Continuum Modeling the Behavior of Carbon Nanotubes in different loading condition

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ABSTRACT

Molecular dynamics and quantum mechanics are the best method for analysis the CNTs behavior. Bur because of the difficulties and cost, this task is limited to small structure with limited atoms number. In this paper, continuum mechanics theory base on the Cauchy-born role has been used for this goal according to the experimental and theoretical results. This analysis includes both elastic and inelastic behavior despite serious challenges in inelastic field. In this paper the virtual definition of thickness in SWCNT and MWCNT are reviewed. Then the validity of this definition in different loading and elastic and inelastic region is discussed. Then a FEM model of CNT in different load combination is developed with advanced capabilities like large deformation. The result of this model is compared with some experimental and MD model's results and shows that the continuum mechanic's modeling of nanotubes could help to predict of behavior of nanostructure and nanocomposite despite serious limitation.

Keywords: nanotube, elastic, continuum, modeling

1 INTRODUCTION

Discovered in 1991, carbon nanotubes have continued to receive attention, both theoretically and experimentally [1]. Their special physical properties have led to suggestion of numerous applications. Theoretically, various parameters, such as Young's module and Poisson's ratio, as well as deformation modes, have been determined by several atomistic techniques, including classical molecular dynamics (MD) with empirical potentials [2–4]. Attention has also been given to continuum descriptions of nanotubes, based on the theory of shells. Yakobson et al. [5] computed analytical expressions on the energy of a shell in terms of local stresses and deformations. Thus, attempts to reconcile continuum theory with atomistic simulations [2] had to use uncertain parameters like the effective thickness of the shell, the physical origin of which was doubtful at first.

The continuum approximation can be very valuable and may be the only feasible approach toward large and complex systems like composites, but its applicability deserves further scrutiny [6]. The elastic domain in behavior of the CNT is very extensive and they are remarkably resilient, sustaining extreme strain with no signs of brittleness or plasticity. But after a limit, non-reversible behavior occurs resulting in a nano-plasticity/nano-fracture. The transition of the system from the initial pre-yielding state to the final post-yielding state occurs through a series of bond breaking and rearrangement processes. Nanotubes under large strain go through two kinds of structural changes. The first practice is structural elastic buckling in compression. The second possibility is the rearrangement of bonds under large strains, permanent damage, plastic deformation and yielding in tension or compression. Plasticity of nano-material is a complex phenomenon that requires a multiscale description involving microscopic, mesoscopic and macroscopic modeling [2]. Obviously initiation and extension this nano-plasticity differ with the macro plasticity but the there are some similarities between them. Effect of temperature, strain rate is very important in nano plasticity and its main reason is breaking and rearranging the bonds and vacancy in nanostructure. Mielke et al. [11] investigated the effect of vacancy and holes in the fracture of carbon nanotubes. Srivastava et al. [7] investigated the tensile strength of nanotube in the different temperatures and strain rates. Dumitric and Yakobson investigated the strain-rate and temperature dependent plastic yield in carbon nanotubes from ab initio calculations. This nano-plasticity has been observed in tension, compression, bending, torsion and etc by many researchers

2 CONTINUUM AND PLASTICITY IN NANOTUBES

The yield and plasticity in nanotubes could be considered in different fields like tension, compression and combined loading. In the tension aspect, MD calculations show the tensile yield strain of perfect SWCNT's to be as much as 20-30%. But experimental results report smaller tensile yield strain (about 5-6%).the main explanation of this huge difference is described by the role of defects [14]. The yielding or failure of CNT's is mainly depending on the activation and propagation of defects, such as Stone-Wales bond rotation and/or vacancies defects [14]. The formation of a SW defects in a nanotube or graphene lattice typically involves in a bond rotation with breakage of two existing C-C bonds and formation of two new ones [14]. This mechanism is explained by formation of heptagon-pentagon pair defects in the walls of the nanotubes. The formation energy of such a defect is decreased with the applied strain. It also depends on the diameter and chirality of the nanotube. This transformation, shown in Figure 1, can occur in all types of chirality nanotube. Farther more, the

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plastic flow and continuous formations of defects continue until the necking and breaking of the nanotube.

