CONTINUUM SIMULATION OF TENSILE, BENDING AND TORSIONAL RIGIDITIES OF MULTI-WALLED CARBON NANOTUBES

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Keywords: Multi-walled carbon nanotubes, Finite element analysis, Representative volume element

Abstract. *In this paper, continuum mechanics are combined with molecular mechanics to evaluate the tensile, bending and torsional rigidities of multi-walled carbon nanotubes (MWCNTs). Analysis is conducted by means of beam FE models. The elastic moduli of carbon-carbon bonds are derived using a linkage between molecular and structural mechanics while the van der Waals forces between adjacent tubes are simulated using the Lennard-Jones potential. The adopted approach is successfully verified against results from the literature. A significant effect of van der Waals forces on the elastic behavior of MWCNTs is found for small strains. On the contrary, for large strains, the effect diminishes and the behavior of MWCNTs is equal to the aggregated behavior of the constituent nanotubes. Besides the useful information about the elastic behavior of MWCNTs, the paper proposes a simplified method for representing MWCNTs as continuum mediums. In order to demonstrate the method, the tensile response of a representative volume element of a MWCNT-reinforced polymer is modeled.*

1 INTRODUCTION

In view of the prospective use of carbon nanotubes (CNTs) as reinforcements in the next generation of composite materials, their effectiveness in this role is currently being extensively studied. The performance of a composite material system is critically controlled by the characteristics of the interface between the reinforcement and the matrix. However, in cases where multi-walled CNTs (MWCNTs) are used as reinforcements, an equally critical issue is the load transfer between the adjacent tubes; an increased load transfer is required in order for a portion of loading to be transferred from the outer to the inner tubes. Contrary to the application of MWCNTs as reinforcements, their use in nanoelectromechanical devices as support shafts in rotational actuators [1], linear bearings [2] and torsion springs in resonant oscillators [3] requires an easy slide or rotation of the adjacent tubes with respect to each other. In any case, the precise knowledge of the load transfer between the tubes of MWCNTs and how it may be affected by the structural characteristics of the tubes necessitates. The need is increased by the fact that many geometrical and structural characteristics of the CNTs are still undetermined.

Towards the establishment of MWCNTs' role in the above mentioned applications, there is a demand for developing efficient modeling techniques. During the first years of CNT research, atomistic models have being solely used. However, in the last few years, they are being progressively replaced by continuum methods mainly due to the huge computational effort they require. Continuum methods used so far may be classified into three categories: atomistic-based continuum methods, analytical/micromechanical methods and numerical methods. In the first category belong the models that draw data from atomistic methods, such as molecular dynamics and force-fields, for the behavior of CNTs and the interfacial load transfer between the nanotube and the matrix, and assign them in a representative unit cell whose elastic properties are evaluated using continuum methods. For example, Odegard et al. [4] modelled the nanotube, the local polymer near the nanotube and the nanotube/polymer interface as an effective continuum fibre by using an equivalent-continuum model. The

effective fibre retains the local molecular structure and bonding information, as defined by molecular dynamics, and serves as a means for linking the equivalent-continuum and micromechanics models. The micromechanics method is then available for the prediction of bulk mechanical properties of single-walled CNT/polymer composites. The main drawback of the atomistic-based continuum methods is that they involve very complicated analyses and huge computational efforts imposed by the incorporated atomistic method. In the second category, belong the analytical and micromechanical models well established in fiber-reinforced composites. These methods have been mainly used for modelling the interfacial load transfer between the nanotube and the matrix. Exception is the work of Seidel and Lagoudas [5] who obtained the effective elastic properties of CNT-reinforced composites through a variety of micromechanical techniques. Although the analytical/ micromechanical methods provide detailed information about the interaction between the nanotube and the matrix, they are locally oriented, thus being inapplicable in larger scale systems such as nanocomposite specimens. Contrary to the previous two methods, for which a considerable number of works have been published, the use of numerical approaches is restricted to the use of the FE method either as supporting method to obtain necessary data [6] or as verification method [5].

