Chapter 6

Carbon Nanotubes Under Simple Tension and Torsion – Molecular/Structural Mechanics and the Finite Element Method

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Additional information is available at the end of the chapter

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1. Introduction

The intended applications of carbon nanotubes have steadily increased since their discovery by Ijima [4]. They range from the nanoscale, as in the tip of an atomic electron microscope, to the macroscale, as in the preliminary design of the space elevator cable.

In modeling CNTs, molecular as well as quantum mechanics have been the primary tools for analysis. Also, closed form expressions were developed to study the response of CNTs in different environments [3,8,12].

On the other hand, some attempted to use structural mechanics, and built corresponding finite element models, to study the behavior of CNTs, as evident in several publications [5-8]. Some of these publications simplified the property relations between molecular mechanics and structural mechanics. They assumed the structural bending stiffness EI/a to be a constant and set it equal to the molecular bond bending stiffness C.

However, in [1], with a simple proof, we showed that the main assumption used by various authors to equate the element bending stiffness to the bond bending stiffness ($C= EI/a$) does not hold. In addition, in our previous publications (Kasti [1,2]), we related some of the mechanical properties used in molecular and structural mechanics.

In [1], we derived an expression for the axial deformation of zigzag CNTs that accounts for the axial and bending structural stiffnesses under simple tension. While molecular mechanics uses the bond angle between two bonds to describe bond bending deformations, struc-

tural mechanics uses the bending within one 3D frame element for this definition. Comparing the deformation equation in structural mechanics to the equivalent equation derived for molecular mechanics, leads us to a "consistent" frame bending stiffness for an infinitely long zigzag CNT. For large diameter tubes, the frame bending stiffness tends to half the bond bending stiffness. This later case is representative of a graphene sheet. For small diameters, EI/a changes with the bond bending stiffness C, the torsional angle φ and the lattice translational index n. The expression for the axial deformation was then expanded to include the torsional stiffness of 3D frame elements. This provided us with an equation for the "elastic modulus" of an infinitely long zigzag CNT. It included the axial, bending and torsional deformations. Then, in [2], we extended the work to the case of simple torsion of zigzag carbon nanotubes. The expression relating the molecular bond bending stiffness C and the structural bending stiffness EI/a was derived. It was found to be different from the case of simple tension. The structural bond bending stiffness was both load and chirality dependent. However, for the particular configuration of a graphene sheet, the relation of simple tension was recovered, namely $EI/a=C/2$. We concluded the work by presenting the expression for the deformation of the tube when axial, bending and torsional structural stiffnesses are accounted for. We noticed in this case of simple torsion that the axial stiffness couples with the bending and torsion stiffnesses, unlike simple tension.

In a recent paper (Chen et al., [9]), the radial elastic modulus of the original Molecular Structure Mechanics model (MSM) was compared to the one from the Molecular Dynamics (MD) simulation. In that paper, it was pointed to the fact that a modification to the original MSM model was suggested in our previous paper (Kasti, [1]).

In this chapter, we extend our previous work to armchair carbon nanotubes under simple tension. In addition, we summarize the equivalent results for zigzag CNTs under simple tension and torsion.

We start with a brief review of molecular and structural mechanics and we refer to the work of Chang and Gao [3]. Then, the relation between the structural bending stiffness EI/a and the molecular bond bending stiffness C is derived for the case of simple tension. This shows that EI/a depends on the bond bending stiffness C and the torsional angle φ. In the limit of an infinite tube radius, which represents a graphene sheet, we recover the previous relation, i.e., EI/a tends to $C/2$. Finally, an expression for the Young's modulus is presented that accounts for the axial, bending and torsional deformations. We conclude the chapter with numerical simulations that validate the results.

2. Bond Energies and the Finite Element Method

This section deals with the molecular and structural mechanics formulations of bond energies. Also, a short review of the finite element method is presented as it applies to the modeling of carbon nanotubes subjected to mechanical loading.

