Estimation of mechanical properties of single wall carbon nanotubes using molecular mechanics approach

P SUBBA RAO^{1,2,*}, SUNIL ANANDATHEERTHA³,
G NARAYANA NAIK¹ and S GOPALAKRISHNAN¹

¹Department of Aerospace Engineering, Indian Institute of Science,
Bangalore 560012, India

²Structures group, ISRO Satellite Centre, Bangalore 560017, India

³Department of Mechanical Engineering, PES University, Bangalore 560085, India
e-mail: subbarao@isac.gov.in; subbarao_pendyala@yahoo.com

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Abstract. Molecular mechanics based finite element analysis is adopted in the current work to evaluate the mechanical properties of Zigzag, Armchair and Chiral Single wall Carbon Nanotubes (SWCNT) of different diameters and chiralities. Three different types of atomic bonds, that is Carbon–Carbon covalent bond and two types of Carbon–Carbon van der Waals bonds are considered in the carbon nanotube system. The stiffness values of these bonds are calculated using the molecular potentials, namely Morse potential function and Lennard-Jones interaction potential function respectively and these stiffness's are assigned to spring elements in the finite element model of the CNT. The geometry of CNT is built using a macro that is developed for the finite element analysis software. The finite element model of the CNT is constructed, appropriate boundary conditions are applied and the behavior of mechanical properties of CNT is studied.

Keywords. Molecular mechanics; single wall carbon nanotube; mechanical properties; finite element method.

1. Introduction

Carbon nanotubes regarded as one of the most exciting nanomaterials with exceptional mechanical, physical, thermal and electronic properties are broadly classified into two types, Single Walled Carbon Nanotubes (SWCNTs) and Multi Walled Carbon Nanotubes (MWCNTs). There are three well-known configurations of SWCNTs namely Armchair, Zigzag and Chiral (Hamada *et al* 1992). Many works have been carried out regarding the estimation of their mechanical properties by various methods. Mielke *et al* (2004) employed density

*For correspondence

functional theory (DFT) calculations and estimated the tensile strength and maximum tensile strain as 110 GPa and 30% for (5, 5) Armchair SWCNT and 105 GPa and 20% for (10, 0) Zigzag SWCNT. Ogata & Shibutani (2003) also used the same method and estimated the tensile strength and maximum tensile strain as 115 GPa and 29.5% for (8, 8) Armchair SWCNT and 107 GPa and 20.8% for (10, 0) Zigzag SWCNT. Liew *et al* (2004) used molecular dynamics (MD) method and estimated that their values to be 140.4 GPa and 28% for (10, 10) SWCNT and 110 GPa and 20% for (12, 12) SWCNT. Xiao *et al* (2005) developed an analytical molecular structural mechanics model and predicted the tensile strengths of 126.2 GPa for Armchair nanotubes and 94.5 GPa for Zigzag nanotubes. The failure strain for Armchair nanotubes (23.1%) is found to be greater than that of Zigzag nanotubes (15.6–17.5%) in their analysis. Natsuki & Endo (2004) presented a structural mechanics approach based on continuum shell model and evaluated the tensile strength of Armchair (10,10) and Zigzag (17, 0) nanotubes as 90 GPa and 67 GPa respectively. By thermally inducing the vibration of cantilevered MWCNT, Treacy *et al* (1996) measured the Young's modulus of carbon nanotubes in the range of 0.4–4.15 TPa. Krishnan *et al* (1998) used the same method to calculate the Young's modulus of SWCNTs and obtained an averaged value of 1.3 TPa. Mielke *et al* (2004) using DFT calculations found a Young's modulus of 0.96 TPa for (5, 5) SWCNT and 0.94 TPa for (10, 0) SWCNT. Jin & Yuan (2003) used molecular dynamics (MD) simulations and calculated the Young's modulus for Armchair SWCNTs as 1.350 TPa and 1.238 TPa. Meo & Rossi (2006a) (Composites Science and Technology) used molecular mechanics (MM) based finite element analysis and predict a Young's modulus of 0.920 TPa for Armchair nanotubes, 0.912 TPa for Zigzag nanotubes and 0.915 TPa for chiral nanotubes.