Recently, Papanikos et al. [7] proposed a concept to evaluate equivalent beams possessing identical mechanical behavior with CNTs. Using the concept, CNTs are replaced with beams that can be analyzed by classical continuum methods, such as the FE method, thus simplifying the efforts required to model CNT-based applications. In this paper, the concept is extended to MWCNTs.

2 THE EQUIVALENT BEAM

The concept of the 'equivalent beam' is based on the condition of identical mechanical behavior between the CNT and the beam, which corresponds to identical tensile, bending and torsional behaviors. As for elastic beams, these behaviors are designated by the corresponding rigidities and in order to fully define the equivalent beam, it suffices to evaluate its equivalent properties (geometrical characteristics and elastic moduli) from the nanotube's rigidities.

2.1 FE analysis of CNTs: derivation of bond rigidities

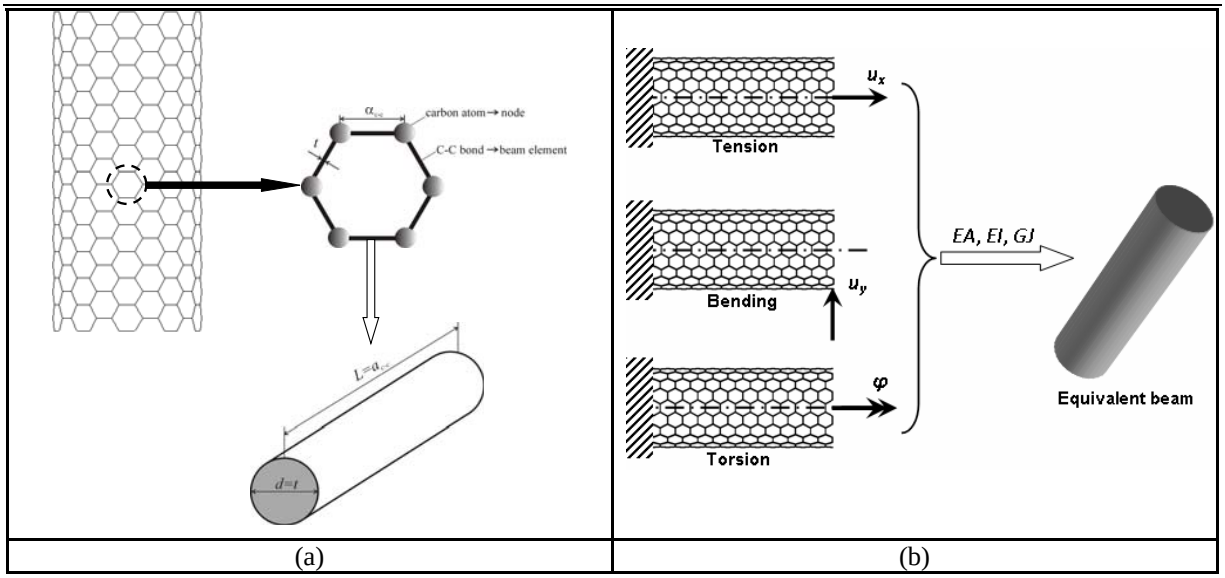
In order to derive the nanotube's rigidities, a 3D FE model, which treats CNTs as space-frame structures, is created, as shown in Figure 1(a). Using 3D elastic beam elements and the ANSYS commercial FE code, the exact atomic structure of the nanotubes is modeled. The elastic moduli of the beam elements are determined using a linkage between molecular and continuum mechanics. The following relationships between the structural mechanics parameters and the molecular mechanics parameters are obtained

$$\frac{E_b A_b}{\ell} = k_r, \qquad \frac{E_b I_b}{\ell} = k_\theta, \qquad \frac{G_b J_b}{\ell} = k_\tau \tag{1}$$

Here, ℓ is the bond length equals to 0.1421 nm; E_b and G_b are the bond's Young's modulus and shear modulus, respectively; I_b and J_b are the moment of inertia and polar moment of inertia, respectively, and k_r , k_θ and k_τ are the bond stretching, bond bending and torsional resistance force constants, respectively. Assuming a solid circular cross-sectional area of the beams with diameter d and setting $A_b = \pi d^2 / 4$, $I_b = \pi d^4 / 64$ and $J_b = \pi d^4 / 32$, Eqs.(1) give

$$d = 4\sqrt{\frac{k_\theta}{k_r}}, \quad E_b = \frac{k_r^2 \ell}{4\pi k_\theta}, \quad G_b = \frac{k_r^2 k_\tau \ell}{8\pi k_\theta^2} \tag{2}$$

