INELASTIC CONTINUUM MODELING OF CARBON NANOTUBE'S BEHAVIOR USING FINITE ELEMENT METHOD

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Abstract This paper describes a continuum model for analyzing the inelastic behavior of a single walled carbon nanotube (SWCNT) in different loading conditions. Because of limitations in using molecular dynamics (and other atomic methods) to model the failure load of the SWCNT, continuum mechanics methods are considered in this paper. Based on some experimental and theoretical results, an elasto-plastic model was used to analyze inelastic behavior of carbon nanotubes. 3D FEM model of SWCNT including the "Vander-Waals" interactions was developed with advanced capabilities. The results obtained by this model in different conditions have been compared with other numerical and experimental results. The comparison shows that this method is efficient and could be expanded for numerical modeling of nano-composites.

Keywords Nanotube, Continuum, FEM, Elasto-Plastic, Inelastic

چکیده این مقاله به کاربرد مکانیک محیط پیوسته در تحلیل رفتار غیر الاستیک نانوتیوب های تک جداره در بارگذاری های گوناگون و مقایسه آن با سایر بارگذاری ها می‌پردازد. با توجه به محدودیت های روش های دینامیک مولکولی و روش های مشابه اتمی در مدل سازی این رفتار، از روش مکانیک محیط پیوسته استفاده شده است. بر پایه نتایج تئوری و عملی، مدل رفتاری الاستو پلاستیک برای این منظور مناسب تشخیص داده شده و دو مدل سه بعدی اجزای محدود با قابلیت های ویژه نظیر تغییر شکل های بزرگ برای تحلیل رفتار نانوتیوب های تک جداره در کشش و خمش ساخته شده است. در ادامه نتایج تحلیل ها در این دو حالت بارگذاری ارائه شده و با نتایج آزمایشگاهی و تئوری (دینامیک مولکولی) مقایسه شده اند. این مقایسه بیانگر سازگاری نتایج به میزان قابل قبولی بوده و مبین این مهم است که این روش می تواند به شیوه موثری در تحلیل های مشابه به کار رفته و توسعه یابد.

1. INTRODUCTION

Discovered in 1991, carbon nanotubes have continued to receive attention, both theoretically and experimentally [1]. Their special physical properties have led to suggestions of numerous applications such as nano-composites and nano-machines. Much research has been carried out on the remarkable carbon-nanotubes CNT mechanical properties in terms of its high strength, high stiffness, and large elastic strain [2,3]. Many analytical analyses on the modeling of CNTs have been conducted besides experimental work.

Two main classes of theoretical methods for analyzing these structures are atomistic based [4] and the continuum mechanics based methods [5]. The computational complexity limited the former to number of atoms in very small scale of time and length. In other hand; although some simulation results have been achieved based on the atomic models, these methods are limited to systems with a small number of molecules and atoms. Therefore these methods are restricted to a study of small-scale modeling. Unlike molecular dynamics and other atomic methods, the continuum model is the most /useful practical method for analyzing large-

scale atomic systems.

Among these continuum studies, a carbon nanotube is either modeled as a cylindrical shell [4-8] a beam or many truss members [9]. Two critical parameters in the shell model, namely the elastic modulus and virtual shell thickness, are determined by fitting the tensile and bending stiffness obtained from molecular dynamics simulations [4].

These continuum models are used several times in modeling nanotube behavior in elastic domain.

Based on some experimental and analytical results, the elastic domain in mechanical behavior of the CNT is large (more than 10-30 percent strain for perfect nanotubes [5-7]) and they are remarkably resilient, sustaining extreme strain with no signs of plasticity and other inelastic behavior.

The mathematical support of using continuum mechanic methods is achieved by energy methods and the Cauchy-born rule and their results in elastic domain as having a good agreement with other results.

Because of high stiffness of nanotubes, this structures absurd a considerable magnitude of stress during loading in composites especially after cracking. This matter may lead to inelastic behavior in tension and bending and may also cause some local and global inelastic buckling that are shown in Figure 1. In this figure, the nanotube-cracks interaction is presented. During crack opening, some buckling and inelastic behavior is observed in nanotubes and after a long elastic domain, non-reversible behavior occurs. This inelastic behavior is reported with energy absorption and more displacement till fracture that is called nano-plasticity. Plasticity of nano-material is a complex phenomenon that requires a multi-scale description involving microscopic, mesoscopic and macroscopic modeling [4] and its modeling using molecular dynamics is a tough job.

This is the reason for modeling this complex phenomenon using continuum mechanics.

