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Modeling of Randomly Oriented Carbon Nanotube Reinforced Composites

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One of the most important issues in micromechanics is the characterization of the global behavior of the material. Even though Voigt and Reuss models give us a limit, different characterization methods are used to determine the actual behavior of the material. Of these methods, the representative volume method is one approach. It has the goal of characterizing the material by analyzing it by means of a numerical model. As another approach the heterogeneous structure is characterized at a local scale again using a numerical simulation and then to obtain global behavior, the structure is homogenized using an Eshelby-based method like Mori-Tanaka. In this second method, generally one directional modulus of elasticity is determined. Which is inadequate for a highly anisotropic structure. In this study, the data generated at local level will be used to characterize the local model as an anisotropic building block.

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1.Introduction

Being one of the allotropes of carbon element, carbon nanotubes (CNT) are a mesh distribution of carbon atoms with a cylindrical shape and hexagonal symmetry. They have become popular after Iijima's work in 1991 [1]. Main reason of this popularity are their high electrical and thermal conductivity, high tensile strength, high elasticity (18% of elongation until break), high modulus of elasticity etc. [2]. They are currently being used in various industries including but not limited to aerospace, military, construction, and sports equipment industries.

In order to make use of these favorable properties of CNT, they must be considered as a reinforcement agent due to their scale at nano-level. For design purposes, it is not feasible to model a CNT reinforced composite considering both nano and macro level properties at the same time. Therefore, the effective elastic properties must be calculated at macro level. The micromechanics field, which has been established by the work of Eshelby in 1957 [3], deals with this problem which is also called homogenization.

Homogenization can be done analytically like Eshelby's solution [3] for dilute concentrations and like Mori Tanaka [4] and self-consistent methods [5] for denser reinforcements. On the other hand, it can be done numerically for more complex geometries of reinforcements based on the Hill-Mandel [6] condition which requires a representative model to be built so that the model is large enough to be statistically representative of the macro level material.

On the numerical side somehow disregarding the Hill Mandel condition, Fisher (2003) [7] presented a study on characterization of CNT reinforced composites by means of a representative volume element (RVE) with only a single

reinforcement, though only longitudinal modulus of elasticity was considered.
In this study this approach will be further investigated by dealing with not only isotropic but also anisotropic behavior of the RVEs with single reinforcements. First, the material parameters will be determined through application of basic boundary conditions on the RVE. Later a least-squares based approach will be used to extract anisotropic coefficients and the generalization capability of using volume averages will be discussed.

2. Numerical characterization - Representative volume element

2.1. Hill-Mandel Condition

When the geometries of the reinforcements are complex, it is not possible to homogenize the composite material using analytical methods. According to Hill-Mandel [6] condition, if you create a small representative model, which is large enough so that overall elastic behavior is same statistically throughout the global model, then elastic energy of the body subject to either kinematic uniform boundary condition (KUBC)

$$u^0(x) = E.x \quad (1)$$

or static uniform boundary condition (SUBC)

$$n = t^0(x) = \Sigma.n \quad (2)$$

can be calculated using volume averages of the strain and stress in the model:

$$< \sigma >:< \varepsilon >=< \sigma : \varepsilon > \quad (3)$$

where < > denotes volume average and : is double dot product.

2.2 Fisher's RVE with Single Reinforcement

In 2003 Fisher published a study where he examined the effect of curvature of CNTs inside polymer matrices [7]. He did so by creating an RVE with a single CNT inside (Figure 1). Then he extracted effective longitudinal modulus of elasticity due to the curvature by simply applying a displacement boundary condition and calculating effective modulus from basic rule of mixtures.

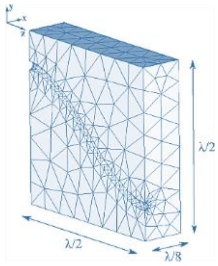

Fig 1. Fisher's RVE with single reinforcement

Due to their highly complex geometry, CNT reinforced composites are expected to behave anisotropically. In the next section details on anisotropic characterization will be given.

3. Anisotropic Characterization

3.1 Conventional Approach

Even though Hill-Mandel condition requires a statistically equivalent RVE model, this condition will be ignored in the case study and the usual boundary conditions and loads will be applied to the structure.
In order to minimally restrict the model, symmetric boundary conditions will be applied at 2 sides. To obtain the modulus of elasticity along each main direction, a uniform displacement load will be applied. Finally after the evaluation of reaction forces using finite element method, the elastic coefficients will be obtained by:

$$E = \frac{R.L}{d.A} \quad (4)$$

where R is the reaction force obtained from finite element analysis, d is the applied displacement, L is the length along the main deformation axis and A is the cross secional area of th RVE.