In this paper, we have considered the effect of non-bonded Lennard-Jones atomic interactions (van der Waals interactions) as well, which has been neglected in previous research works (Odegard *et al* 2002; Chang & Gao 2003; Xiao 2005; Meo & Rossi 2006b (Engineering Fracture Mechanics); Rossi & Meo 2009). Furthermore, the work carried out by Natsuki & Endo (2004), Xiao *et al* (2005) and Sun & Zhao (2005) in the direction of evaluation of CNT mechanical properties, such as ultimate tensile strength, have not considered any effects of van der Waals interactions in their simulations. In this paper, we have paid due consideration to the effect of these non-bonded interactions.

This paper is organized as follows. Following the introduction in section 1, section 2 discusses the methodology of basic molecular mechanics adopted in this work as applied to modeling the carbon–carbon bonded interactions of carbon nanotube. Here, the details of Morse potential and Lennard-Jones potential functions are presented. This is followed by section 3, highlighting the adoption of molecular mechanics method to finite element analysis and some of the novelties of molecular mechanics based finite element analysis. This is followed by section 4 on numerical simulation, where the method used to calculate the Young's modulus and tensile strength is discussed. The obtained results are presented and discussed in section 5 followed by conclusions in section 6.

2. Molecular mechanics methodology

Molecular mechanics based finite element analysis is adopted in the current work to evaluate the above-mentioned mechanical properties of Zigzag, Armchair and Chiral SWCNTs of different diameters and chiralities.

Firstly, the geometry of SWCNT is built using the macro that is developed for the finite element analysis software named ANSYS. Later, three different types of atomic bonds are

identified in the carbon nanotube system. They are Carbon–Carbon Covalent bond and two types of Carbon–Carbon van der Waals bonds. The two latter types of bonding are differentiated by the difference in the inter-atomic separation distance. Note that, such an interaction has never been considered by previous researchers (Odegard *et al* 2002; Chang & Gao 2003; Xiao *et al* 2005; Meo & Rossi 2007) in their molecular mechanics based finite element model.

In the finite element analysis, spring elements represent the covalent and the van der Waals bonding. The stiffness values of these elements are calculated using the molecular potentials, namely Morse potential function and Lennard-Jones 6–12 interaction potential function, the details of which are explained. Once the Finite Element model of the SWCNT is constructed, appropriate boundary conditions are applied and the mechanical properties of SWCNT are calculated.

2.1 Molecular mechanics model

Figure 1(a) shows two carbon atoms separated by a distance r . While one of the atoms is constrained against deformation, the other is subjected to an axial stretch, Δr as shown in figure 1(a). $F_{\Delta r}$ is the reaction force generated due to the imposed stretch deformation and $K_{\Delta r}$ is the axial stiffness of the bond opposing the deformation. Figure 1(b) shows a system of three carbon atoms contained in a CNT. Under deformation of CNT, atoms C1, C2 and C3 move out of their equilibrium positions by $(\Delta X_{C1}, \Delta Y_{C1}, \Delta Z_{C1})$, $(\Delta X_{C2}, \Delta Y_{C2}, \Delta Z_{C2})$ and $(\Delta X_{C3}, \Delta Y_{C3}, \Delta Z_{C3})$ respectively. This results in a change in the bond angle $\Delta\theta$ between C1–C2 and C1–C3 covalent bonds. This $\Delta\theta$ results in a change in the bond-angle potential, $V_{\Delta\theta}$. The modified Morse potential V_{MP} is written as (Belytschko *et al* 2002),

$$V_{MP} = V_{stretch} + V_{angle} = V_{\Delta R} + V_{\Delta\theta} \quad (1)$$

where $V_{\Delta R}$ (i.e. $V_{stretch}$) and $V_{\Delta\theta}$ (i.e. V_{angle}) are bond stretch and bond angle potentials respectively.

Figure 1. (a) Spring elements representing bond – stretching and (b) bond bending.

