TECHNICAL NOTE

STRESS TRANSFER MODELING IN CNT REINFORCED COMPOSITES USING CONTINUUM MECHANICS

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Abstract Because of the substantial difference in stiffness between matrix and nanotube in CNT composite, the stress transfer between them controls their mechanical properties. This paper investigates the said issue, analytically and numerically, in axial load using representative volume element (RVE). The analytical model was established based on the modified Cox's shear lag model with the use of some simplified assumptions. Some, in the developed shear lag model, the CNT assumes hollow fiber. Solving the governing differential equation, led the high shear stress in interface especially in the CNT cap. In addition, some finite element models were performed with different aspect ratios and the shear stress pattern especially in interface was calculated numerically. Despite some simplified assumptions that were performed with these two models such as elastic behavior and full connectivity, and the comparison of their results with other numerical models show adequate agreement.

Keywords Nanotube, Continuum, FEM, RVE, Shear-Lag

چکیده در کامپوزیت های مسلح شده توسط نانوتیوب های کربنی، به علت سختی قابل توجه نانوتیوب ها نسبت به ماتریس، تنش نسبی زیادی به نانوتیوب ها وارد می‌شود. با توجه به اینکه کارکرد بهینه نانوتیوب در کامپوزیت به چگونگی انتقال تنش بستگی دارد، میزان پیوستگی نانونیوب و ماتریس بر رفتار مکانیکی کامپوزیت به میزان زیادی موثر است. در این مقاله چگونگی انتقال تنش مابین نانوتیوب و ماتریس در قالب مکانیک محیط پیوسته به صورت تحلیلی و عددی بر روی المان نماینده حجمی کامپوزیت بررسی شده است. یک مدل تحلیلی بر پایه مدل برش جداره کاکس بر اساس شرایط هندسی نانوتیوب ها که توخالی هستند، توسعه یافته است. به طوری که نتایج مدل، تمرکز تنش در منطقه مرزی ماتریس و نانوتیوب را در دو سر نانوتیوب نشان می‌دهد. این نتیجه در مدل اجزای محدود سه بعدی ساخته شده برای المان نماینده حجمی نیز مشاهده شده است. مقایسه نتایج ایندو مدل با سایر نتایج تحلیلی و عددی مبین تطابق مناسب آنها است. نتیجه تحقیق، نمایان گر قدرت روش مکانیک محیط پیوسته در مدل سازی ماکروی کامپوزیت های نانوتیوب می‌باشد.

1. INTRODUCTION

Carbon nanotubes have special mechanical properties and they have been used as reinforcements in matrices to form a so-called "nanocomposite materials". It has been theoretically and experimentally confirmed that, carbon nanotubes possess exceptional high stiffness and strength. Their exceptional mechanical properties as well as their high stiffness, low density and highly ductile deformation suggest that carbon nanotubes may hold a promising characteristic as reinforcement for nanocomposites [1]. The improvements in stiffness and strength due to the addition of carbon nanotubes in brittle and ductile matrixes have been demonstrated by some experimental and analytical results [2]. There has been tremendous interest in the modeling and simulations of the CNT composites in order to characterize their mechanical properties for potential engineering applications. There are many researches dealing with the elastic properties of the carbon nanotube through various means, in elastic and inelastic behavior [3]. To understand the properties of nanotube reinforced composites, a fundamental challenge exists in the characterization and modeling of these materials at the nanoscale. Both molecular dynamics and continuum mechanics and their combinations have been attempted for this purpose. Among the available literature, Lordi, et al [4] used force-field-based molecular mechanics to model the interactions between nanotubes and several different kinds of polymers. Wise, et al [5] used molecular dynamics simulation to address the local changes in the interface of a single-walled nanotube surrounded by polyethylene molecules. These approaches typically involve extensive computations and tend to be configuration specific.