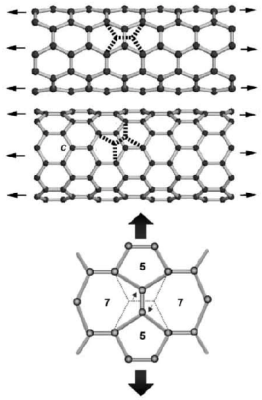

Figure 1: Initial of plastic deformation in SWCNT in tension in different chirality (Stone-Wales phenomena) [10]

Yield strain is strongly depends on the activation energy. Analysis in the references show that the yield strain of a tensile strained CNT strongly depends on the temperature and the applied strain rate. Furthermore, calculations show that such defects can bifurcate and migrate along the tube, and their aggregation becomes energetically favorable at high strains [15]. In the compression, the plasticity could be described by reconstructing of graphitic (sp2) bonds to (sp3) bonds [12] is similar to the rearrangement of bonds in the tension but their shape are inverse. That is done by the relaxation of the accumulated strain energy in the uncollapsed section of the tube and is very similar to plasticity phenomenon in macro structures [12]. The similar procedure happens in the compression side of SWCNT in the bending process. It is observed by high-resolution electron microscopy, when the bending deformation is due to a series of buckling in the compressive side. According to (Speck et al. 1989), the minimum radius of curvature of graphite sheets in elastic bending is thought to be 15 nm. For lower radius, inelastic behavior is seen [13].

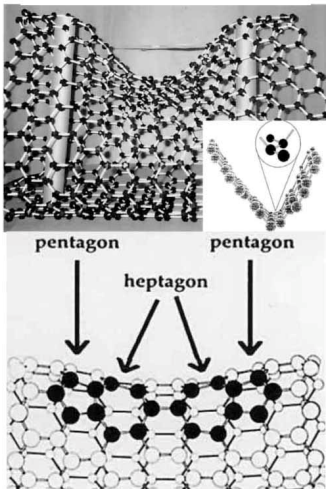

Figure 2: (Left) Stone-Wales defect in the buckling and compression side (Right) Schematic shape of structure in the buckling [12]

3 MULTISCALE ANALYSIS AND VALIDATION THE CONTINUUM

The key rule for the using the continuum mechanics for analysis the lattice system (like the atomistic system in the nanotubes) in the Cauchy-born rule. By this rule, the displacement of a discrete system could be expresses as a continuum system. This transformation is briefly showed in figure 3. In this figure, the mapping function Φ, changes the displacement from initial undeformed space $\Omega_0 CR^n$ ΩCR^n, (n could be 1, 2 or 3). The relationship of two space is defined by the $\Omega = \Phi(\Omega_0)$. Therefore if the X is a point in the undeformed space in Ω_0, after transformation its coordinated would be changed to $x = \Phi(X)$. In this space, F in considered the gradient of deformation and is defined by $F = D\Phi = \frac{\partial \Phi}{\partial X}$. Therefore we could say the $dx = F(dX)$.

By using the appropriate tangential gradient we could express the deformation in the continuum space. This is the main subject of the continuum crystal elasticity that has been used for the analyzing the elastic behavior of the crystals. During the recent decade, many researchers expand and extend this theory for the analysis the elastic and inelastic behavior of nanotubes.

