobson, Brabec and Berholc (1996); Yakobson, Campbell. Brabec and Bernholc (1997)], and thermal vibration [Chen and Cao (2006)].

As to continuum mechanics based on finite element method, there are three kinds of theories widely used in the CNT simulation: the classic beam, truss, and shell theory. Li and Chou (2003); Chen and Cao (2006) considered a SWCNT as a frame structure and used beam element to simulate elastic moduli. Based on this frame structure, Li and Chou (2003) further introduced truss rod element to simulate the van der Waals forces between the interlayer of MWCNTs. Besides using beam element as the main frame structure, models based on pure truss rod element have also been investigated. However, the main difference of beam element from truss element is the bending rigidity which is applied for the bond angle force equivalence [Li and Chou (2003)]. In order to correlate the angle variation energy with pure truss element model, Odegard, Gates, Nicholson and Wise (2002) presented a factitious rod in a truss model to study the effective geometry of a graphite sheet. Also, Leung, Guo, He and Kitipornchai, (2005) proposed an idea on spatial periodic strain, and a truss model with factitious rod was established for the mechanical simulation of zigzag SWCNTs. By considering classic shell theory, Yakobson, Brabec and Berholc (1996) introduced a continuous isotropic shell model with a fixed wall thickness, a fixed Young's modulus, and a variable radius for all SWCNTs. Moreover, Pantano, Parks and Boyce. (2004) further the concepts of shell theory into the simulation of MWCNTs. In addition to the above three classic elements, some researchers have tried to analyze nanotubes by using representative cells [Ling and Atluri (2006)], novel four-node elements [Nasdala, Ernst, Legnick and Rothert (2006)], quasicontinuum approach based on high order triangular elements [Park, Cho, Kim, Jun, and Im (2006)], or repetitive finite areas [Theodosiou and Saravanos (2007)].

Besides the elastic properties simulation of CNTs, the vibrational properties have also been studied by Krishnan, Dujardin, Ebbesen, Yianilos and Treacy (1998) and the amplitude of thermal vibrations of cantilevered nanotubes has been used for predicting their Young's modulus. But the potential of carbon nanotubes as high-frequency resonators has not been explored by experiments. Accordingly, based on beam theory, Li and Chou (2003) proposed a frame-like structure and simulated

the vibrational behavior of SWCNTs by molecular-structural-mechanics method. The results showed that the fundamental frequencies of carbon nanotubes could reach the level of 10 GHz – 1.5 THz depending on the nanotube diameter and length. Li and Chou (2004) further introduced the beam element model combined with truss element to simulate the vibrational behavior of MWCNTs. Yoon, Ru and Mioduchowski (2002) also investigated the interlayer vibration of MWCNTs by a multiple-elastic beam model. Besides, Sohlberg, Sumpter, Tuzun and Noid (1998) theoretically studied the vibration of CNTs by assuming nanotube as solid slender rods. Snow, Campbell and Novak (2002) applied a continuum shell model with Young's modulus of 1.0 TPa to study the vibration responses of SWCNTs as atomic force microscope probes.

In this research, an equivalent-spring structure is represented while applying the atomistic-continuum mechanics (ACM). A spring element is applied to transform the covalent bonds in the carbon nanotubes in order to describe the interatomic force between adjacent carbon atoms, and then the originally discrete atomic structure is analyzed in the continuum level. Moreover, in order to describe the bond-angle behavior of the covalent bonds, a factitious spring element between the carbon atoms along the two sides of each bond-angle is added. For the material properties of the spring element in the SWCNT structure, the Brenner's second-generation reactive empirical bond order (REBO) potential energy [Brenner, Shenderova, Harrison, Stuart, Ni and Sinnott (2002)] is selected to describe the binding energy between carbon atoms, including both the bond-stretch and the bond-angle term. In addition, according to the ACM and the finite element method, the ACM model is applied to investigate Young's moduli of zigzag and armchair type SWCNTs, and the modal analysis is also achieved within an affordable computational time by means of personal computers. Moreover, by comparing the results of Young's modulus and modal analysis based on structural dynamics, the ACM method shows good agreement in the two analyses which verifies the capability of applying ACM method in the nanostructure simulation.