The bond stretch potential is given by the relation (Belytschko *et al* 2002),

$$V_{\Delta r} = D_e \left[\left(1 - e^{-\beta \cdot \Delta r} \right)^2 - 1 \right] \quad (2)$$

where ' D_e ' is the equilibrium binding energy, ' β ' is the fitting parameter and ' Δr ' is $(r - r_o)$, where r_o is the equilibrium distance of separation between the two carbon atoms in the CNT ($r_o = 0.1421$ nm) and ' r ' is the distance of separation between the two carbon atoms after stretch. This Δr results in a change in the bond potential function $V_{\Delta r}$ given by Eq. (2). The values of these constants are $D_e = 6.03105 \times 10^{-10}$ N nm, $\beta = 2.625 \times 10^{10} \text{m}^{-1}$ (Belytschko *et al* 2002).

The bond angle potential is given by the relation (Belytschko *et al* 2002; Meo & Rossi 2006a)

$$V_{\Delta \theta} = 0.5k_{\theta} \Delta \theta^2 (1 + k_{sextic} (\Delta \theta^4)) \quad (3)$$

where $\Delta \theta$, i.e. $(\theta - \theta_0)$ is the variation in C–C–C bond angle (see figure 1(b)); θ is the angle of separation between the two bonds after deformation and θ_0 is the equilibrium bond angle of separation between the two bonds. k_{θ} is the bond stiffness for angular deformations ($k_{\theta} = 0.9$ nN-nm/rad²). The value of the constant k_{sextic} in Eq. (3) was provided by Belytschko *et al* (2002) as 0.745 rad^{-4}

The Lennard-Jones 6–12 potential function (Lau *et al* 2004) is written as

$$U_{ij} = 4\epsilon \left[\left(\frac{r_c}{r_{ij}} \right)^{12} - \left(\frac{r_c}{r_{ij}} \right)^6 \right] \quad (4)$$

where U_{ij} is the van der Waals interaction potential between the i^{th} and j^{th} atoms of a system of two carbon atoms, separated by a distance of r_{ij} . ϵ is the Lennard-Jones parameter, ($\epsilon = 3.825 \times 10^{-4}$ nN – nm) (Brcic *et al* 2009), whose value determines the strength of Lennard-Jones interaction. r_c is the cut-off distance, which is equal to 0.34 nm for calculating the Lennard-Jones interactions.

3. Molecular mechanics based finite element modeling

In the present work, two types of finite elements are used to represent the covalent and van der Waals inter-atomic interactions respectively. They are chemical bond element and Lennard-Jones element.

3.1 Novelities of molecular mechanics based finite element approach

1. The finite elements are governed by structural equivalents of molecular potential functions; thereby the inter-atomic interactions are accurately depicted.
2. Since the nanoscale inter-atomic interactions are one to one, a single finite element can represent the individual interactions. Thus, the total number of finite elements in the nanoscale structure would be the same as the total number of nanoscale inter-atomic interactions, which eliminates the discretization errors.
3. Very large domains of the nanoscale structure can be analyzed at a fraction of the computational time and resources as opposed to methods such as molecular dynamics and density functional theory.

3.2 Calculation of covalent bond stiffness

First, to obtain the bond stiffness of the chemical bond element, Eq. (2) has to be differentiated twice with respect to Δr . Differentiating $V_{\Delta r}$ in Eq. (2) with respect to Δr ,

$$F_{\Delta r} = \frac{dV_{\Delta r}}{dr} = 2\beta D_e e^{-\beta \Delta r} (1 - e^{-\beta \Delta r}) \quad (5)$$

where $F_{\Delta r}$ is the force generated by the C–C covalent bond against the deformation r ,

Next, differentiating $F_{\Delta r}$ with respect to Δr , we get the bond stiffness, $K_{\Delta r}$ of the chemical bond element.

$$K_{\Delta r} = \frac{dF_{\Delta r}}{dr} = \frac{d^2 V_{\Delta r}}{dr^2} = \beta^2 D_e e^{-\beta \Delta r} (2e^{-\beta \Delta r} - 1) \quad (6)$$