Eqs.(2) give all necessary input parameters for the beam elements. In the present study, the following values were used for the force constants [8,9]: k_r =6.52 x 10^{-7} N/nm, k_θ =8.76 x 10^{-10} N nm/ rad $^{-2}$, and k_τ =2.78 x 10^{-10} N nm/ rad $^{-2}$. However, since the modeling of the bond is done using beam elements, it is clear that the results of the analyses would be the same as long as the rigidities $E_b A_b$, $E_b I_b$, $G_b J_b$ of the bond are the same. The constant values of the rigidities arise directly from Eqs.(1): $E_b A_b$ =92.65 nN, $E_b I_b$ =0.1245 nN nm^2 and $G_b J_b$ =0.0395 nN nm^2.



(a) (b)

Figure 1. Finite element modeling of the nanotube as a space-frame structure: (a) bond modeling, and (b) the equivalent beam concept.

2.2 Derivation of CNT rigidities

Since the nanotube possess a linear behavior, to derive the rigidities it is sufficient to apply in the FE model an arbitrary displacement such as to load the nanotube in tension, bending and torsion. The boundary and loading conditions for each case are depicted in Figure 1(b). To simulate tension, an axial displacement u_x is applied at one nanotube's end having the other end fixed. Evaluating the reaction force F_x from the FE analysis, the tensile rigidity is evaluated as $EA = F_x L / u_x$, where L is the nanotube length. To simulate bending, a transverse displacement u_y is applied at one nanotube's end having the other end fixed. Evaluating the reaction force F_y from the FE analysis, the bending rigidity is evaluated as $EI = F_y L^3 / u_y$. To simulate torsion, an angle of twist φ is applied at one nanotube's end having the other end fixed. Evaluating the reaction torque T from the FE analysis, the torsional rigidity is evaluated as $GJ = TL / \varphi$.

The intertube vdW forces are simulated using the "6-12" Lennard-Jones potential $U(r)$ and the vdW forces are given by

$$F_{vdW} = -\frac{dU(r)}{dr} = 24\frac{\lambda}{\sigma}\left(2\left(\frac{\sigma}{r}\right)^{13} - \left(\frac{\sigma}{r}\right)^{7}\right) \tag{3}$$

where r is the distance between the interacting atoms and λ, σ are the Lennard-Jones parameters, which for the carbon atoms are equal to 3.864×10^{-4} nNnm and 0.34 nm, respectively. In the current simulation of vdW forces and in order to reduce the modeling time, the forces are applied directly on the interacting atoms in the direction of the line connecting them. The displacement at the loading end of the nanotube is applied in steps and the vdW forces are updated for each load step according to the new distance between the atoms.

2.3 Equivalent solid cylindrical beam

Consider an equivalent solid cylinder with diameter D. Its cross-section area, secondary and polar moments of inertia are given by $A = \pi D^2 / 4$, $I = \pi D^4 / 64$ and $J = \pi D^4 / 32$, Using these expressions and the rigidities values evaluated from the FE analysis, we can evaluate the equivalent diameter as $D = 4\sqrt{EI / EA}$. Then, it is easy to evaluate the modulus of elasticity and the shear modulus of the equivalent beam.

Recently, Papanikos et al. [7] evaluated the specific expressions for the rigidities for armchair and zig-zag SWCNTs as a function of the chiral index n. These expressions are:

$$(EA)_s = \alpha\left(n - n_0\right),\ (EI)_s = \beta\left(n - n_0\right)^3,\ (GJ)_s = \gamma\left(n - n_0\right)^3 \tag{4}$$

where α, β, γ and n_0 are constants for each type of nanotube (armchair or zig-zag) and can be found in [7]. The subscript s denotes the SWCNT. These simple expressions allowed the derivations of expressions for the mechanical properties and dimensions of the equivalent beams. It is clear that, in the absence of van den Waals forces, the rigidities of the MWCNTs could be easily evaluated as the sum of the rigidities of their constituents.