Based on many MD calculations [10] transition from an elastic state to the final failure state in nanotubes occurs through a series of bond breaking and bond rearrangement processes [10]. This bond breaking is called Stone-Waales defect and is the most common defect formation in nanotubes. Formation of Stone-Waales defects in a nanotube

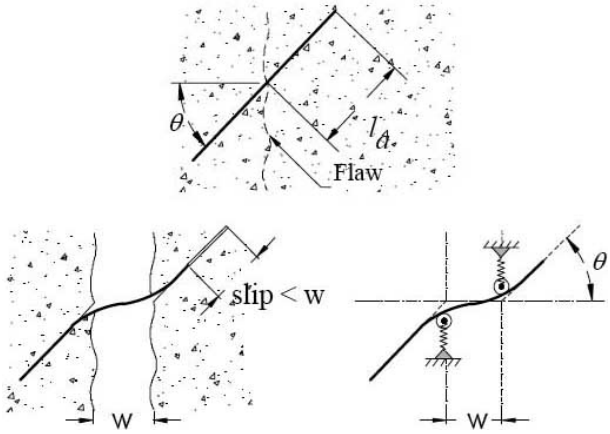

Figure 1. Interaction between nanotube and matrix in nanotube composite that may cause some inelastic buckling and tensile forces in nanotube.

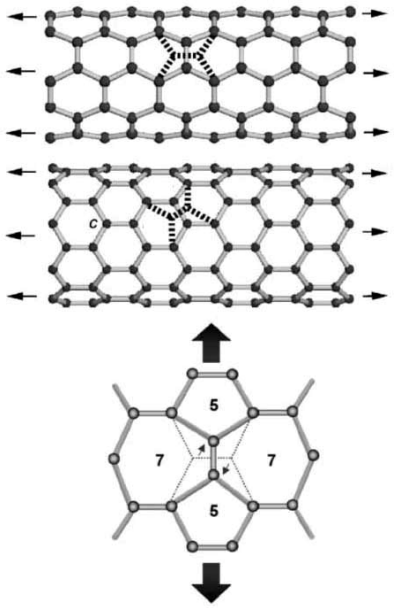

Figure 2. Starting of plastic deformation in SWCNT in tension in different internal structures (Stone-Waales phenomenon) [10,11].

typically involves a bond rotation with breakage of two existing C-C bonds and formation of two new ones that creates heptagon-pentagon pair defects in the walls of the nanotubes [10]. This

transformation is shown in Figure 2 and can occur in all types of nanotube.

In compressive loads, the plasticity could be described by reconstructing of bonds similar to tensile conditions, but their shapes are reversing [12]. Similar status happens in compression sides of SWCNT in the pure bending [12]. It is observed by high-resolution electron microscopy, when the bending deformation is due to a series of buckling in the compressive side. The minimum radius of curvature of a nanotube wall in elastic bending is thought to be 15 nm. For lower radius, inelastic behavior is seen [13]. Therefore, a nanotube bends without any change in the bonding state up to a certain critical curvature. This transformation is schematically shown in Figure 3.

In following parts of this paper, after some description of a Cauchy-born role and validation of the continuum mechanics, one simple method for modeling the inelastic behavior of carbon nanotubes is presented.

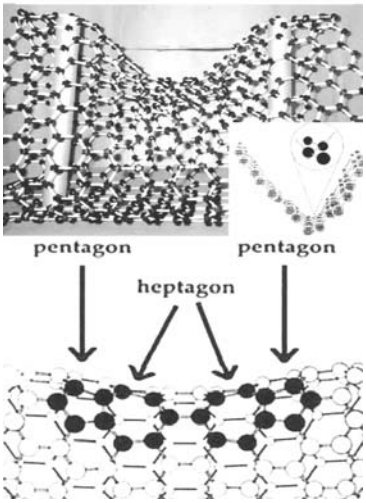

Figure 3. (Left) Stone-Waales defect in the buckling and compression side (Right) Schematic shape of structure in the buckling [13,14].

2. VALIDATION OF USING CONTINUUM MECHANICS IN CNT'S BEHAVIOR MODELING

The key rule for using the continuum mechanics in discrete systems (like the nanotube) is the Cauchy-born rule. By this rule, the displacement of a discrete system could be expressed as a continuum system. This transformation is briefly shown in Figure 4. In this figure, the mapping function Φ, changes the displacement from initial unreformed space $\Omega_0 CR^n$ to deformed space ΩCR^n, (n could be 1,2 or 3). The relationship of two spaces are defined by the $\Omega = \Phi(\Omega_0)$. If the X is a point in the undeformed space, after transformation its coordinates would be changed to $x = \Phi(X)$. In this space, F in considered the gradient of deformation and is defined by $F = D\Phi = \frac{\partial \Phi}{\partial X}$ that $dx = F(dX)$.