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2.1. Characterization of the Atomic Structure and Molecular/Structural Mechanics of Carbon Nanotubes (CNTs)

The geometry of a CNT could be described with the pair (*n*,*m*), the lattice translational indices, and the bond length *a*. In general, the diameter *d* of a CNT is defined using the expression

$$d = \frac{\sqrt{3}a}{\pi}\sqrt{\mathrm{n}^2 + \mathrm{m}^2 + \mathrm{nm}} \tag{1}$$

For zigzag CNTs (Fig. 1a), the value of *m* is zero. In this case, the diameter is simply given by the formula $d = \frac{\sqrt{3}an}{\pi}$. However, for armchair CNTs (Fig. 1b), the value of *m* is equal to *n*. In this case, the diameter is given by the formula $d = \frac{3an}{\pi}$.

The bond energies between carbon atoms include the stretching U_a, bending U_b and torsional U_t energies. For small distortions from equilibrium, these energies could take the forms:

$$\begin{aligned} U_a &= \frac{1}{2}K(r - r_o)^2 \\ U_b &= \frac{1}{2}C(\Theta - \Theta_o)^2 \\ U_t &= \frac{1}{2}C_t(\Phi - \Phi_o)^2 \end{aligned} \tag{2}$$

where *K*, *C*, and C_t are the bond stretching, bending and torsional stiffnesses.

r, Θ, and Φ are the stretched position, bending and torsional angles, respectively.

The subscript "$_o$" refers to the initial equilibrium configuration.

As far as structural mechanics, the linear elastic deformation is assumed to be the combination of axial, bending and torsional deformations. Their corresponding strain energies are expressed as:

$$\begin{aligned} U_{axial} &= \frac{1}{2}\int EA\left(\frac{du}{dx}\right)^2 dx \\ U_{bending} &= \frac{1}{2}\int EI\left(\frac{d\theta}{dx}\right)^2 dx \\ U_{torsion} &= \frac{1}{2}\int GJ\left(\frac{d\phi}{dx}\right)^2 dx \end{aligned} \tag{3}$$

where *EA*, *EI*, and *GJ* are the axial, bending and torsional stiffnesses; and u, θ and φ are the axial, bending and torsional deformations, respectively.

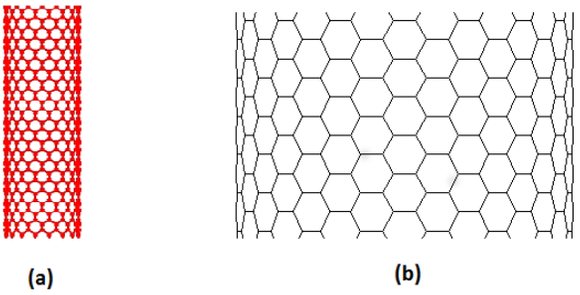

Figure 1. Carbon Nanotubes: (a) Zigzag, (b)Armchair.

2.2. Review of the Finite Element Method for 3D Space Frames

For linear elastic behavior of 3D space frames, the axial, bending and torsional strain energies can be expressed as in equation (3).

The bonding between two carbon atoms is modeled by placing a 3D space frame element between them, Fig. 2. When this procedure is repeated throughout the tube, a finite element mesh is obtained with the carbon atoms becoming the nodes in the mesh.

Each node is assumed to have six degrees of freedom, three translational and three rotational.

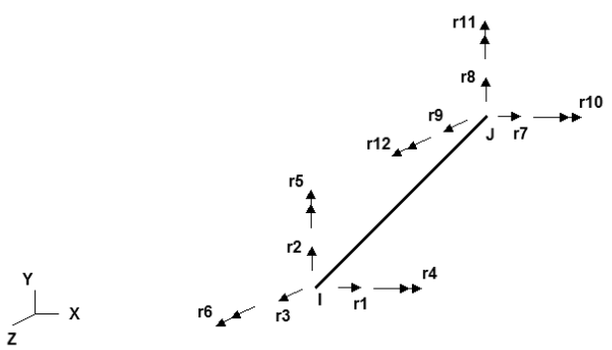

Figure 2. Space frame element.

The stiffness matrix *K* relating the degrees of freedom to their corresponding forces and moments at both ends of a 3D frame element is a 12x12 matrix.

$$K = \begin{bmatrix} K_{ii} & K_{ij} \\ K_{ij}{}^{T} & K_{jj} \end{bmatrix} \tag{4}$$

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3. Work of Chang and Gao [3]

Chang and Gao derived closed form expressions for carbon nanotubes subjected to simple tensile loading using molecular mechanics.