It is the scope of this work to evaluate the effect of the van den Waals forces on the mechanical behaviour of MWCNTs.

2.4 Numerical results

To evaluate the mechanical behaviour of MWCNTs, a number of nanotube with two walls were modelled. Early analyses revealed that nanotubes with more than two walls behave similarly to those of two walls. To evaluate the effect of intertube spacing several DWCNTs were examined, i.e. armchair (5,5)-(n,n) with n=10 to 14 and zig-zag (5,0)-(n,0) with n=14 to 18. In this way, we were able to examine intertube spacing ranging from 0.34 to 0.6 nm. Figure 2 shows a typical DWCNT and the axial displacement distribution in the case of tensile loading.

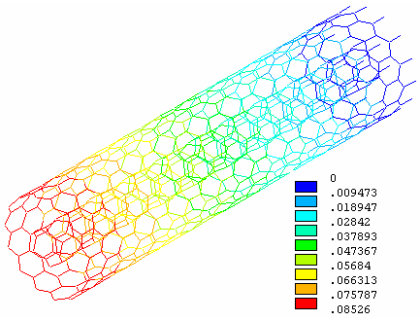


Figure 2. Typical axial displacement distribution for the (5,0)-(14,0) nanotube.

Figure 3 shows the evaluated tensile rigidities of the (5,5)-(10,10) and (5,0)-(14,0) nanotubes. The corresponding values of the rigidities without considering the effect of the vdW forces are also presented. These values are constant with respect to the applied strain and were evaluated from the summation of the rigidities of the SWCNTs using Eqs. (4). It is clear that the effect of the vdW forces is significant for small strains and diminishes for strains larger than 2%. When nanotubes are used as reinforcement in structural elements, this can be significant as the applied strains are usually small. An interesting aspect of the effect of vdW forces is shown in Figure 4, where the normalized rigidities are plot as a function of 1/strain. It is clear that the relationship is linear. Fitting the computed values with a straight line provides the following approximate relations for the tensile rigidities:

$$EA/(EA)_{s+} = B/\varepsilon + 1 \tag{5}$$

where ε the axial strain, B a fitting parameter and $(EA)_{s+}$ is the sum of the rigidities of the SWCNTs as evaluated from Eqs. (4). This relationship holds for all the nanotubes modelled. The values of the fitting parameter are presented in Figure 5 as a function of the chiral index and the corresponding intertube spacing for both armchair and zig-zag nanotubes. As expected, the smaller the spacing the more significant is the effect of the vdW forces on the tensile behaviour of the nanotube.

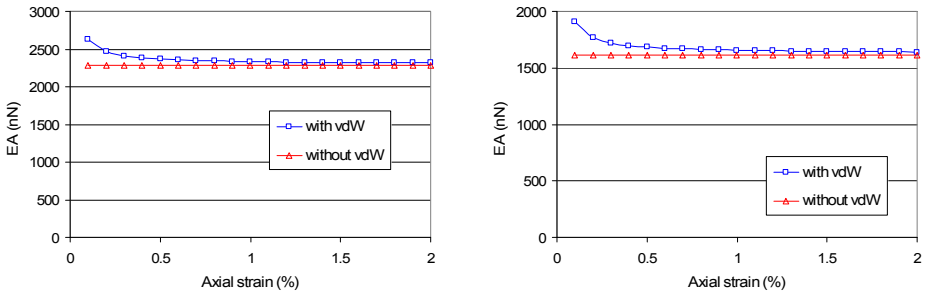
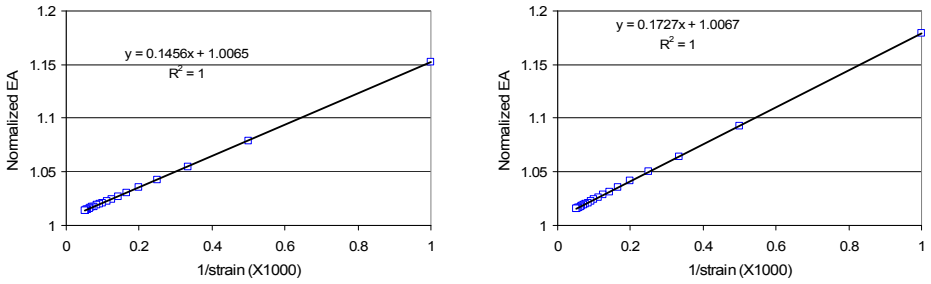
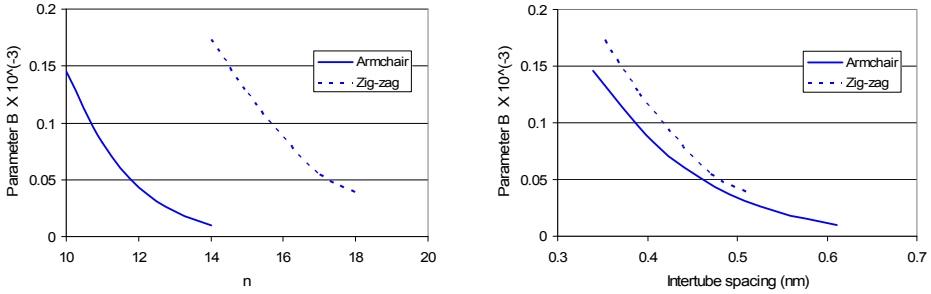