2 Atomic Structure of Carbon Nanotubes

A SWCNT can be view as a rolled-up graphene sheet. A multi-wall carbon nanotube (MWCNT) can be considered as an assembly of multiple concentric SWCNTs with layer spacing about 0.34 nm. The atomic structure of nanotubes can be described in terms of tube chirality, which is defined by the chiral vector $\mathbf{C}_h$ and the chiral angle θ [Dresselhaus, Dresselhaus and Saito (1995)]:

$$\mathbf{C}_h = n\mathbf{a}_1 + m\mathbf{a}_2 \tag{1}$$

$$\theta = \tan^{-1}\left(\frac{\sqrt{3}m}{2n+m}\right) \tag{2}$$

The chiral vector is defined in terms of the integers (n, m) and the basis vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ are two unit vectors related to the hexagonal structure in the graphitic lattice. The chiral angle can be used to determine the arrangement of hexagonal cells in nanotube. Depending on the value of θ, a nanotube is defined as zigzag type when θ = 0˚, armchair type when θ = 30˚ and generally chiral type for any other value of θ between 0˚ and 30˚. On the other hand, the zigzag nanotube can be denoted by (n, 0) and the armchair nanotube (n, n) in terms of the chiral vector. The chiral vector can also define the diameter of nanotube d as Eq. 3,

$$d = \frac{|\mathrm{C}_h|}{\pi} = \frac{\sqrt{n^2+m^2+nm}}{\pi} \cdot \sqrt{3}a_{c-c} \tag{3}$$

where a_{c-c} is the distance between two nearest carbon atoms and is approximately equal to1.42Å for nanotube.

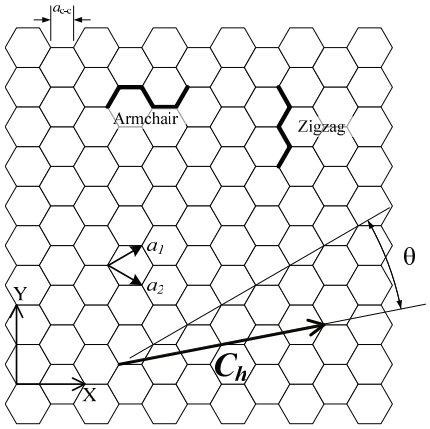


Figure 1: The 2D hexagonal structure of a graphene sheet with chiral vector $\mathbf{C}_h$ and chiral angle θ

3 Interatomic Potential for Carbon Atoms

There have been numerous literatures in molecular mechanics devoted to searching the reasonable numerical forms of the potential energy between atoms in molecules. In general, the total potential energy can be expressed as the sum of energies due

to valence or bonded interactions and nonbonded interactions [Cornwell, W. D.; Cieplak, P.; Bayly C. I.; Gould, I. R.; Merz, K. M.; Ferguson, D. M.; Spellmeyer, D. C.; Fox, T.; Caldwell, J. W.; Kollman, P. A. (1995)]:

$$E_{total} = \sum U_r + \sum U_\theta + \sum U_\phi + \sum U_{non-bond} \tag{4}$$

where U_r is for a bond stretch interaction, U_θ for a bond angle interaction, U_ψ for a dihedral angle torsion, and $U_{non-bond}$ for nonbonded interactions, including electrostatic interaction and van der Waals forces. In this research, the second-generation REBO [Brenner, Shenderova, Harrison, Stuart, Ni and Sinnott (2002)] is selected to describe the potential energy between carbon atoms in the nanotube due to the capability of REBO in defining the bond energy in the solid state carbon, such as graphene and carbon nanotubes. REBO determined the interatomic potential for carbon atoms as represented by Eq. 5:

$$E_b = \sum_i \sum_{j(>i)} [V^R(r_{ij}) - b_{ij} V^A(r_{ij})] \tag{5}$$

For atoms i and j, r_{ij} is the distance between atoms i and j, V_R and V_A are the respective repulsive and attractive pair terms given by Eq. 6 and 7, and b_{ij} is a bond order between atoms i and j as represented by Eq. 8:

$$V^R(r) = f^c(r)(1 + Q/r) A e^{-\alpha r} \tag{6}$$

$$V^A(r) = f^c(r) \sum_{n=1,3} B_n e^{-\beta_n r} \tag{7}$$

$$b_{ij} = \frac{1}{2}\left[b_{ij}^{\sigma-\pi} + b_{ji}^{\sigma-\pi}\right] + b_{ij}^{\pi} \tag{8}$$