3.2 Least Square Based Characterization

Any linear elastic material behavior can be represented by a 4th order tensor. Due to symmetries matrix-based Voigt notation can be used. Due to the fact that in this study only a 2D case study will be evaluated, so the constitutive relation of a 2D linear elastic material is

$$\begin{bmatrix}\sigma_1\\ \sigma_2\\ \sigma_3\end{bmatrix} = \begin{bmatrix}E_1 & E_4 & E_5\\ E_4 & E_2 & E_6\\ E_5 & E_6 & E_3\end{bmatrix}\begin{bmatrix}\varepsilon_1\\ \varepsilon_2\\ \varepsilon_3\end{bmatrix} \quad (5)$$

where index 3 for stress and strain denotes shear. At most 6 of these coefficients can be independent. That means in order to evaluate those 6 coefficients by volume averages of stress and strain distributions, data from at least 2 analysis with different boundary conditions/loads must be obtained. But to have a more general idea about the validity of the coefficients, much larger amount of data will be generated. Those large amount of data will be used in a least squares approach where the unknown coefficients will be elastic coefficients. So, the usual constitutive relation is rearranged to fit the least squares form:

$$\begin{bmatrix}\sigma_1\\ \sigma_2\\ \sigma_3\end{bmatrix} = \begin{bmatrix}\varepsilon_1 & 0 & 0 & \varepsilon_2 & \varepsilon_3 & 0\\ 0 & \varepsilon_2 & 0 & \varepsilon_1 & 0 & \varepsilon_3\\ 0 & 0 & \varepsilon_3 & 0 & \varepsilon_1 & \varepsilon_2\end{bmatrix}\begin{bmatrix}E_1\\ E_2\\ E_3\\ E_4\\ E_5\\ E_6\end{bmatrix} \quad (6)$$

To find the elastic coefficients, Moore-Penrose pseudo inverse of the strain matrix must be calculated and multiplied by the stress vector on the left-hand side.

4. Results

4.1 Benchmark problem

For the sake of simplicity the characterization approach has been evaluated using a plane stress model. As can be seen in the Fig. 2, the mesh consists of 6 rows and 5 columns. Each node has translational degrees of freedom along x and y axes. As a simple example, the reinforcement elements have been assigned different elastic properties and they are listed in Table 1. The geometry of the reinforcements has been selected like the letter S in order to mimic the curvature of a CNT.

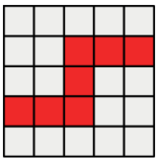

Fig. 2 Two-dimensional example RVE

Table 1. Elastic coefficients of the constituents

Phase	E [GPa]	ν
Matrix	3	0.3
Reinforcement	800	0.3

Boundary conditions and loads were different in conventional and least squares settings and will be detailed in the following sections.

4.2 Conventional approach

When Hill-Mandel conditions are considered in a conventional setting, one of KUBC, SUBC or periodic boundary condition (PBC) is applied. In this study KUBC is used. Also, in order to maintain equilibrium without additional restrictions along boundaries, symmetry boundary conditions have been applied as can be seen in Fig. 3.

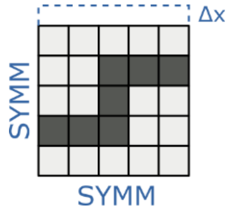

Fig. 3 Conventional method - boundary conditions and loads

Using equation (4), the calculated elastic coefficients along x and y directions is listed in Table 2.

Table 2. Elastic coefficients by conventional approach

Elastic Coef.	Value [GPa]
$\mathbf{E_x}$	13.78
$\mathbf{E_y}$	6.86

4.3 Least squares method

As mentioned in the previous sections, at least 2 different analyses must be made to determine elastic coefficients of a 2-dimensional material. But this is valid for a homogeneous material. If the material is composite, meaning it has 2 or more phases, it is not possible to extract exact coefficients with any 2 conditions. Instead we must obtain data from higher numbers of conditions and also, we must accept the fact that the result will be a compromise, meaning least squares will try to find the coefficients of a linear equation with minimum of sum of squared error values.

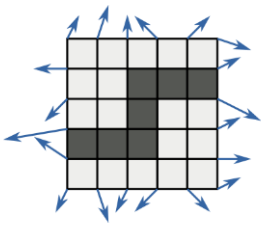

Fig. 4 Least squares method – random boundary conditions

In this study 4500 different displacement boundary conditions have been generated randomly and applied to all boundary nodes. The elastic coefficients are determined after calculating volume averages of stress and strain for each case. The results can be seen in Table 3 and Table 4:

Table 3. Elastic coefficients by least squares

Elastic Coef.	Value [GPa]
E_x	170
E_y	173.6

Table 4. Stress level and error

	Value [GPa]
Mean Abs Stress	323.875
Means Abs Error	78.223
St.Dev. Abs Error	63.422

As the results show, random boundary conditions resulted in substantially different coefficients. Compared with the average stress level, error level (which are calculated by simulating calculated coefficients on test data) is quite high with high standard deviations.

4. Conclusion

The results have shown that for composites with single reinforcements, a usual approach of application of basic boundary conditions is far less representative of the composite. On the other hand, a wide range of analysis data doesn't help either.

The reason may be due to the loss of information when doing volume averages. More case studies for different geometries must still be done though. Also purely random boundary conditions may not reflect the major elastic deformation shapes so that each constituent has a considerable effect.

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