Figure 3. Tensile rigidity as a function of the axial strain: (a) (5,5)-(10,10), and (b) (5,0)-(14,0).



(a) (b)

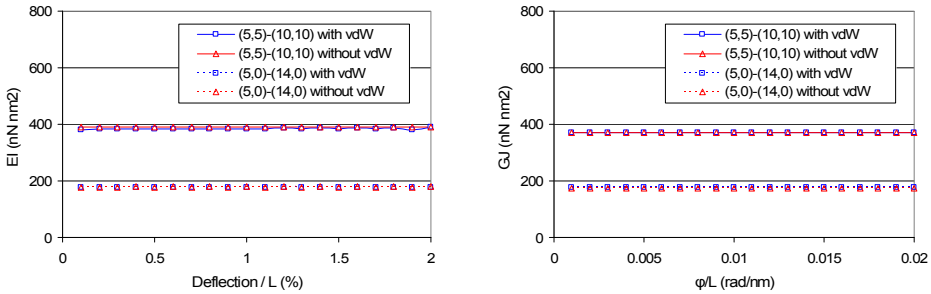
Figure 4. Normalized tensile rigidity as a function of the axial strain: (a) (5,5)-(10,10), and (b) (5,0)-(14,0).



(a) (b)

Figure 5. Parameter B as a function of (a) chiral index, and (b) intertube spacing.

Unlike the tensile rigidity, it was found that the influence of the vdW forces on the bending and torsional rigidities was negligible. Typical results are presented in Figure 6. Early examination reveals that for small transverse displacements and angles of twist, the distance between the atoms of the tubes change much less than for the case of small axial strains.



(a) (b)

Figure 6. Typical (a) bending, and (b) torsional rigidities.

2.5 Comparison with literature

It should be noted here that there are only a small number of papers dealing with the evaluation of the mechanical behaviour of MWCNTs, e.g. [10,11]. Even though there are many articles dealing with the experimental evaluation of the mechanical behaviour, the results show a large scatter and are not suitable for comparison. Using the values of the tensile rigidity as evaluated from Eq. (5) for the (5,5)-(10,10) nanotube we evaluate first the "modulus of elasticity" E by simply divided by the corresponding cross-section area as considered in [11], i.e.

$$A=\frac{\pi}{4}\left(\left(d_{1010}+\sigma\right)^2-\left(d_{0505}-\sigma\right)^2\right) \tag{6}$$

where d_{0505} and d_{1010} are the diameters of the (5,5) and (10,10) nanotubes, respectively and σ is the assumed wall thickness (=0.34 nm). The results of the "modulus of elasticity" E are shown in Figure 7. The literature values given (without considering the effect of axial strain) are 1.16 TPa [10] and 1.04 TPa [11]. These values

are within the values evaluated from the current study.

