Evaluation of Axial Young's Modulus of CNT-based Composites using Square, Hexagonal and Cylindrical Representative Volume Elements

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Abstract: ***In the present work, finite element (FE) analysis has been performed for evaluating effective axial Young's modulus of CNT-based composites considering different types of representative volume elements (RVEs). Different types of matrix materials from low strength to high strength have been considered to observe the effect of axial Young's modulus on matrix materials. Effect of volume fraction on axial Young's modulus has also been investigated. The present computational results are also compared with the theoretical results obtained based on rule of mixture (ROM). It has been found that the cylindrical RVE underestimated the Young's modulus but the square and hexagonal RVEs give more closer results to those obtained based on ROM. It has also been observed that the axial Young's modulus of CNT-based composites for all the RVE models increase with increase in volume fraction.***

Keywords: CNT-based composite, Representative Volume Elements, Axial Young's modulus, Finite Element method, Rule of Mixture.

1. Introduction

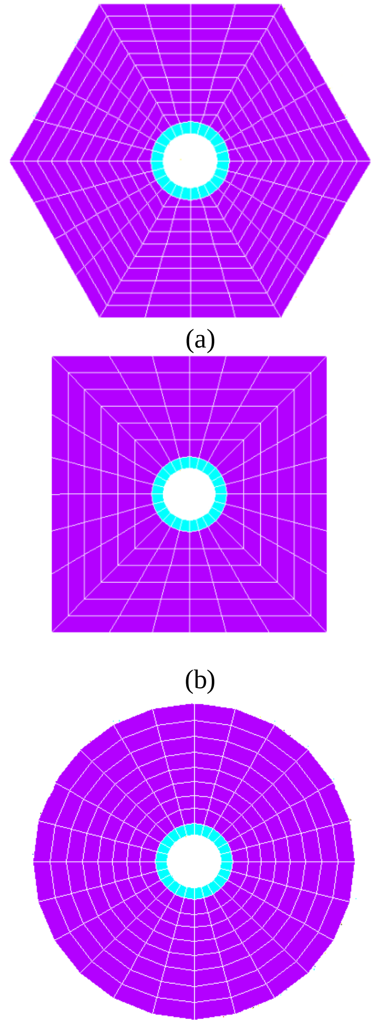
Development of CNT-based composites is one of the most promising challenges of real life application in near future. Since the discovery of CNT by Iijima [1], it has become a focused area in the field of nanotechnology. With its unique structure and high aspect ratio, CNT possesses exceptionally high mechanical, thermal and electrical properties [2-4] which makes the CNT as excellent reinforcing material. A number of works have been published in the board area of CNT-based composites using different types of matrix materials. A huge number of works have been reported in the evaluation of elastic properties of CNT-based polymer matrix composites [5-9]. Qian et al. [5] conducted experiments and reported that with the addition of only 1 wt. % of CNT in polystyrene, the elastic modulus of CNT/polystyrene composites could be increased by 36% to 42% compared to the elastic modulus of pure polystyrene. Xiadong et al. [6] conducted experiment and reported that with the addition of 5 wt. % single wall CNT (SWCNT) in epoxy the elastic modulus and hardness of CNT/epoxy composites could be increased by 75% and 30% when compared to the Young's modulus of pure epoxy, respectively.Arash et al. [7] reported that the Young's modulus of CNT/polymer composites increases from 3.9 GPa to 6.85 GPa with an increase in the aspect ratio of the CNTs from 7.23 to 22.05, respectively. Hossain et al. [8] conducted experiment and reported that with the addition of 0.3 wt. % of the CNT in epoxy the flexural strength and modulus could be increased by 27% and 14%, respectively compared to pure epoxy. Inam et al. [9] conducted experiment and reported that for CNT/epoxy composites containing long CNTs possess higher tensile strength and elastic modulus as compared to nanocomposites containing short CNTs.

Less number of works has been published on CNT-based metal matrix composites [10-12] compared to CNT/polymer composites. But few papers have also been published on CNT-based ceramic matrix composites [13]. Among the metals magnesium (Mg), aluminum (Al) and titanium (Ti) have been attracting more in the field of nanocomposites. Due to their low density and good mechanical properties, they attracted a lot of attention to using them in aerospace and automobile industry for improving efficiency through weight reduction. Through the successful development of such CNT/metal matrix composites, excellent mechanical properties can be obtained. Goh et al. [10] fabricated lightweight CNT/Mg composites and reported a significant improvement of mechanical properties with the addition of only 1.3 wt. % CNT in Mg. Esawi et al. [11] reported that by adding 5 wt. % of the CNT tensile strength and stiffness of CNT/Alcomposites could be increased by 50% and 23% respectively compared to the pure aluminum. A comprehensive review on CNT/Ti composites has been present by Munir et al. [12] and reported that with the addition of 5 volume% of the CNT in Ti the Young's modulus could be increased by 19% as compared to pure titanium. Kirtania and Chakraborty [13] reported that axial