By using an appropriate tangential gradient; the deformation could be expressed in continuum space. This is the main basis of continuum crystal elasticity. Recently, this theory has expanded for curved structures like nanotubes.

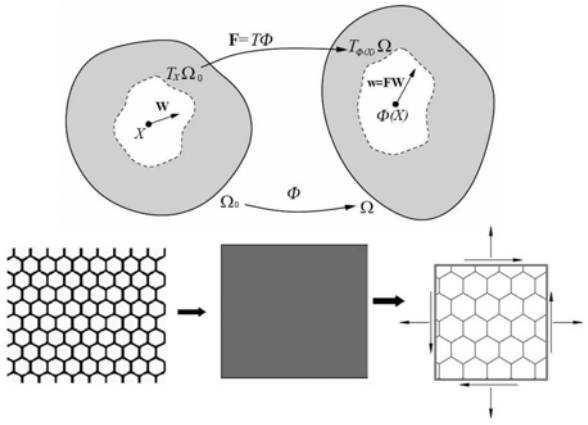

Figure 4. The Cauchy-Born description for continuum analysis of a discrete atomic system.

3. ELASTO-PLASTIC MODEL PARAMETERS

With the starting of the Stone-Waales defect, higher displacement and energy release rate occur. In order to model this defect in continuum mechanics, a simple method was applied based on equal displacement and energy release rates which is shown in Figure 5.

The overall shape of stress-strain curve of nanotube in inelastic region (simple tension) is similar to a material with elastic-plastic behavior.

Therefore with defining the assumed properties of an elastic-plastic model using the energy balance method, these assumed parameters were defined and used in this paper.

The stress-strain relationship in elasto-plastic mode is expressed as per Equation 1:

$$\sigma(\varepsilon) = \begin{cases} E_{elast}\varepsilon & \text{for} \quad \varepsilon \le \varepsilon_Y \\ E_2\varepsilon_Y & \text{for} \quad \varepsilon > \varepsilon_Y \end{cases} \quad (1)$$

In this equation, ε_Y is the yield strain and E_2 is the modulus of elasticity after yielding (see Figure 6).

In one part of this figure, the ideal elasto-plastic model is presented. In addition typical stress-strain curves of nanotubes and equivalent elasto-plastic models for nanotubes are presented in other parts of this figure.

Using this model, total energy variation in the model (the grey hatch in Figure 6) is calculated using this formula:

$$\Pi_{plastic} = t_{eq}.[(\varepsilon - \varepsilon_Y) * \sigma_Y + \frac{1}{2}E_2.(\varepsilon - \varepsilon_Y)^2] \quad (2)$$

This energy is considered as required energy for the Stone-Waales defect. The magnitude of yield strain is a key parameter in this model and depends on many parameters like diameter, internal structure and defect mapping that is assumed to be 8% according to references [4,15]. Another key value in this model is energy absorption during initiation of Stone-Waales defect and has been measured experimentally and numerically by molecular dynamics and assumed as $\Pi_{W-V} = 5.5ev$ [10].

Using these values and assuming elastic modulus as $E_{elast} = 5.5Tpa$, nanotube thickness as $t_{eq} = 0.066nm$, the second modulus of elasticity is calculated as $E_2 = 2.37Tpa$. Using this model, two FEM models are developed and their properties and results presented in the following section.

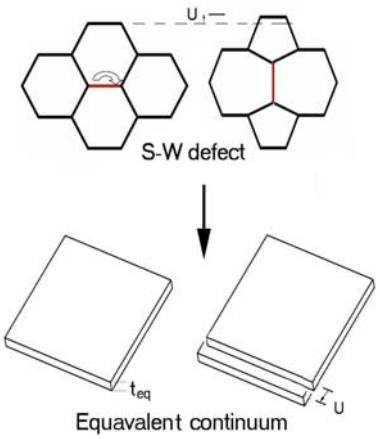

Figure 5. The virtual definition of the plastic deformation regarding the S-W defect.