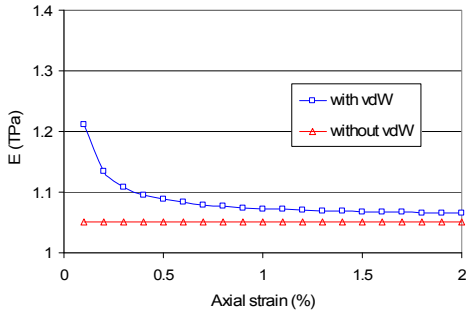
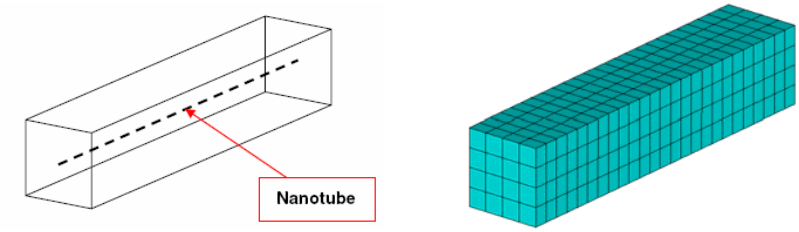


Figure 7. "Elasticity modulus" as a function of the axial strain for the (5,5)-(10,10) nanotube.

3 RVE MODELING

In order to demonstrate the usage of the equivalent beam concept in modeling of MWCNTs, the tensile behavior of an RVE of a MWCNT-reinforced polymer was modeled. The RVE is a rectangular solid whose entire volume is taken up by the matrix. In order to reduce the computational effort and make the RVE more versatile, instead of modeling the nanotube as a solid or hollow cylinder, it is superimposed to the matrix as can be seen in Fig.8(a). 3D isotropic solid elements are used for modeling the matrix while the nanotube is represented by 3D elastic beam elements created by binding the nodes of the matrix. As in the present study implementation was done in the ANSYS commercial FE code, the 3D SOLID45 and BEAM4 elements were respectively used. For the beam elements, a hollow circular cross-sectional area was adopted. A typical FE mesh of the RVE is depicted in Fig.8(b). The behavior of the beam elements was simulated using Eq.(5).



(a) (b)

Figure 8. (a) Reinforcement and (b) mesh of the RVE.

The RVE was loaded in axial tension. In Figure 9, the tensile stress-strain curve of the pure polymer is compared to the curves of the reinforced RVE for the cases of an armchair and a zigzag MWCNT for 10% volume fraction. As can be seen, the addition of MWCNTs increased dramatically the stiffness of the polymer.

Considering the simplicity of the FE model of the RVE, the procedure used for evaluating the behavior of the nanotube and that the analyses lasted a few seconds on a conventional notebook, the advantage of the approach proposed herein over the methods discussed in the Introduction becomes evident.

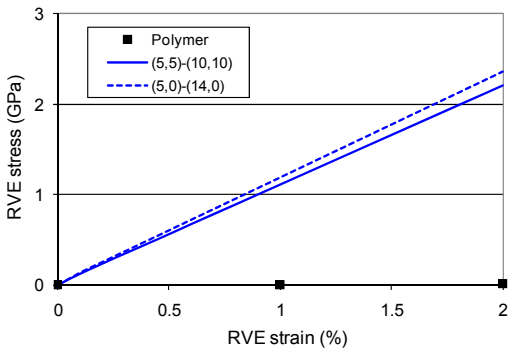


Figure 9. Stress- strain diagram of the RVE for 10% volume fraction.

4 CONCLUSIONS

In this paper, continuum mechanics are combined with molecular mechanics to evaluate the tensile, bending and torsional rigidities of multi-walled carbon nanotubes (MWCNTs) taking into account the effect of the vdW forces and the corresponding deformation. The results of the study reveal the following:

- The tensile rigidity of MWCNTs is influenced significantly by the interaction between the tubes.
- The bending and torsional rigidities of MWCNTs are unaffected by the tube interaction.
- The results of the work can be used to evaluate the mechanical behaviour of carbon nanotube – reinforced composites by simulating the nanotube as an equivalent beam.

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