The MD approach is necessary in the study of nanocomposites, especially for investigating local interactions of CNTs with matrix materials. However, MD simulations at present are limited to small length and time scales due to the limitations of the current computing power [6]. Continuum mechanic approaches can fill this gap and results from such approaches have been shown to be close to those of the atomistic based simulations. Although efficient in computing and able to handle models at larger length scales, simulation results are obtained, using the continuum mechanics approach which should be interpreted correctly. Attention should be given to the overall deformations or load transfer mechanisms rather than local properties. There are some recent efforts to develop the continuum theories to modeling nanoscale composites [9-14]. Pipes, et al [9] characterized the mechanical properties of CNT composites using a continuum mechanics approach. Applying the traditional textile-mechanics approach and anisotropic elasticity theory, they studied the behavior of CNT composite stress distributions and effective elastic properties were evaluated using continuum mechanics approach.

Liu, et al [12-14] applied the finite element and boundary element methods (FEM/BEM) for the study of CNT composite models, where representative volume element (RVE) were modeled as thin elastic layer in the shape of a capsule (for short CNT). Effective elastic properties of the CNT composites are evaluated and compared with the rules of mixtures. The detailed FEM models in [13,14] reveal that the ‘‘stress’’ gradient cross the interface of the CNT and matrix is very high. All the above mentioned investigations have focused on RVE (representative volume element) as a typical representative of CNT composite.

The analysis of the RVE model is the first step in analyzing the macro scale short fiber composites including CNT composite [12-14]. In Figure 1, the real situation of CNT in matrix is schematically shown.

The aim of this paper is to develop such a shear-lag model using a representative volume element (RVE) of a concentric composite cylinder embedded with a capped carbon nanotube. Therefore, in order to find the stress transfer between matrices in this paper, the modified Cox's shear lag model is developed upon the assumption of hollow cylinder instead of the solid fiber assumption in previous works and stress transfer between matrix and nanotube is evaluated. Then a Finite Element Method (FEM) model was performed to analyze the stress transfer in the RVE model in axial loads. Results of these computational models were compared with other experimental and computational results.

2. ANALYTICAL MODEL

Regarding the complex geometry of RVE model of CNT composites, it is difficult to establish and solve the governing differential equations of continuum mechanics in a closed form. This is why shear lag models have been extensively used to analyze the stress transfer problem in short fiber composites, like CNT composites. The computational efficiency of the shear lag models stems in part from simplifying the assumption of one-dimensional displacement and stress fields. The Cox model is the most used shear lag model for a solid fiber embedded in matrix, subjected to uniform load/displacement in the fiber direction [15-17]. Based on Cox's model, we have established an RVE model which is used in the following analytical part as shown in Figure 2.

Some simplified assumptions performed in this model are as follows:

- Both SWCNT and matrix are considered linear-elastic.
- The nanotube is assumed as a hollow thin cylinder with specified thickness
- The load acts only axially at the side of the RVE model.
- The nanotube-matrix bonds are perfect with full connectivity. A cylindrical coordinate (r, θ and z) is defined, with the z axis representing the SWCNT axial direction.

The governing equations for the axisymmetric problem, in a displacement formulation and in terms of the polar coordinates, include the equilibrium equations (in the absence of body forces) [18]:

$$\begin{aligned}&\frac{\partial\sigma_{rr}}{\partial r}+\frac{\partial\tau_{rz}}{\partial z}+\frac{\sigma_{rr}-\sigma_{\theta\theta}}{r}=0\\&\frac{\partial\tau_{rz}}{\partial r}+\frac{\partial\sigma_{zz}}{\partial z}+\frac{\tau_{rz}}{r}=0\end{aligned}\qquad(1)$$

Which σ_{rr}, $\sigma_{\theta\theta}$, σ_{zz} and τ_{rz} are respectively the axial and shear stress components. Upon integration of the equilibrium equation with respect to r from r_i to r_o, (Which r_i is internal radius and r_o is external radius of nanotube) the equilibrium of forces for nanotube in Z direction could be written as Equation 2:

$$\int_{r_i}^{r_o}\frac{\partial\sigma^n_{zz}}{\partial z}(2\pi r)dr+\int_{r_i}^{r_o}\frac{1}{r}\frac{\partial}{\partial r}(r\tau_{rz})(2\pi r)dr=0\qquad(2)$$

Using these equations and considering the definition of average axial stress in matrix, the interfacial shear stress $\tau^n_{rz}(z)$ will be found as:

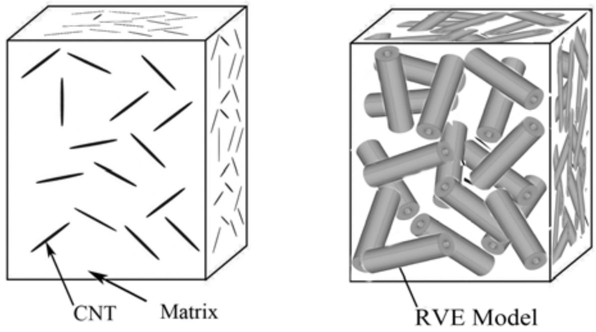

Figure 1. The schematic random dispersion of CNT (Left) and virtual RVE (Right) in CNT composites.

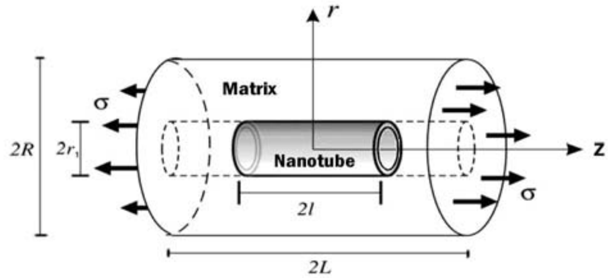

Figure 2. The parameter used in RVE analysis.

$$\frac{d\bar{\sigma}^n_{zz}(z)}{dz}=-\frac{2}{t_n}\tau^n_{rz}(z)\qquad(3)$$

The integration of Equation 1 with respect to r from r_o to R using boundary condition yields:

$$\frac{d\bar{\sigma}^m_{zz}(z)}{dz}=\frac{2r_o}{R^2-r_o^2}\tau_i(z)\qquad(4)$$

In Equation 4, $\bar{\sigma}^m_{zz}(z)$ is the average axial stress in the matrix. Substitution of Equation 4 with Equation 1 and integration concludes as:

$$\tau^m_{rz}=\frac{t_o}{R^2-r_o^2}\left(\frac{R^2}{r}-r\right)\tau_i\qquad(5)$$

In this equation, τ_i is the interfacial stress. If w is assumed as the displacement in z direction and u assumed as the displacement in r direction; upon assumption of $\left|\frac{\partial u}{\partial z}\right| << \left|\frac{\partial w}{\partial r}\right|$, the shear strain (and displacement) can be related to shear stress simply as:

$$\tau_{rz}^{m} = G_m \frac{dw_m}{dr} = \frac{E}{2(1+\upsilon_m)} \frac{dw_m}{dr}$$
$$\tau_{rz}^{n} = G_n \frac{dw_n}{dr} = \frac{E}{2(1+\upsilon_n)} \frac{dw_n}{dr} \tag{6}$$

Using Equation 5 and the integration of Equation 6 with respect to r from r_o to R, and using the RVE boundary condition, it can be concluded that:

$$\tau_i = G_m \frac{R^2 - r_o{}^2}{t_n[R^2 \ln(R/r_o) - 0.5(R^2 - r_o{}^2)]} (w_R - w_{r_o})$$
$$\tau_m = G_m \frac{(w_R - w_{r_o})}{R^2 \ln(R/r_o) - 0.5(R^2 - r_o{}^2)} \left(\frac{R^2}{r} - r\right) \tag{7}$$

Using τ_i as interfacial shear stress τ_m as the shear stress in matrix and using Equation 7 and upon integration with respect to r from r_o to r, the displacement of matrix can be found as:

$$w_m = w_{r_o} + \frac{R^2 \ln(\frac{R}{r_o}) - \frac{1}{2}(r^2 - r_o)}{R^2 \ln(\frac{R}{r_o}) - \frac{1}{2}(R^2 - r_o)} \tag{8}$$
$$((w_m^{zz})_{r=R} - (w_m^{zz})_{r=r_0})$$