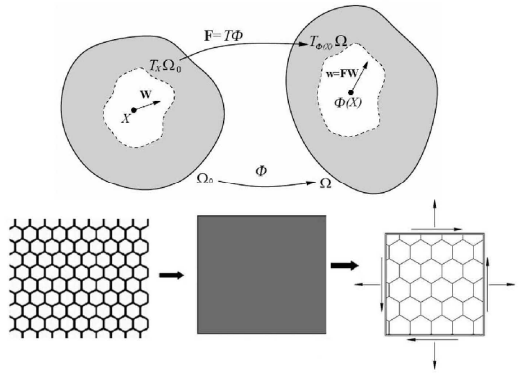

Figure 3: the Cauchy-Born description for continuum analysis of a discrete system

Another important aspect in this field is multiscale problem. In the multiscale analysis, two concurrent domains are employed: a nanoscale continuum domain for the defect free condition, and an atomic scale domain that models the localized phenomena. On of the best models for this multiscale modelling is the stick-slip model of Gao and co-workers that employed to yield nanoscale material moduli that are a function of internal variables which are in turn based on the changes in the bond lengths and bond angles that occur because of the local state of deformation. Multi-body interatomic potentials of the Tersoff-Brenner type are employed in mentioned model.

4 FINITE ELEMENT MODEL

For modeling, a three-dimensional FEM analysis was performed using the standard software package. In this analysis, two types of elements were used.. (I) Four-node shell element was used to modeling the nanotube's Shell element has six degrees of freedom at each node and advanced capability such as large deformation, local and global buckling and plasticity. This element type is suitable for analyzing thin to moderately thick shell structures.

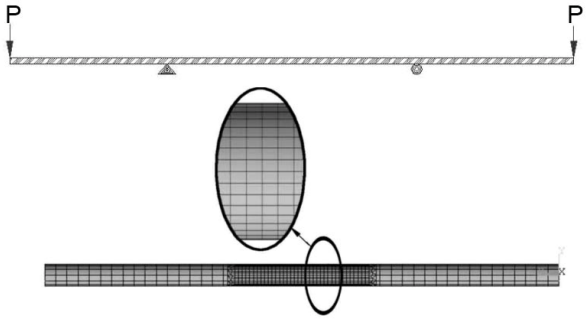

Figure 4: schematic loading of SWCNT in pure bending

(II) Non-linear elastic links for Van der Waals interactions. This element is a unidirectional element with nonlinear generalized force-deflection capability. The element has longitudinal capability in three-dimensional applications. The element has large displacement capability for which there can be two or three degrees of freedom at each node.

For modeling the pure bending condition and elimination the shear effects, two concentrate loads inserted to the one-span with two consoles beam. In figure 4, the schematic boundary condition, loading and elements of the model are shown. Because of the large deformation, rotation, and plasticity, a fine mesh is selected.

Physical properties, such as thickness and Poisson's ratio, are traditionally associated with the macroscopic-length scale, where the characteristic dimensions of a continuum solid are well defined. The determination of these properties has been attempted in many of the studies cited above without proper regard to an acceptable definition of the nanotube geometry. In many studies, it has been assumed that the nanotube ''wall thickness'' is merely the inter-planar spacing of two or more graphene sheets [9], which is about 0.34 nm in single-crystal graphite. In this analysis Poisson's ratio is assumed as 0.3 and the diameter of this nanotube is 10 nm.

In large deformations of the SWCNT, effect of the van der Waals forces is obvious. These interactions are often modeled using the general Lennard–Jones ''6–12'' potential, providing a smooth transition among the attraction and repulsion regions. Based on the Lennard–Jones Potential, the van der Waals force between interacting atoms can be written as [8].

$$F(r) = -\frac{dU_r}{dr} = 24\frac{\varepsilon}{\sigma}[\left(\frac{\sigma}{r}\right)^{13} - \left(\frac{\sigma}{r}\right)^{7}]$$

Non-linear springs that connect the two interacting atoms with hinged end joints

5 RESULTS AND DISCUSSION:

The results of FEM model consist of deformed shaped, plastic regions and sections are shown in figures 5 and 6. In addition, the moment-rotation and strain energy-rotation diagrams are shown in figures 10 and 11.