Young's modulus of the CNT/alumina (Al_2O_3) composites increase with the increase in volume fraction ofCNT. Elastic properties of CNT-reinforced composites have also been reported in some earlier works considering different types of RVE models [14-16]. Harsha et al. [14] used hexagonal RVE and reported that with the addition of only 3.6% volume fraction of the CNT in the matrix, the stiffness of the composites could be increased by 33% for long CNT. Liu and Chen [15] used three-dimensional (3D) nanoscale RVEs based on continuum mechanics for evaluation of elastic properties of CNT-based composites and reported that with the addition of CNT in a matrix, the stiffness of the composites could be increased from 0.7 times to 9.7 times. Kirtania and Chakraborty [16] reported that with the addition of only 3.06% volume fraction of CNT, the effective axial Young's modulus as well as axial coefficient of thermal expansion (CTE) of composites could be increased and decreased by 776.61% and 91% compared to the Young's modulus and CTE of the pure epoxy, respectively. Literature review reveals that a number of works have been published in the determination of elastic properties of CNT-based composites. But there is less number of works available in determination of elastic properties using different types of RVE models. Therefore, present work aims at estimation of elastic properties of CNT-based composites considering different types of RVE models and recommended for the better RVE model.

2. Finite element modelling of RVEs

In the present analysis, three types of RVE models have been considered viz. hexagonal, square and cylindrical. In the present RVE models, the CNT is assumed to be surrounded by matrix materials. Figure 1 shows the front view of different types of RVEs with FE mesh of the CNT-based composites for a constant volume fraction of 3.06%. Where, the CNT is placed at the center of RVE. SOLID45 element embodied in ANSYS has been used for modelling both the CNT and the matrix materials. SOLID45 element is an eight-nodal element having three degrees of freedom at each node. The diameter of CNT has been considered as 1.88 nm which is equal to the diameter of zigzag (24, 0) CNT. Thickness and length of the CNT are taken as 0.34 nm and 200 nm [16] respectively. RVEs have been modelled in such a way that the volume fraction changes from 0.5% to 10% by changing the volume of the surrounding matrix materials. Figure 2 shows a pictorial view of a hexagonal RVE with FE mesh for a constant volume fraction of 3.06%.



(a)

(b)

(c)

Figure 1:Front view of CNT-reinforced composites with FE meshes (a) hexagonal, (b) square and (c) cylindrical RVE models.

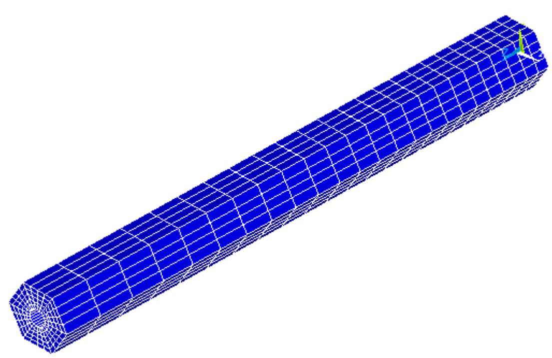


Figure 2: Pictorial view of a hexagonal RVE with FE mesh

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3. Boundary conditions

For evaluating the effective axial Young's modulus of CNT-based composites, all the nodes at $z=0$ are fully constrained and the nodes at $z=L$, a uniform tensile load (P_z) is applied, where L is the length of the RVE in z-direction. Figure 3 shows a pictorial view of a square RVEs along with applied boundary conditions. The average displacement at $z=L/2$ obtained from FE simulations are used to evaluate the effective axial Young's modulus of the CNT-based composites.

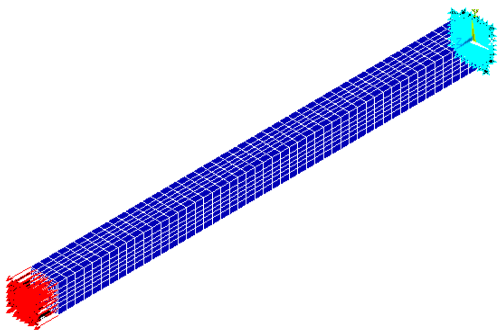

Figure3: Pictorial view of square RVE along with the applied boundary condition.

4. Formulations

In the present study, for the evaluation of axial Young's modulus of CNT-based composites, three types of RVE models have been considered with a long CNT along the length of the RVEs. Figure 4 shows the cross-sectional area of a hexagonal RVE.