For simplicity, it is assumed that the "σ_{rr}, + $\sigma_{\theta\theta}$ << σ_{zz}". Therefore, the stress can easily be concluded as:

$$\sigma_{zz}^{n} = E_n \frac{\partial w_n}{\partial z}$$
$$\sigma_{zz}^{m} = E_m \frac{\partial w_m}{\partial z} \tag{9}$$

With differential, this equation and number 8 with regards 'z' and multiplying it to elastic modulus will conclude in:

$$\sigma_m^{zz} = \sigma_{r=r_o}^{zz} +$$
$$\frac{R^2 \ln(\frac{R}{r_o}) - \frac{1}{2}(r^2 - r_o)}{R^2 \ln(\frac{R}{r_o}) - \frac{1}{2}(R^2 - r_o)} [(\sigma_m^{zz})_{r=R} - (\sigma_m^{zz})_{r=r_0}] \tag{10}$$

Using the equilibrium between applied stress and the stress in the nanotube and matrix, it can be concluded that:

$$\sigma_0 R^2 = (r_0^2 - r_i^2)\sigma_n + \sigma_m(R^2 - r_o^2) \tag{11}$$

With substitution, the stress of matrix from Equations 2, 10 and 11

$$(\sigma_m^{zz})_{r=R} = (\sigma_m^{zz})_{r=r_o} +$$
$$\frac{R^2 \ln(\frac{R}{r_o}) - \frac{1}{2}(R^2 - r_o{}^2)}{R^4 \ln(\frac{R}{r_o}) - \frac{1}{4}(R^2 - r^2{}_o)(3R^2 - r_o{}^2) + t^2(R^2 - t^2)} *$$
$$[R^2\sigma_o - t^2 \bar{\sigma}_{zz}^{f} - (R^2 - a^2)(\sigma_m^{zz})_{r=r_o}] \tag{12}$$

Using this equation and considering the boundary condition, after some calculation the governing differential equation was found. When solving the governing equation in two different areas (the area with nanotube and area without nanotube in two caps) the shear stress in interface is calculated as:

$$\tau_i = \frac{t\,\alpha \sin h\,(\alpha z)}{2 \cos h\,(\alpha L_t)} \left(\frac{(1 - \frac{E_m}{E_f})(R^2 - r_o{}^2)(\frac{t}{r_o})}{t^2 + \frac{E_m}{E_f}(R^2 - r_o{}^2)}\right)\sigma \tag{13}$$

$$\alpha_m{}^2 = \frac{1}{1+\nu_m} \cdot \frac{R^2 - r_o{}^2}{t^2} *$$
$$\frac{R^2}{R^4 \ln(\frac{R}{r_o}) - \frac{1}{4}(R^2 - r^2{}_o)(3R^2 - r_o{}^2) + t^2(R^2 - t^2)} \tag{14}$$

Results of this model are compared with other results in the following parts.

3. FINITE ELEMENT MODEL RESULTS AND DISCUSSION

The Finite element method (FEM) is a numerical approach which can be used to analyze the complex geometry of continuum mechanic problems, when the exact solution of a complicated differential equation is difficult, if at all possible [12-14]. This method could solve these problems within acceptable precision and it is used in this paper to compare with the results of the analytical model as well as other results. It is clear that the results of FEM should be interpreted precisely, considering the overall results rather than the locals. Therefore, some finite element models were established using "Ansys" FEM software. These 3D models were built with a couple of geometries and aspect ratios.

In FEM models, two different types of elements were used; the matrix is modeled using 20-nodded 3D solid element and the nanotube is modeled using 8 nodded shell elements. Both these element types have mid-nodes for more efficient modeling of curvature volumes and surfaces which is our case. Like the analytical model, full connectivity between the nanotube and matrix is assumed. The mechanical properties for these materials are listed in Table 1.

The schematic loading, elements and boundary condition of these models are shown in Figure 3.

The results of Fem models including the stresses and displacements are shown in Figure 4 to 6. The axial stress in the nanotube because of unit load on the RVE model is presented in Figure 4. According to this figure, the stress in the middle of the nanotube is more than 10 times the applied stress because of its high relative stiffness. In this figure, the axial stress variation in the two edges of the nanotube is more than that of the middle and the stress intensity is quite high around the nanotube's cap.