The parameter Q, A, α, B_n and β_n are determined from the known physical properties of single (from diamond), conjugated double (from graphite), full double (from ethene), and triple (from ethyne) bonds. The function f^c is a smooth cutoff function to limit the range of the potential.

The values for the functions $b_{ij}^{\sigma-\pi}$ and $b_{ji}^{\sigma-\pi}$ depend on the local coordination and bond angles for atoms i and j, respectively. The function b_{ij}^{π} is further written as a sum of two terms as given by Eq. 9:

$$b_{ij}^{\pi} = \Pi_{ij}^{RC} + b_{ij}^{DH} \tag{9}$$

The value of the first term Π_{ij}^{RC} depends on whether a bond between atoms i and $j$has radical character and is part of a conjugated system. The value of the second term b_{ij}^{DH} depends on the dihedral angle for carbon–carbon double bonds.

According to the REBO potential for solid carbon, the interatomic potential function including bond stretching, angle variation, and dihedral term can be obtained. Moreover, van der Waals and electrostatic interactions between carbon atoms can be derived from Lennard-Jones "6-12" potential [Jones (1924)] and typical electrostatic potential, respectively. However, for a SWCNT that is subjected to axial loadings at small strains, dihedral, van der Waals, and the electrostatic potential can be neglected and it has been proven by Brenner, Shenderova, Areshkin, Schall and Frankland (2002). Accordingly, in this research, only bond stretching and angle variation terms are considered in the system potential energy.

4 Atomistic-Continuum Mechanics (ACM)

Based on the finite element method, the atomistic–continuum mechanics is developed to simulate the mechanical characteristics of nanoscale structures, such as Young's modulus and Poisson's ratio. The ACM method transfers an originally discrete atomic structure into an equivalent continuum model by suitable atomistic-continuum transfer elements. It simplifies the complexities of the interactive potential energies among the atoms, while keeping the calculation accuracy still acceptable and the computational time affordable.

One can generate the potential energy equations for a typical static constant-strain finite element. The total potential energy can be defined as a function (π_p) of the nodal displacements x, y and z such that $\pi_p = \pi_p(x,y,z)$. Here the total potential energy is given by Eq. 10,

$$\pi_p = U + \Omega_b + \Omega_p + \Omega_s \tag{10}$$

where U, Ω_b, Ω_p and Ω_s represent the strain energy, the potential energy of the body force, the potential energy of the concentrated load and the potential energy of the distributed load, respectively. The above equation can be rewritten as a finite element integrated form as Eq. 11 shown:

$$\pi_p = \frac{1}{2}\iiint_V \{d\}^T [B]^T [D] [B] \{d\} dV - \iiint_V \{d\}^T [N]^T \{F\} dV - \{d\}^T \{P\} - \iint_S \{d\}^T [N_S]^T \{T_S\} dS \tag{11}$$

where $\{d\}$ represents the nodal displacement vector, $[B]$ is the strain-displacement matrix, $[D]$ is the modulus of the elasticity matrix, $[N]$ is the shape function matrix, $\{F\}$ is the body force vector, $\{P\}$ is the external load vector and $\{T_s\}$ is the traction force vector. The ACM method transfers the interatomic potential function into a

force-displacement curve so as to create the material properties for an equivalent atomistic-continuum transfer element. Afterwards, the equivalent nanoscale model can be analyzed by FEM.