Representing units of zigzag and armchair carbon nanotubes are shown in Fig. 3 with α and β being the internal angles. Equivalent equations to the ones of Chang and Gao will be derived in the next section for the armchair CNT.

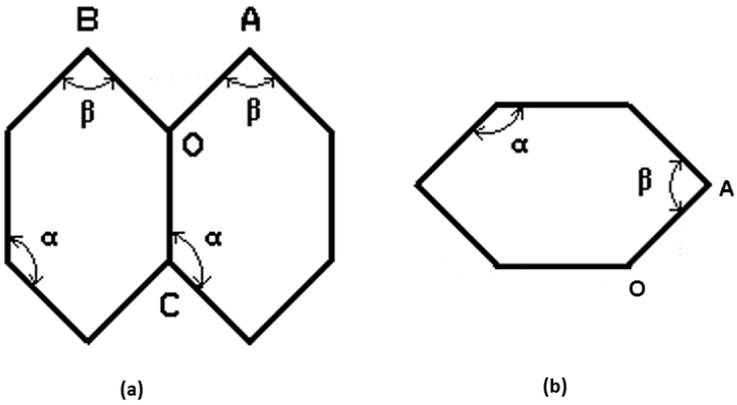

Figure 3. a) Two units of a zigzag CNT. (b) One unit of an armchair CNT.

4. Axial and Bending Stiffnesses of Armchair CNTs: Molecular versus Structural Mechanics

We start by expressing the results of Chang and Gao [3] in a more suitable form using the principle of minimum total potential energy. We will split the approach into bond stretching and bond bending deformations.

4.1. Bond Stretching – Molecular/Structural Mechanics

Due to bond stretching, it is easy to verify that $K = EA/a$.

We start with the molecular energy expression

$$\Pi = \sum_1 \frac{1}{2} K(u - u_o)^2 - \sum_2 F\Delta \tag{5}$$

where F is the axial load applied to a single carbon atom, Δ is the deflection of the end of the tube, Σ_1 is a summation over the number of bonds and Σ_2 is the summation over the number of atoms with applied loads.

Expression (5) takes the following form in structural mechanics:

$$\Pi = \sum_1 \frac{1}{2} (EA/a)(u - u_o)^2 - \sum_2 F\Delta \tag{6}$$

Since both K and EA/a are conjugate to the axial deformation between carbon atoms in the energy equation, they represent the same axial stiffness. Thus,

$$K = EA/a \tag{7}$$

To determine the tube deformation, we let n_u be the number of vertical units of Fig. 3 in a carbon nanotube and n_v equal to $(2n_u–1)$. The deflection at the end of the tube due to axial bond deformations can be expressed as:

$$\Delta = \frac{2n_v F \sin^2(\alpha/2)}{(EA/a)} \tag{8}$$

4.2. Bond Bending – Molecular Mechanics

Due to bond bending, the total potential energy is written as:

$$\prod = \sum_1 \frac{1}{2} C(\alpha - \alpha_0)^2 + \sum_2 \frac{1}{2} C(\beta - \beta_0)^2 - \sum_3 F\Delta \tag{9}$$

Let n_x be the number of units along the circumference and n_v the number of vertical units. Then, for an infinite cylinder with no end effects,i.e., all units have the same deformation, Π will be equal to:

$$\prod(\alpha, \beta, \Delta) = \frac{1}{2}[2n_x(2n_v - 1)]C(\alpha - \alpha_0)^2 + \frac{1}{2}[4n_x(2n_v - 1)]C(\beta - \beta_0)^2 - (2n_x F)\Delta$$

Minimizing the total potential energy with respect to α gives

$$d\Pi/d\alpha = n_x[(2n_v - 1)C(\alpha - \alpha_0) + 2(2n_v - 1)C(\beta - \beta_0)d\beta/d\alpha - Fd\Delta/d\alpha] = 0$$

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Since cosβ = -cos(π/2n)cos(α/2) and cosφ = tan(α/2)/tan(β), we get dβ/dα = cosφ/2, where φ is the torsion angle between the planes of adjacent units of an armchair nanotube (Fig. 3).