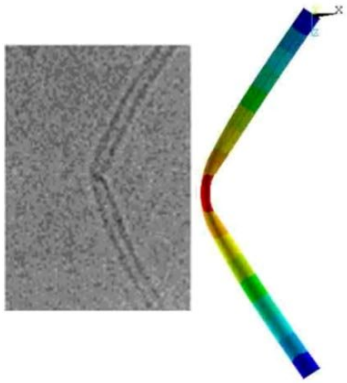

Figure 5: Comparison between (Left) a real plastic deformation of SWNT with (Right) deformed shaped of FEM model

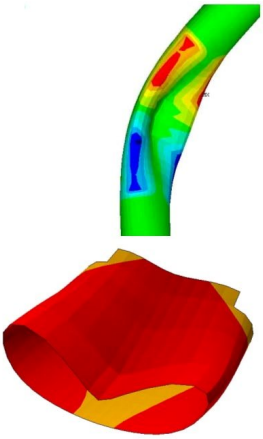

Figure 6: Result of FEM model :(Top) Plastic regions, (Below) Section of the middle part

In figure 5, the finial deformed shape of FEM model compared with the image of real bent SWCNT. The global shape of deformation is similar, but in the kinks location; there are some differences that relate to the limitation and assumption of macro modeling of SWCNTs. But huge inelastic rotation in the kinks region is significant. According to the FEM results, the in more than 60 degrees, and the rotation in the kinks boundary exceeded from elastic limit and inelastic behavior in observed.

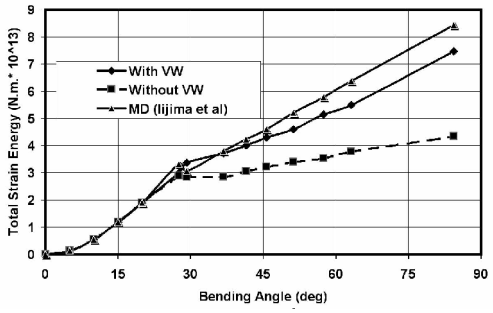

Figure 7: Bending angle & total strain energy

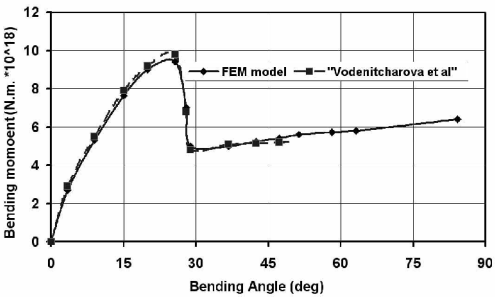

Figure 8: Bending angle & total strain energy

During kink's initiating, the ovalization deformed to an irregular shaped and the walls will be closer. The graphite layer's distance (0.34 nm.) is the lower limit for closing two opposite walls. Because of the large repulsive force, the stiffness of structure will be increase relative to macro structure and that is one reason for large deformation capability of SWCNT. When kink happens, the absorbed energy during bending is linear and corresponding to the bending angle. During this phenomena, some plasticity (witch consisting the initiation and extension of S-W defects will be occurred. This plasticity was not reported in the pervious molecular dynamics (MD) modeling and this is the main deference in FEM model's and MD's results. Regarding these results, some plasticity will happen and during unloading procedure, these defects will remain in the nanotube structure. These defects may decrease the stiffness in the subsequent loading. This matter (reduction of stiffens in the Stone-walls defects and vacancies) will reduce the bending stiffness in the next loading.

6 CONCLUSION:

This paper has established an inelastic FEM model to analysis inelastic behavior of SWNT deferent loading condition. A new concept of this paper is using the macro plasticity in analyzing the inelastic behavior of SWCNT. This method because of its simplicity and capabilities in absence of analytical methods is suitable method for modeling the inelastic behavior of nanotubes. Results of this model show that the macro plasticity could help us to analysis the complex nano structure. This method is strongly dependents to artificial definition of yield stress, plasticity rule and elastic limit. This method could develop to modeling the inelastic behavior of nano-composites.

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