5 SWCNT Numerical Modeling

In this section, an ACM model is constructed to simulate Young's modulus and perform the modal analysis of SWCNTs. A single-walled carbon nanotube, which can be viewed as a graphite sheet rolled into a tube, is usually indexed by a pair of integers (n, m), which was so-called the chirality of CNTs. Based on the geometry described by the integers (n, m), the positions of carbon atoms in the SWCNT ACM model could be obtained.

In a carbon nanotube, covalent bonds are the main chemical bonds between each carbon atoms with characteristic bond length, bond angle, and dihedral angle building up hexagonal structure on the cylindrical wall of the nanotube. By directly transforming the covalent bonds into beam [Li and Chou (2003] or truss [Odegard, Gates, Nicholson and Wise (2002)] elements, a nanotube could be simulated by classic continuum mechanics and finite element method. Instead, a typical spring element is chosen as the equivalent atomistic-continuum transfer element in this research. The distinct characteristics of a spring element from truss or beam element are that it is not allowed to be bent, the cross-sectional area need not be defined, and the potential between atoms is the same as spring element. According to the former two characteristics, a spring element could represent a more realistic equivalent model since the chemical bond could neither be bent nor be defined by a cross-sectional area [Murray (1993)]. Moreover, based on the present potential theory, the last feature makes the transformation between the atomistic and the continuum method easier and more direct.

In the SWCNT ACM model, the chemical bond between carbon atoms can be transformed into the spring element as shown in the Fig. 2. The carbon atom is transformed into the node between spring elements, and can be viewed as the pin-joint which cannot resist any bending moment but can only transmit uniaxial tensile or compressive forces. In addition, the factitious spring elements are needed to equate the angle variation potential, and also make the equivalent-spring model stable. Fig. 3 show a zigzag and armchair SWCNT of the SWCNT ACM model, respectively, where the hexagon is a representative structure of SWCNT. The solid and the dashed line in the hexagon unit represent the bond stretching and angle variation, respectively. Furthermore, a spring element with nonlinear generalized force-displacement (F-D) capability is chosen in this research to reflect the nonlinear force-displacement behavior between carbon atoms. The F-D curve of SWCNT can be derived from the first derivative of the potential energy as Eq. 5.

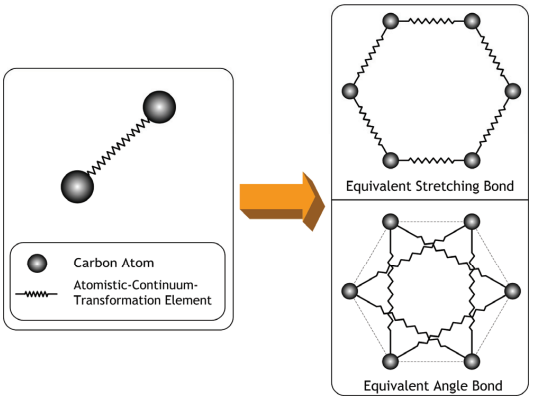
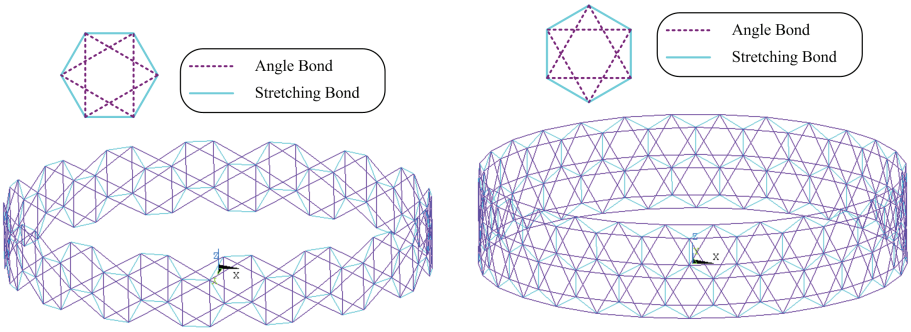


Figure 2: The equivalent-spring structure for atomistic-continuum mechanics model of hexagonal structure in carbon nanotubes.



(a) Armchair type (b) Zigzag type

Figure 3: The representative ACM model of the two types SWCNT structure.