For obtaining the bond bending stiffness, it is required to differentiate Eq. (3) twice with respect to $\Delta \theta$. Differentiating $V_{\Delta \theta}$, we get $M_{\Delta \theta}$, moment function,

$$M_{\Delta \theta} = \frac{dV_{\Delta \theta}}{d\Delta \theta} = k_\theta \Delta \theta (1 + 3k_{sextic} \Delta \theta^4) \quad (7)$$

Next, differentiating $M_{\Delta \theta}$ we get, $K_{\Delta \theta}$ the bond bending stiffness with varying bond angle $\Delta \theta$. It is written as

$$K_{\Delta \theta} = \frac{dM_{\Delta \theta}}{d\Delta \theta} = k_\theta (1 + 15k_{sextic} \Delta \theta^5) \quad (8)$$

3.3 Calculation of Lennard-Jones stiffness

Differentiating U_{ij} in Eq. (4) with respect to r_{ij} , we get the Lennard-Jones force of interaction.

$$\frac{dU_{ij}}{dr_{ij}} = F_{r_{ij}} = 24 \frac{\epsilon}{r_c} \left[-2 \left(\frac{r_c}{r_{ij}} \right)^{13} + \left(\frac{r_c}{r_{ij}} \right)^7 \right] \quad (9)$$

Differentiating $F_{r_{ij}}$ with respect to r_{ij} , we get the Lennard-Jones element stiffness

$$\frac{d^2 U_{ij}}{dr_{ij}^2} = \frac{dF_{r_{ij}}}{dr_{ij}} = K_{r_{ij}} = 24 \frac{\epsilon}{r_c^2} \left[26 \left(\frac{r_c}{r_{ij}} \right)^{14} - 7 \left(\frac{r_c}{r_{ij}} \right)^8 \right] \quad (10)$$

Figures 2(a) and (b) show the finite spring elements used in the present analysis. Two types of Lennard-Jones finite elements viz. Type 1 (LJSE1) and Type 2 (LJSE2) of lengths 0.2461 nm and 0.2842 nm respectively are used. The respective stiffness values calculated using Eq. (10) for the above-mentioned lengths are 183.1685 nN/nm and 23.067 nN/nm respectively. Similarly, at deformed covalent bond lengths of 0.1421 nm (that is, at $\Delta r \rightarrow 0$) it can be seen from Eq. 6, that the bond stiffness is 831.4514 nN/nm. From the above discussion, it is concluded that the stiffness of LJSE1 and LJSE2 is not negligible in comparison to the stiffness of the C–C covalent bond and hence are considered in the present study. The relation between the element load vector $\{Q\}$, the element stiffness matrix $[K]$ and the element displacement vector $\{q\}$ is written as $\{Q\} = [K] \{q\}$.

Figure 2. (a) Lennard-Jones Spring Elements-Type 1 (LJSE1) ($r_{ij} = \sqrt{3}L_{C-C} = 0.2461$ nm) and Type 2 (LJSE2) ($r_{ij} = 2L_{C-C} = 0.2842$ nm). $L_{C-C} = 0.1421$ nm. The continuous thick lines represent chemical bonds modeled by Eq. (6). Dashed thick lines represent LJSE1 while dashed thin lines represent LJSE2; both modeled by Eq. (10). (b) 3D extensional spring element in its local co-ordinate system.

4. Numerical simulation

For numerical simulation studies, SWCNTs of different chirality and diameters are considered. ANSYS software is used for the finite element simulations. Geometry of the SWCNT is constructed using the macro written in software's Parametric DesignLanguage (APDL). Finite elements COMBIN39 and COMBIN14 are chosen for analysis. COMBIN39 is a non-linear spring element defined with the help of force deflection behavior obtained using Eq. 6. COMBIN14 is a linear spring-damper element and is employed with its damping coefficient value set to zero. The stiffness values of the springs are calculated using Eqs. (6) and (10). Molecular Mechanics based finite element analysis is carried out to study the effect of chirality and diameter on the tensile strength, maximum tensile strain and Young's modulus.