The vertical deformation of the tube can be expressed as:

$$\Delta = H - H_0 = (2n_v)a(\sin(\alpha/2) - \sin(\alpha_0/2)) \tag{10}$$

where H_o,H are the initial and current heights of the tube, respectively. Differentiating Eq. (10) with respect to α

$$d\Delta \Big/ d\alpha = \frac{1}{2}(2n_v)a\cos(\alpha \Big/ 2)$$

Solving for $\Delta\alpha$ by minimizing the total potential energy, we get

$$\Delta\alpha = \alpha - \alpha_0 = Fa\cos(\alpha/2)/(2C + C\cos^2\phi) \tag{11}$$

Substituting $\Delta\alpha$ in Eq. (10) above, we get the following expression for the vertical deflection of an infinitely long CNT (due to bond bending only)

$$\Delta = \frac{(2n_v)Fa^2\cos^2(\frac{\alpha}{2})}{4C + 2C\cos^2\phi} \tag{12}$$

In the next Section, we will derive an equivalent expression in terms of the material properties of structural mechanics. This will allow us to deduce a relation between *EI*/*a* and *C*.

4.3. Bond Bending - Structural Mechanics: Armchair Carbon Nanotube under Simple Tension

Let *O* and *A* be two atoms on the CNT with coordinates (*R*cos(-θ/2), *R*sin(-θ/2), *0*) and (*R*cos(-π/*n*+θ/2), *R*sin(-π/*n*+θ/2), *a sin*(α/2)), respectively. The angle θ is given by $2R^2(1-\cos\theta)=a^2$.

Also, let *u* be the unit vector from *O* to *A* expressed as:

$$\boldsymbol{u} = u_1\boldsymbol{i} + u_2\boldsymbol{j} + u_3\boldsymbol{k} \tag{13}$$

where *i*, *j* and *k* are the unit vectors in the Cartesian coordinate system.

For an infinite cylinder and due to symmetry, the radial and tangential rotations at *O* and *A* are zero.

In addition, due to multiple symmetries (for n=4,8,12,16,..), we assume the displacement and rotation fields at O and A take the following forms:

$$\begin{aligned} \boldsymbol{\delta r}_o &= \delta \boldsymbol{i} \\ \boldsymbol{\delta r}_A &= \delta \sin(-\pi / n)\boldsymbol{i} + \delta \cos(-\pi / n)\boldsymbol{j} + \Delta \boldsymbol{k} \end{aligned} \tag{14}$$

and

$$\begin{aligned} \boldsymbol{\theta}_o &= \theta \boldsymbol{k} \\ \boldsymbol{\theta}_A &= -\theta \boldsymbol{k} \end{aligned} \tag{15}$$

where (δr_o, δr_A) and (θ_o, θ_A) are the displacements and rotations vectors at O and A respectively. In this work, small displacements and rotations are assumed. Without loss of generality, the tensile load at each carbon atom is assigned a value of one.

Following a similar procedure to Kasti [1], one can show that θ is equal to zero.

And, the only force in the inclined member OA in Fig. 3 is the vertical force F and the moment is (1/2)F.a.sin(α/2).

Due to multiple symmetries (for n=4,8,12,16,..), and after some simplifications, the axial deflection at the end of the whole CNT is given by:

$$\Delta = \frac{(2n_v)Fa^2 \cos^2(\frac{\alpha}{2})}{12(EI/a)} \tag{16}$$

and the corresponding elastic modulus Y_s

$$Y_s = \frac{8EI \sin(\frac{\alpha}{2})}{a^3 \cos^2(\frac{\alpha}{2})} \tag{17}$$

Zigzag CNTs under simple tension

The corresponding axial deformation at the end of a zigzag CNT under simple tension is given by [1]:

$$\Delta = \frac{(n_v + 1)Fa^2 \sin^2 \alpha}{(EI/a)[24 - 36\gamma/(1+\gamma)]} \tag{18}$$