During the computations, the initial carbon-carbon bond length is taken as 1.42 Å [Dresselhaus, Dresselhaus and Saito (1995)] under the equilibrium state without any loading. As to the bond angle transformation, it is chosen as 120° at the initial state and is converted from force-angle relation into F-D curve by the law of cosines while assuming the bond length is fixed under the small deformation assumption.

As boundary conditions for Young's modulus analysis, one end of the SWCNT is fully fixed, and the other end is applied constant small strain (0.1%) only along axial direction, only in the axial direction of SWCNTs. Only half of the SWCNT ACM model was used, together with symmetrical boundary conditions. This was done to reduce the CPU time during the simulation. In the modal analysis, the fix-ends

condition is chosen and the nanotube is under stable state without any prescribed strain. Meanwhile, by considering the atomic structure of carbon atom, the mass of carbon nucleus (m_{carbon} = 1.99 × 10-23 g), neglecting the mass of electrons, is assumed to be concentrated at the center of atom which is equivalent to the mass of node in the ACM model.

6 Simulation Results

6.1 Young's Modulus of SWCNT

In this section, Young's modulus of SWCNTs was analyzed. Young's modulus of a material is defined as the ratio of the normal stress to the normal strain in a uniaxial tension condition as,

$$Y = \frac{\sigma}{\varepsilon} = \frac{F/\pi dt}{\Delta H/H} \tag{12}$$

where F is the total force acting on the atoms at one end of the SWCNT, H is the initial length, ΔH is the elongation under tensile loading, d is the tube diameter, and t is the thickness. The thickness is taken as the interlayer spacing of MWCNT, 0.34 nm [Dresselhaus, Dresselhaus and Saito (1995)]. Two geometric variables, namely, radius and length, with respect to zigzag-type and armchair-type single-walled carbon nanotubes, were analyzed in this research. In the case of the radius-variable, the length of SWCNT is chosen as 5 nm. Moreover, in the case of the length-variable, the integers of SWCNT are selected as (10, 10) and (18, 0) as shown in Tab. 1.

Table 1: The variable table for the Young's modulus analysis

Variables	Model case	
	Radius-variable	Length-variable
Radius	Armchair (n, n): n = 3,4,...,16 Zigzag (n, 0): n= 6,8,...,28	Armchair: (10, 10) Zigzag: (18, 0)
Length	5 nm	10,15,...,40 nm

The results of Young's modulus versus the radius for zigzag and armchair SWCNT are shown in Fig. 4. The results of Young's modulus versus the length for zigzag and armchair SWCNT are shown in Fig. 5. Computations on the elastic deformation of SWCNT reveal that Young's moduli of both zigzag and armchair carbon nanotubes remain constant within a specific range of both 0.2∼1.1 nm (radius) and 10∼40 nm (length). The average Young's modulus is about 1,030 GPa for armchair

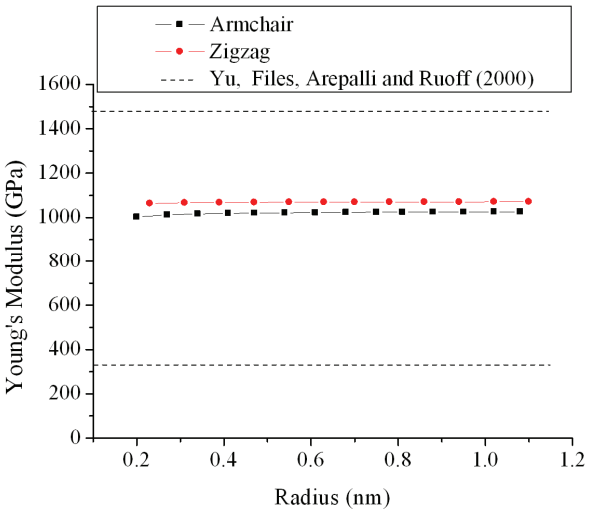


Figure 4: The result of Young's modulus vs. radius for a zigzag-type and armchair-type SWCNT.