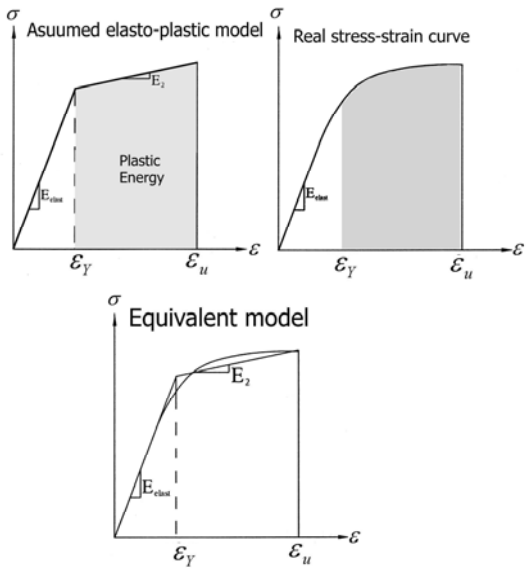

Figure 6. (Up-Left) The ideal elasto-plastic model and its main parameters: (Up-Right) The typical stress-strain graph of nanotube in tension: (Down) The mixture of upper graph.

4. FINITE ELEMENT MODELS

Two 3D FEM models were developed to analyses inelastic behavior of the single walled nanotubes in tension and pure bending using the Ansys software. In these analyses, two types of elements were used [17]:

- Four-node shell element-It was used to model the nanotube shell with six DOFs at each node and advanced features such as large deformation, buckling and plasticity.

- Non-linear links for Vander Waals interactions, this element is a uni-directional element with nonlinear force-deflection capability. The element has large displacement capabilities.

The first FEM model was performed for modeling inelastic behavior of single-walled nanotubes in simple tension. The results of this model are presented in Figure 7 and have been compared with other atomic results [16] which are presented in the lower part of this figure.

Comparison results in this figure show good compatibility between the simple FEM model and complicated atomic model. Another FEM model was performed to model the inelastic pure bending behavior of a SWCNT. To elimination shear effects, the presented beam in Figure 8 was performed. The schematic boundary condition, loading and elements of this model are shown in that figure.

Thickness and mechanical properties of this model are similar to pervious ones but Vander-Waals interactions were considered in this model. These interactions are often modeled using the Lennard–Jones potential. Non-linear springs which connect two interacting atoms (with hinged ends) simulate these interactions. The effects of these interactions are significant when opposite walls of nanotubes approach each other after kink starting.

Results of this FEM model consist of deformed shapes and plastic regions are shown in Figures 9 and 10. In addition, the moment-rotation degree curve and energy-rotation degree diagrams are shown in Figures 11 and 12.

Figure 8 shows the final deformed shape of the FEM model as compared with the image of the real deformed SWCNT in pure bending. In general, the deformed shape of the nanotube in the FEM model is similar to the real deformed shape and the overall shape of the buckled area is similar too.

According to FEM model results; there is a departure from elastic to inelastic behavior in global rotation greater than 30 degrees because of significant rotation and deformation of walls.

Also according to the results, as kinks occur,

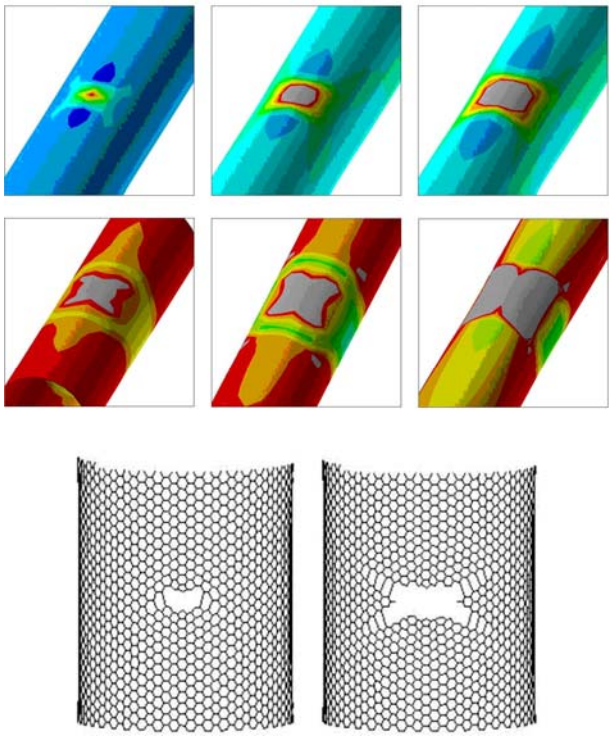

Figure 7. (Up) Results of inelastic FEM model of SWCNT in simple tension. (Down) MD results of fracture of same nanotube in tension [16].