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$$\text{with} \quad \gamma = 2\left(1-\cos\left(\pi/n\right)\right)/\left(3-2\left(R/a\right)^2\sin^2\left(\pi/n\right)\right) \tag{19}$$

Zigzag CNTs under simple torsion

The tangential deformation at the end of a zigzag CNT unit under simple torsion is given by following expression for Δ_B [2]:

$$\Delta_B = -\frac{Fa^2(1+2\cos^2\left(\frac{\pi}{2n}\right))}{48.(\frac{EI}{a}).\cos^2(\frac{\pi}{2n})}. \tag{20}$$

5. Discussion and Validation of the Results obtained in Section 4 – Armchair CNTs

Comparing the molecular mechanics expression Eq. (12) with the structural mechanics Eq. (16), we obtain

$$\frac{EI}{a} = \frac{C}{6}[2+\cos^2\phi] \tag{21}$$

Thus, in general, the bending stiffness to be used in the structural mechanics varies with the bond bending stiffness C and torsional angle φ.

For long CNT tubes with large diameters, $cos^2(\varphi) \rightarrow 1$ and $EI/a \rightarrow C/2$, which is the same result derived by Kasti [1] for the particular case of a graphene sheet.

To validate the closed form solution Eq. (16), we compared the axial deformation of member OA (Fig. 3) and the change in radius to the results from a finite element model in ABAQUS [14]. The results are shown in Tables 1 and 2 below for C=1.42 nN.nm.rad^{-2}. The accuracy obtained is excellent.

Lattice Translational Index, n	Molecular/Structural Mechanics	ABAQUS
4	5.9844	5.9849
8	5.9477	5.9470
12	5.9358	5.9358
16	5.9310	5.9306

Table 1. Vertical deformation of member OA (x10^{-4}).

Lattice Translational Index, n	Molecular/Structural Mechanics	ABAQUS
4	-1.3538	-1.3539
8	-2.6402	-2.6401
12	-3.9383	-3.9383
16	-5.2403	-5.2402

Table 2. Change in radius (x10^{-3}).

Zigzag CNTs under simple tension

For zigzag CNT under simple tension, the equivalent stiffness is given by [1]:

$$\frac{EI}{a} = \frac{4C + 8C\cos^2\phi}{24 - 36\gamma/(1+\gamma)} \tag{22}$$

Thus, in general, the bending stiffness to be used in the structural mechanics varies with the bond bending stiffness C, torsional angle φ and γ.

For long CNT tubes with large diameters, $\cos\varphi \rightarrow 1$, $\gamma \rightarrow 0$ and $EI/a \rightarrow C/2$, which is the same result for the particular case of a graphene sheet.

Zigzag CNTs under simple torsion

For a zigzag CNTs under simple torsion, the corresponding stiffness is given by [2]:

$$\frac{EI}{a} = \frac{C}{6}\left[1 + 2\cos^2\left(\frac{\pi}{2n}\right)\right]. \tag{23}$$

Thus, in general, the bending stiffness to be used in structural mechanics varies with the bond bending stiffness C and lateral translational index n.

For long CNT tubes with large diameters, $n \rightarrow \infty$, $\cos(\frac{\pi}{2n}) \rightarrow 1$ and $EI/a \rightarrow C/2$.

6. Deformation of Armchair CNTs due to Axial, Bending and Torsional Structural Stiffnesses

In Sections 4 and 5, a closed form expression was developed for the deformation of infinitely long armchair CNT under simple tension. It included the axial and bending stiffnesses of 3D frame elements. In this Section, we study the effect of the torsional stiffness of 3D space frames.

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6.1. Bond Bending and Torsion - Structural Mechanics: Armchair Nanotube under Simple Tension

Similar work to Kasti [1] will show that the torsional stiffness does not enter the expression for the deformation of an infinitely long armchair carbon nanotube under simple tension.

When the axial, bending and torsional deformations are combined, we obtain the following formula:

$$\Delta = \frac{2n_v F \sin^2(\alpha/2)}{(EA/a)} + \frac{(2n_v)Fa^2\cos^2(\frac{\alpha}{2})}{12(EI/a)} \tag{24}$$

To validate the closed form expression of Eq. (24), we compared the vertical deformation of member OA (Fig. 3) and the change in radius to the results from a finite element model in ABAQUS. The results are shown in Tables 3 and 4 below for K=652nN.nm^{-1} and C=1.42 nN.nm.rad^{-2}. The accuracy obtained is excellent.