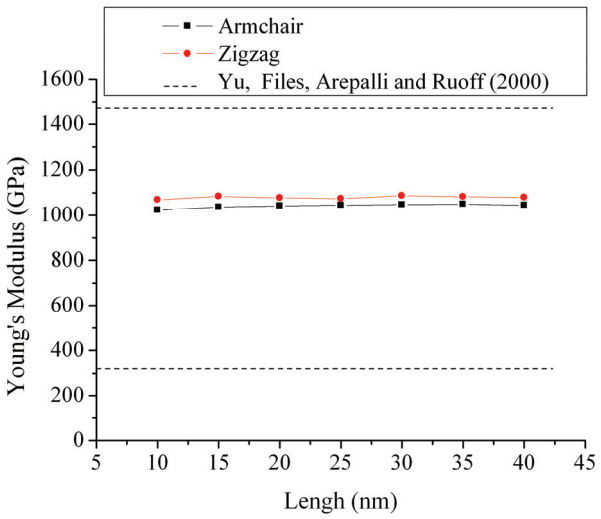


Figure 5: The result of Young's modulus vs. length for a zigzag-type and armchair-type SWCNT.

SWCNTs and 1,070 GPa for zigzag, which falls within the range of Young's modulus as the simulation results by molecular dynamics method [Cornwell and Wille (1997)] and continuum mechanics [Zhang, Huang, Geubelle, Klein and Hwang (2002)], and the experimental results [Yu, Files, Arepalli and Ruoff (2000); Salvetat, Briggs, Bonard, Bacsa, Kulik, Stöckli, Burnham and Forró (1999)]. However, the result is lower than other reported Young's moduli using ACM with a truss [Odegard, Gates, Nicholson and Wise (2002)] or a beam element [Li and Chou (2003)].

The results also show that Young's moduli of armchair and zigzag SWCNT remain constant within the specific range in this research in terms of both radius and length, and make good agreement with the literature [Jin and Yuan (2003), Lu (1997)]. For a given tube radius, Young's modulus of zigzag SWCNT is slightly larger than that of armchair SWCNT. These two results agree with the physical phenomena reported by Chang and Gao (2003) even if the parameter of the tube length is different. In addition, for a given tube length, Young's modulus for zigzag SWCNT is also slightly larger than that for armchair SWCNT.

6.2 Modal Analysis of SWCNT

In this section, modal analysis of SWCNT is performed. The radius and length of SWCNT are chosen as the variables with respect to the armchair and zigzag SWCNT, and the detailed parameters were shown in the Tab. 2. The parameters are selected to make the length-to-radius ratio of SWCNT large enough to ensure that the first mode could be a beam-mode instead of a shell-mode. The results of the first three mode frequency are listed in the Tab. 2 and those shadowed and underlined mode frequency show the mode shape is shell-mode while all else stand for beam-mode. The representative mode shape of beam-mode is shown in the Fig. 7 (a) and shell-mode was shown in the Fig. 7 (b). As given in Fig. 7, the vibrational behavior of a pure atomic structure can be simulated based on proposed ACM models.

By comparing the mode frequency with the same mode shape, the results showed that the mode frequency is proportional to the radius, but inversely proportional to the length. The results agree with the simulation results published by Li and Chou (2003) and the vibrational properties of the Bernoulli-Euler beam derived by the classical structural mechanics [Craig, R. R. Jr. (1981)], which will be detailed in the discussion chapter.

7 Discussion

According to the classic structural mechanics, if the nanotubes are considered as continuum hollow beams, the modal (resonant) frequencies ω_n can be approximately obtained by the Eq. 13 [Craig, R. R. Jr. (1981)]:

$$\omega_n = \frac{\lambda_n^2}{8\pi L^2}\sqrt{\frac{E\left(r_i^2 + r_o^2\right)}{\rho}} \tag{13}$$

where E, r_i, r_o, L, ρ and λ_n represents Young's modulus, the inner radius, the outer radius, the length, the density of nanotubes, and the constant for the nth mode, respectively. For the fix-ends boundary condition, $\lambda_1 = 4.74$, $\lambda_2 = 7.85$, $\lambda_3 = 10.99$, Young's modulus can be obtained from the previous analysis as the approximate value 1,000 GPa. The density is about 2.24 g/cm^3 by assuming that the atomic mass distributes uniformly in the hollow cylinder structure and the wall Thickness is 0.34 nm. Because the continuum model based on beam theory might be too stiff, a shell continuum model is further introduced in this research wherein the parameters used are the same as the beam model. The corresponding first three mode frequencies are listed in Tab. 3.