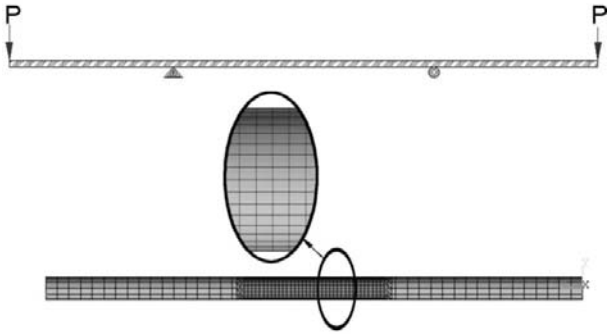

Figure 8. FEM model to analysis pure bending of SWCNT.

the oval shape of cross section deformed to an irregular shape and walls will get closer because of buckling. Because repulsive effects of Vander-Waales interactions, the minimum distance of walls in nanotubes and other atomic carbon sheets is 0.34 nm. Therefore after buckling, lack of stiffness is not similar to the macro structure. This

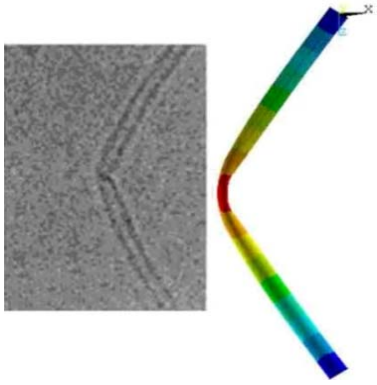

Figure 9. Comparison between (Left) A real plastic deformation of SWNT with [3] (Right) Deformed shaped of FEM model.

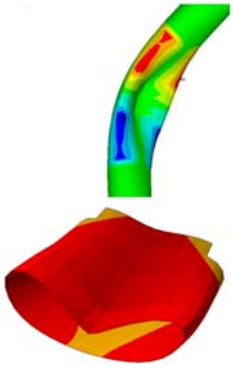

Figure 10. Result of FEM model: (Top) Plastic regions, (Below) Section of the middle part.

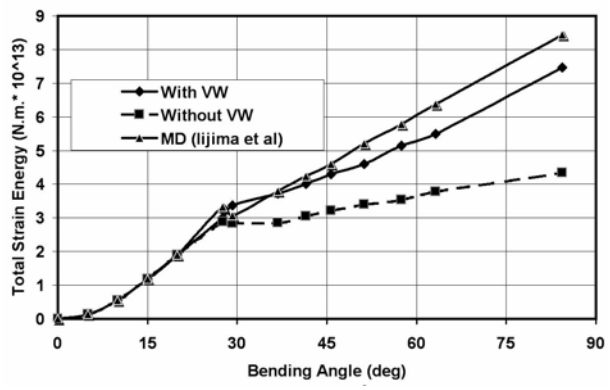

Figure 11. Comparison of the results of pure bending modeling via other results presented in [12] (Bending angle and total strain energy).

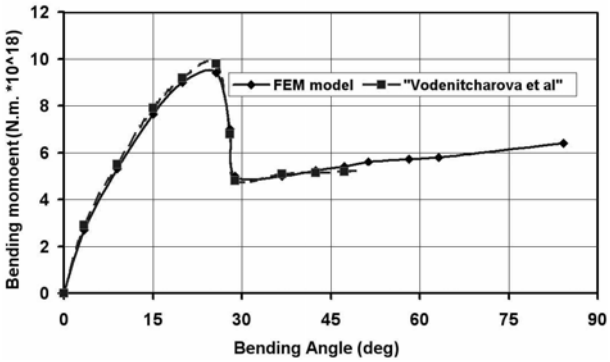

Figure 12. Comparison of the results of pure bending modeling via other results presented in [12] (Bending angle and bending moment).

issue is considered as the main reason of large deformation and significant amounts of ductility SWCNT in bending. Based on these results, after kinks, the magnitude energy absorption is considerable because of the wide area beyond the elastic domain.

5. CONCLUSION

In this paper, a simple elasto-plastic model was used to model inelastic behavior of nanotubes using continuum mechanics. Using this model, two FEM models were performed in simple tension and pure bending.

The results of these models are more or less compatible with other atomic results. For example, the FEM model results show 30 degree as the buckling rotation angle that is similar to MD and experimental results.

The new concept in this paper was the use of macro plasticity in analyzing the inelastic behavior of SWCNT. Results showed that this method is an applicable engineering method and could be developed in modeling the inelastic behavior of nano-composites.

6. REFERENCES

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