Lattice Translational Index, n	Molecular/Structural Mechanics	ABAQUS
4	1.7686	1.7686
8	1.7500	1.7500
12	1.7461	1.7461
16	1.7446	1.7446

Table 3. Vertical deformation of member OA (x10^{-3}).

Lattice Translational Index, n	Molecular/Structural Mechanics	ABAQUS
4	-0.53131	-0.53136
8	-0.96001	-0.96001
12	-1.4088	-1.4088
16	-1.8634	-1.8634

Table 4. Change in radius (x10^{-3}).

The contribution of each of the bond stiffnesses (axial, bending and torsion) to the total vertical deformation of an armchair carbon nanotube is shown in the following example.

Two long carbon nanotubes (40 armchair carbon units) with lattice translational indices "n" equal to 4 and 16, respectively, are modeled using MSC/Nastran [15]. The tubes are supported at the bottom and subjected to tensile loading at the top.

The resulting vertical deformations are compared to the closed form solution of Eq. (24), as shown in Fig. 4. In spite of the difference in boundary conditions between the closed form solution and the finite element modeling, the errors in the results are less than 3%.

Zigzag CNTs under simple tension

Going through the same manipulations as for an armchair CNT, the vertical deformation at the end of a zigzag CNT under simple tension that accounts for bending and torsional deformations can be expressed as [1]:

$$\Delta = \frac{(n_v + 1)Fa^2 \sin^2 \alpha}{(EI/a)[24 - 36\gamma/(1+\gamma)]} \tag{25}$$

where F is the load applied at a carbon atom, n_u is the number of vertical units of Fig. 3 and $n_v = (2n_u - 1)$. However, in this case, γ takes on the following expression:

$$\gamma = 2\left(1 - \cos(\pi/n)\right) / \left(3 - 2(R/a)^2 \sin^2(\pi/n)(1-\lambda)\right) \quad \text{and} \quad \lambda = GJ/EI \tag{26}$$

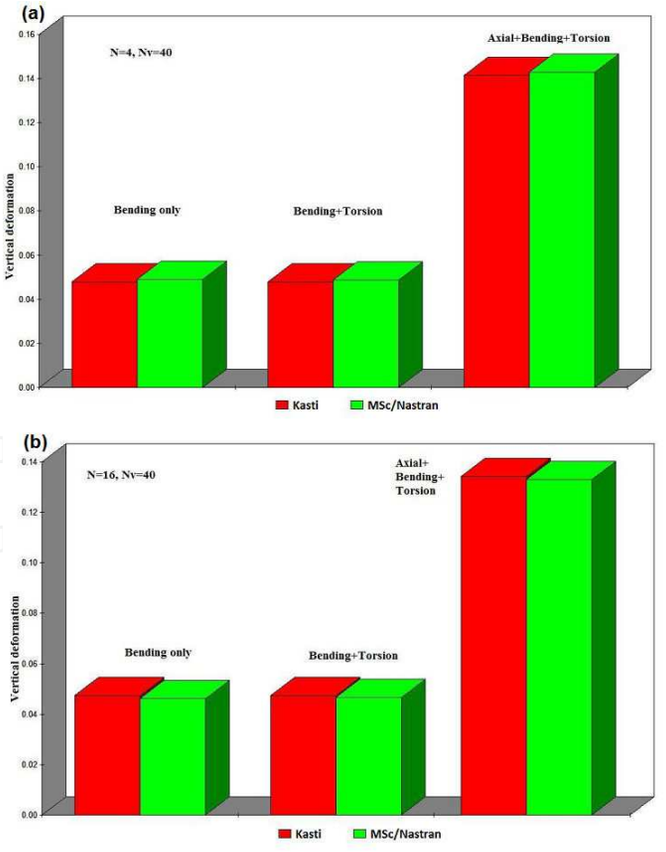

Figure 4. Vertical deformations of armchair carbon nanotubes with lattice translational indices of 4 and 16, respectively. Three cases are considered: 1) bending stiffness only, 2) bending + torsion and 3) axial+bending+torsional.