The axial stress in the matrix is shown in Figure 5 and presents high stress intensity around the nanotube cap for which variation seems considerable.

The shear stress in the interface is presented in Figure 6 which shows significant variation in interface in the CNT caps. This shear stress intensity could be more than 2 times the applied stress on the RVE model.

TABLE 1. Mechanical Properties of FEM Model.

	E (Gpa)	Poison Ratio	Thickness (nm)	Radius (nm)	Length (nm)
Matrix	3.75	0.30	-	5	100
SWCNT	5000	0.30	0.006	2	60

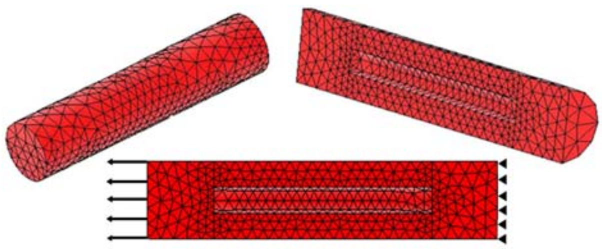

Figure 3. Schematic loading, elements and boundary condition of 3D FEM model.

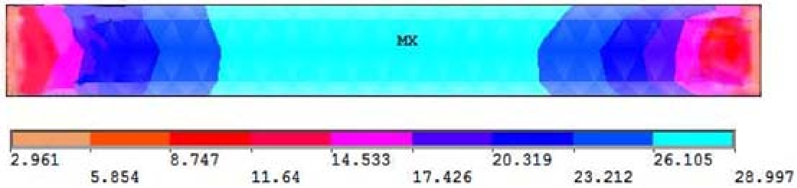

Figure 4. The axial stress in the nanotube due to axial unit tension pressure on RVE.

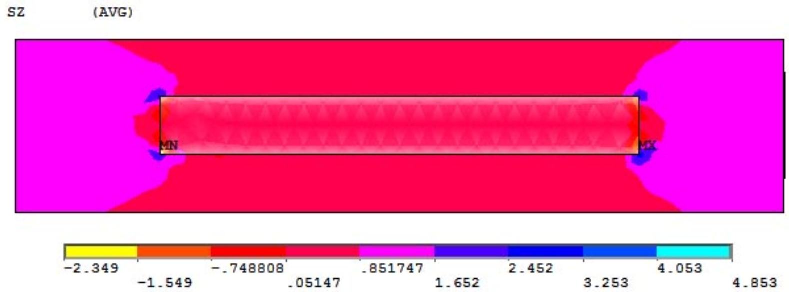

Figure 5. The normalized axial load in matrix due to the unit tension load on RVE.

4. COMPARISON OF RESULTS

In this part, the results of the finite element and analytical model are compared with other FEM models which are presented in reference [11]. For better comparison, the normalized lengths of nanotube and normalized stress level are used. Where the normalized stress is the interfacial stress divided by the maximum interfacial stress. This comparison is depicted in Figure 7, for two aspect ratios. The aspect ratio is defined as the result of CNT's length to its assumed diameter and in this calculation, the diameter is assumed constant (radius of nanotube is assumed 2 nm) and its length is assumed variable.

According to this figure, the general variation of stress is almost similar and some small differences between the analytical model, FEM model and the reference can be distinguished. Also according to this figure, it can be concluded that in the smaller aspect ratio, the length of nanotube is not enough to achieve the anchorage length in the matrix. For a better comparison, the interface shear stress for aspect ratios 50 and 100 are compared in Figure 8. This figure shows high interface shear stress intensity at both ends. Likewise, it is shown that increasing the aspect ratio and length of the nanotube (or increasing the length of nanotube) will cause more stress intensity in the nanotube. But when more anchorage length is achieved, the efficiency of the nanotube increases.