Figure 3(a) shows atomic bonding in the finite element model of (20, 20) Armchair SWCNT containing two unit cells and figure 3(b) shows the finite element model of (6, 6) carbon nanotube. The edges of the regular hexagons represent the C–C covalent bonds while the shorter and longer diagonals of each of the regular hexagons represent LJSE1 and LJSE2 respectively.

4.1 Longitudinal tensile behavior of SWCNTs

In the molecular mechanics based finite element simulation of SWCNTs subjected to longitudinal loading, all atoms on one end are constrained and longitudinal tensile displacement is applied to all atoms on the opposite end. Initially, the geometry of the nanotube is built and the finite elements are defined. The ability of the software ANSYS10.0 to use only certain types of Force-Deflection (FD) types (to which the covalent FD behavior belongs and the Lennard-Jones FD behavior does not belong) is the reason behind the use of non-linear element to simulate Covalent bonds (COMBIN39) and linear spring to simulate Lennard-Jones interactions (COMBIN 14). Then, all atoms on one end of the SWCNT are constrained.

Figure 3. (a) Atomic bonding in the Finite Element Model of (20, 20) Armchair SWCNT Containing two unit cells; (b) Finite Element Model of (6, 6) CNT.

For simulation of tensile behavior, maximum tensile strain (that is, the strain at which the stress–strain curve for that particular nanotube just starts to dip) is applied to the SWCNT. This displacement is applied in suitable steps in the non-linear finite element analysis so as to obtain a smooth and well defined stress–strain behavior. Once, the above displacement boundary conditions are set, finite element analysis is performed. After the completion of analysis, the tensile stress is calculated as follows.

$$\sigma_{\parallel swcnt} = \frac{\sum_{j=1}^k F_j}{\pi D t} \quad (11)$$

where ‘ σ ’ is the stress, the superscript ‘ $\parallel$ ’ corresponds to the SWCNT axial direction, $\sum_{j=1}^k F_j$ is the sum of axial reaction forces on all atoms ($j = 1$ to k). The obtained stress is then plotted against the applied strain in each step of the analysis and the stress–strain behavior is obtained. The tensile stress at the point where the stress–strain curve just starts to dips is taken as the tensile

Table 1. Predicted and literature values of tensile strength and maximum tensile strain of SWCNT.

Different chiralities	(n, m)	Diameter (nm)	Predicted tensile strength	Predicted tensile strain (%)	Reported literature σ_T	Reported literature ϵ_{max}	Method
Arm chair	(5,5)	0.6785	117.05	29.12	110.0 ¹	30 ¹	DFT
	(7,7)	0.9499	118.88	29.62	121.3 ²	20.68 ²	MM
	(9,9)	1.2213	120.45	29.69			
	(11,11)	1.4927	122.53	29.98			
Average			119.73	29.60			
Zigzag	(5,0)	0.3917	101.21	20.56	105 ¹	20 ¹	DFT
	(8,0)	0.6267	101.95	20.64			
	(10,0)	0.7834	102.69	20.75			
	(12,0)	0.9401	103.23	20.78			
Average			102.27	20.68			
Chiral	(5,4)	0.6119	114.22	22.15			
	(10,1)	0.8254	117.96	22.98			
Average			116.09	22.57			

¹Mielke *et al* (2004), ²Meo & Rossi (2007).

strength of the SWCNT. SWCNT geometric parameters – ‘t’ is the thickness of the SWCNT and ‘D’ is the SWCNT diameter.

4.2 Calculation of Young's modulus of SWCNTs

As explained above, the stress–strain behaviors of various SWCNTs are calculated first. Then, from these stress–strain diagrams, the value of Young's modulus is calculated as the slope of the linear region of the curve (the initial region of the curves is taken to be the linear region of the curve).

Figure 4. (a) Tensile stress strain behavior of Zigzag SWCNT; (b) Tensile stress strain behavior Armchair SWCNT; (c) Tensile stress strain behavior of Chiral SWCNT.

5. Results and discussions

The tensile behavior of SWCNTs of Zigzag, Armchair and Chiral configurations of different diameter and chiralities is studied. The longitudinal tensile Young's modulus and maximum tensile strength are calculated and the results obtained are compared with published literature data.