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Zigzag CNTs under simple torsion

When the torsional stiffness of 3D frame elements is included, in addition to the axial and bending deformations, the tangential deformation Δ_B of a zigzag CNT under simple torsion takes the following form [2]:

$$\Delta_B = \frac{N^T KN}{D^T KD} \tag{27}$$

where N and D are 6x1 vectors function of n, the lattice translational index, and a, the bond length. KN and KD are 6x1 vectors of structural stiffnesses. These vectors could be expressed as:

KN = [$(EI/L)^3$ $(EI/L)^2(GJ/L)$ $(EA/L)(GJ/L)^2$ $(EA/L)(EI/L)(GJ/L)$ $(EI/L)(GJ/L)^2$ $(EA/L)(EI/L)^2$]^T

KD = [$(EI/L)^4$ $(GJ/L)(EI/L)^3$ $(EA/L)(GJ/L)^2(EI/L)$ $(EA/L)(EI/L)^2(GJ/L)$ $(EI/L)^2(GJ/L)^2$ $(EA/L)(EI/L)^3$]^T

N = [N1 N2 N3 N4 N5 N6]^T,D = [D1 D2 D3 D4 D5 D6]^T

For example, for n=4,

N = [-21.1721 -24.53 -0.0015 -0.0969 -0.4074 -0.0832]^T

D = [0. $-2.3062\text{x}10^3$ -0.4408 -76.1719 497.0279 -62.4643]^T

One point worth mentioning is that when the torsional stiffness is neglected, i.e. $GJ/L \to 0$, Δ_B from Eq. (27) takes the form:

$$\Delta_B = \frac{N1*(EI/L)^3 + N6*(EA/L)*(EI/L)^2}{D6*(EA/L)*(EI/L)^3} = \frac{N1/D6}{(EA/L)} + \frac{N6/D6}{(EI/L)}.$$

Thus, in this case of negligible torsional stiffness, the axial and bending deformations are decoupled.

6.2. Elastic Modulus of an Armchair CNT

Similar to the previous work by Kasti [1], an elastic modulus Y_s (Tpa.nm) could be defined that doesn't include the thickness of CNTs, and is expressed as:

$$Y_s = \frac{F_t}{2\pi R(\Delta/L)} = \frac{2L}{3a\Delta} \tag{28}$$

where F_t (equal to 2nF with F=1) is the total load applied, L and R are the length and radius of the tube, respectively.

For a finite length cylinder, the elastic modulus obtained from the closed form expressions of Eq. (28) and ABAQUS are compared in Table 5 for a lattice translational index of 4 and variable tube length. The following values of stiffnesses were used:

EA/a = 652 nN.nm^{-1}, EI/a = 0.875 nN.nm.rad^{-2} and GJ/a = 0.278 nN.nm.rad$^{-2.}$

The closed form results compare very well with the values from ABAQUS.

Lattice Translational Index, n	n_v=40,60 (Eq. 28)	n_v=40 (ABAQUS)	n_v=60 (ABAQUS)
4	358.12	358.284	358.307

Table 5. Elastic Modulus (nN.nm^{-1}).

Zigzag CNTs under simple torsion

Similar to the definition of an elastic modulus Y_s (Tpa.nm) that doesn't include the thickness of CNTs [1], an elastic shear modulus Gs (Tpa.nm) could be defined as [2]:

$$G_s = \frac{T}{(\frac{\varphi}{L})*2\pi R^3} = \frac{nFR}{(\frac{\varphi}{L})*2\pi R^3} = \frac{n}{(\frac{\varphi}{L})*2\pi R^2} \tag{29}$$

where T is the torsional moment applied to the tube, F is the tangential load applied to a single carbon atom which can be taken as unity, L and R are the length and radius of the tube, respectively.

7. Conclusions

Relations between the structural bending stiffness EI/a and the molecular bond bending stiffness C for carbon nanotubes were derived for the cases of simple tension and torsion. In addition, expressions for the deformations and "Young's moduli" of these nanotubes were presented that account for the axial, bending and torsional effects.

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