From the modal analysis results in Tab. 2 and Tab. 3, the first-mode frequencies in the ACM model agree with the above beam and shell models by. This consistence implies the Young's modulus derived from ACM model by modal analysis is almost the same as the one we applied in beam and shell models, which is 1,000 GPa obtained from the previous tensile analysis. This also indicates that the ACM method could provide a realistic atomic model without cross-sectional area equivalent process for truss element or further Young's modulus equivalent procedure for beam element, but only by applying the potential energy from molecular mechanics into spring element. Besides the application in SWCNT simulation in this reserach, the ACM method has been used in DNA [Chiang, Yuan, Han, Chou and Cui (2006)] or nano-metallic structure [Chiang, Chou, Wu and Yuan (2006); Lin and Chiang (2007)] and in good agreement with the existing experimental results.

(a) Beam mode (b) Shell mode

Figure 6: The representative mode shape of SWCNT ACM model.

Table 2: Modal analysis results of SWCNT. Those shadowed and underlined frequencies represented the mode shape was shell-mode while the else stood for beam-mode

$\mathbf{C}_h$	D	L	Mode frequency (GHz)		
(n, m)	(nm)	(nm)	1	2	3
(8,8)	1.1	80	4.75	13.04	25.43
		90	3.74	10.29	20.09
		100	3.03	8.34	16.30
(15,15)	2.2	80	8.84	12.39	15.51
		90	6.98	12.16	14.40
		100	5.66	12.01	13.69
(14,0)	1.1	80	4.72	12.96	25.2
		90	3.75	10.32	20.15
		100	3.03	8.35	16.31
(26,0)	2.2	80	8.75	20.09	23.80
		90	6.97	19.01	19.79
		100	5.64	15.42	19.58

Table 3: Modal analysis based on structural dynamics. Those shadowed and underlined frequencies represented the mode shape was shell-mode while the else stood for beam-mode

Continuum	D	L	Mode frequency (GHz)		
model	(nm)	(nm)	1	2	3
Beam model	1.1	80	4.92	13.51	26.47
		90	3.89	10.67	20.92
		100	3.15	8.64	16.94
	2.2	80	9.52	26.11	51.18
		90	7.52	20.63	40.44
		100	6.09	16.71	32.76
Shell model	1.1	80	4.71	12.94	25.27
		90	3.72	10.24	20.01
		100	3.05	8.38	16.39
	2.2	80	9.24	25.11	48.38
		90	7.31	19.94	38.55
		100	5.99	16.37	31.73

8 Summary

In this research, an atomistic-continuum mechanics (ACM) model based on the finite element method with an equivalent-spring element is proposed to investigate Young's modulus and the modal analysis of SWCNT. The results agree with several experimental and atomistic studies based on ab-initio, MD, and the continuum mechanics. Through the comparison of results from ACM and equivalent continuum models, the validation of ACM method has been proven.

The advantages and unique feature of applying spring element in ACM method is that a more realistic equivalent model between atomistic and continuum mechanics could be obtained without further equivalent process like truss or beam element, and same analytical model can be used for both tensile and vibration analyses. The natural frequencies can be calculated directly from ACM numerical model with no prior inputs such as Young's Modulus and density, etc., however, the frequency obtained from experiment will be a must for other approaches. Besides, the time-saving benefit would make nanotube with length in hundreds nanometers possible within an affordable computational time by means of personal computers. Moreover, the present approach is not only limited to SWCNT since other atomistic studies that provide potential in atomic bonds can be similarly incorporated in the present ACM models with this equivalent-spring element.

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