5.1 Longitudinal tensile behavior

Table 1 shows the values of longitudinal tensile strength and maximum failure strain for various SWCNTs obtained using the present method, wherein, the Lennard-Jones inter-atomic interactions are also considered. The table also provides a comparison of the obtained values with those of published literature. From the comparison, it can be seen that the obtained values of longitudinal tensile strength and maximum tensile strain are in very good agreement with the published literature values.

Figure 4(a), (b) and (c) respectively shows the tensile behavior of Zigzag, Armchair and Chiral SWCNTs. Tensile strength and maximum tensile strain of Armchair SWCNTs are greater than that of Zigzag and Chiral SWCNTs as reported in numerous published literatures (Mielke *et al* 2004; Ogata *et al* 2003; Meo & Rossi 2007).

5.2 Estimation of Young's modulus

Young's modulus of Zigzag, Armchair and Chiral SWCNTs is calculated using the slope of the stress strain diagram. The obtained values of Young's modulus are provided in table 2. It can be seen from table 2 that, the Young's modulus of Zigzag SWCNTs are greater than that of Armchair and Chiral SWCNTs. It can also be seen that its value is sensitive to the SWCNT diameter.

Table 2. Predicted SWCNT Young's modulus.

Different chiralities	(n, m)	Diameter (nm)	Predicted Young's modulus $E^{\parallel}$ (TPa)	Reported literature $E^{\parallel}$ (TPa)	Method
Armchair	(5, 5)	0.6785	1.2289	1.28 – 1.48 ¹	MD
	(7, 7)	0.9499	1.2678	1.293 ²	DFT
	(9, 9)	1.2213	1.2767	0.92 ³	MM
	(11, 11)	1.4927	1.2811	1.01 ⁴	DFT
				1.320 ²	DFT
Average			1.2636		
Zigzag	(5, 0)	0.3917	1.2436	0.912 ³	MM
	(8, 0)	0.6267	1.2641	1.306 ²	DFT
	(10, 0)	0.7834	1.2778	1.1 ⁵	DFT
	(12, 0)	0.9401	1.2895		
Average			1.2688		
Chiral	(5, 4)	0.6119	1.1627	0.915 ³	MM
	(10, 1)	0.8254	1.2097		
Average			1.1862		

¹Wang *et al* (2005), ²Peng *et al* (2006), ³Meo & Rossi (2007), ⁴Treacy *et al* (1996) and ⁵Mielke *et al* (2004).

6. Conclusions

Molecular mechanics based finite element analysis is carried out for all three chiralities of SWCNT (armchair, zigzag and chiral) of different diameters. Mechanical properties such as tensile strength and Young's modulus are calculated using SWCNT tensile behavior. The effect of non-bonded Lennard-Jones interactions is also considered for study. The effect of inclusion of these non-bonded interactions is studied by making the numerical stiffness of these bonds to negligible levels and found that they significantly reduce the mechanical properties. Thus, the importance of inclusion of Lennard-Jones interactions is highlighted in this paper. All further calculations are carried out by considering the full effect of these non-bonded interactions. It is found that the longitudinal tensile strength and maximum tensile strain of Armchair SWCNTs is greater than that of Zigzag and Chiral SWCNTs and its value increases with increasing SWCNT diameter. The average value of longitudinal tensile strength of Armchair SWCNTs is found to be 17.07% and 3.13% greater than that of Zigzag and Chiral SWCNTs. The average value of longitudinal tensile strength of Armchair, Zigzag and Chiral SWCNTs is 119.73, 102.27 and 116.09 GPa respectively. The average value of maximum tensile strain of Armchair SWCNTs is found to be 43.16% and 31.18% greater than that of Zigzag and Chiral SWCNTs. Its average values for Armchair, Zigzag and Chiral SWCNTs correspond to 29.6%, 20.6% and 22.5% respectively. The longitudinal Young's modulus of SWCNTs is calculated as the slope of the linear region of the stress-strain diagram. Its averaged values for Armchair, Zigzag and Chiral SWCNTs are 1.26, 1.26 and 1.18 TPa respectively. The calculated values of the mechanical properties listed above agree well with the published literature data.

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