5. CONCLUSION

In this paper, the stress transfer between SWCNT and matrix in CNT composites were considered analytically and numerically using representative element models (RVE). At first, the essentiality of using continuum mechanics was discussed and then one analytical shear lag model was developed using the modified Cox's shear lag model. The result of the analytical model parametrically shows the high stress intensity at both ends of the nanotube in axial loads, which increases when the aspect ratio increases. Moreover, the most axial force in the CNT was found to be in the middle because of the accumulation of the shear interface stress. Because of the limitation of the analytical model which comes from its basic simplified assumptions, one 3D FEM model was performed

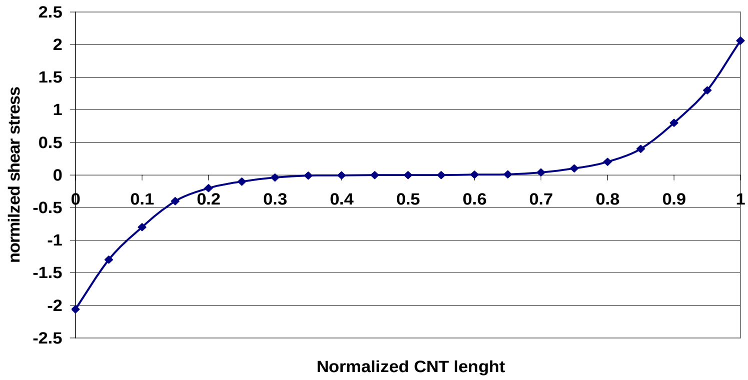

Figure 6. The shear stress in the interface caused by unit pressure tension applied in RVE model.

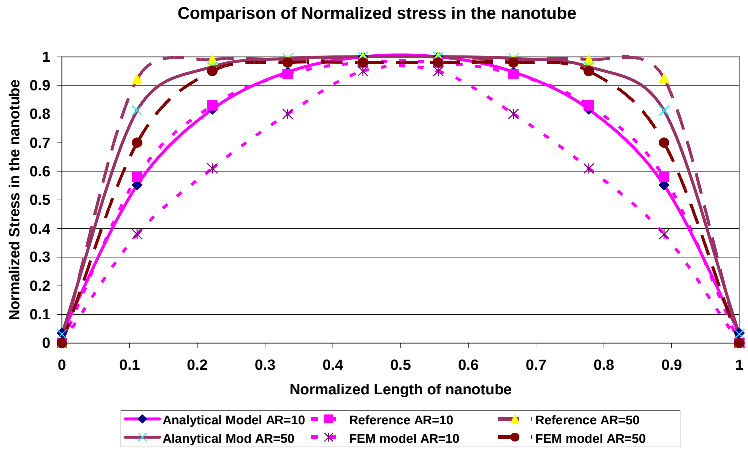

Figure 7. The normalized stress in nanotube with two different aspect ratios in results of FEM, analytical model and reference [19].

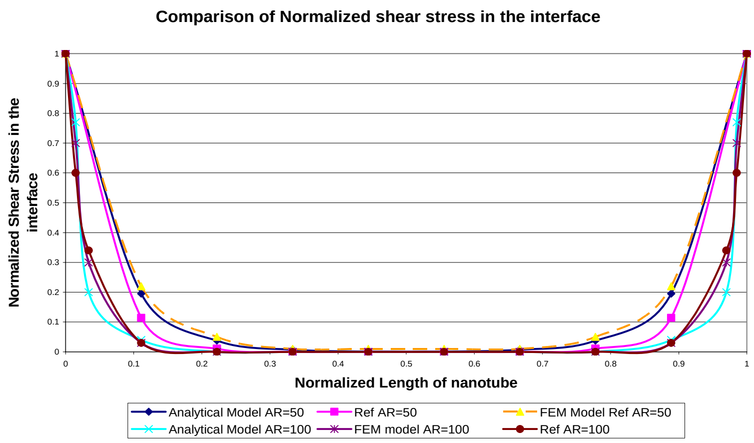

Figure 8. Compression of the shear interface in interface with two aspect ratios in results of FEM, analytical model and reference [19].

in order to better understand the stress transfer phenomena especially in boundaries. The results of the FEM models confirmed the results of the analytical models. These results were compared with other theoretical results and almost confirmed. Based on the mentioned results, the axial force in the nanotube which is a result of the summation of shear stress in the interface makes a relatively high axial stress. High stress in the nanotube, weak confinement and its curvature are the main reasons for their buckling.

6. REFERENCES

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