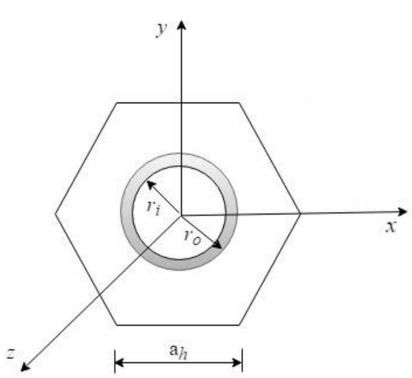

Figure 4: Cross-section of a hexagonal RVE

Cross-sectional areas of different types of RVEs can be calculated using following equations.

$$A_h = 1.5\sqrt{3}a_h^{\,2} - \pi r_i^{\,2} \text{ (Hexagonal RVE)} \quad (1)$$

$$A_s = a_s^2 - \pi r_i^2 \text{ (Square RVE)} \quad (2)$$

$$A_c = \pi(R^2 - r_i^2) \text{(Cylindrical RVE)} \quad (3)$$

Where, $a_h$is thewidth of one side of the hexagonal RVE, a_s is the width of one side of the square RVE, R is the radius of the cylindrical RVE, $r_i$and $r_o$are the inner and outer radius of the CNT. The volume fraction of CNT [14, 15 and 16] in hexagonal, cylindrical and square RVEs can be found using the following equation.

$$V_h = \frac{\pi(r_o^2 - r_i^2)}{1.5\sqrt{3}a_h^{\,2} - \pi r_i^{\,2}} \quad (4)$$

$$V_C = \frac{\pi(r_o^2 - r_i^2)}{\pi(R^2 - r_i^2)} \quad (5)$$

$$V_s = \frac{\pi(r_o^2 - r_i^2)}{a_s^2 - \pi r_i^2} \quad (6)$$

For calculation of effective axial Young's modulus of the CNT-based composites, average displacements are taken from the FE simulation and the same has been calculated by using the following equation.

$$E_1 = \frac{P_z L}{A \Delta L} \quad (7)$$

Where, P_z is the total tensile load applied at one end of the RVE, A is the cross-sectional area of the RVE and ΔL is the average displacement of all nodes in the cross-section at $L=L/2$ in the z-direction.

For a fiber based composites under axial loading, axial Young's modulus of the composites can be estimated by using ROM. The axial Young's modulus of composites with a long CNT can be estimated by using the following equation.

$$E_1 = E_{nt} v_{nt} + E_m v_m \quad (8)$$

Where E_{nt} and E_m are the Young's modulus of CNT and matrix material, respectively; $v_{nt}$and $v_m$are the volume fractions of the CNT and matrix materials, respectively.
Where

$$v_{nt} + v_m = 1 \quad (9)$$

Results obtained using ROM are used to verify the present computational axial Young's modulus of the CNT-reinforced composites.

5. Results and discussion

The effective axial Young's modulus of CNT-based composites has been evaluated considering hexagonal, square and cylindrical RVE models usingFE method. Different types of matrix materials, i.e. from low strength to high strength (epoxy, magnesium, aluminum, titanium and alumina) have been considered for the present analysis. Both the CNT and matrix materials are assumed to be isotropic and homogenous with perfect bonding at the interface between CNT and matrix. The effect of volume fraction of the CNT on the axial Young's modulus of composites has also been investigated. SWCNT has been considered in the present analysis. The properties of SWCNT and the matrix materials are listed in Table 1.

Table 1: Properties of SWCNT and matrix materials.

Material	Young's modulus (GPa)	Poisson ratio
SWCNT	1000	0.28
Epoxy	3.89	0.37
Magnesium	45	0.29
Aluminum	70	0.33
Titanium	116	0.32
Alumina	375	0.22

5.1 Validation of the present RVE models

For validation of the present RVE models, results obtained fromFE simulation are compared with the published work ofKirtania and Chakraborty [16]. They used only square RVE and evaluated elastic properties of CNT-based composites.Axial Young's modulus of CNT/epoxy composites for present RVE models, earlier published work [16] and theoretical based on ROM are listed in Table 2 for a constant volume fraction of 3.06%.

Table 2: Ratio of axial Young's modulus *(E_1/E_m)* of CNT/epoxy composites and matrix.

Present RVE models			Square RVE [16]	Theoreti--cal (ROM)
Hexagonal	Square	Cylindrical		
8.763	8.752	8.739	8.766	8.825

From Table 2, it could be observed that the results obtained from the present RVE models are in good agreement with earlier published work [16] and also with the theoretical results based on ROM. Therefore, the present RVE models validated.

5.2 Effective axial Young's modulus at a constant volume fraction of 3.06%.

Effective axial Young's modulus of CNT-based composites has been evaluated for the three RVE models at a constant volume fraction. Axial Young's modulus of CNT-based composites obtained from FE simulations are listed in the Table 3. For comparison, axial Young's modulus of composites has been calculated based on ROM and listed in the Table 3. Table 3 shows that the ratio of computed axial Young's modulus of the composites to the axial Young's modulus of the matrix (E_1/E_m) at a constant volume fraction of 3.06% for hexagonal, square and cylindrical RVE models.

It could be observed from the Table 3 that with the addition of 3.06% of the CNT in the matrix, there is a significant increase in axial Young's modulus of the composites compared to the matrix materials. The axial Young's modulus of CNT/epoxy composites could be increased by 8.763, 8.752 and 8.739 times compared to the Young's modulus of pure epoxy for hexagonal, square and cylindrical RVE models, respectively. While for CNT/alumina composites the axial Young's modulus could be increased by 1.053, 1.053, 1.046 times for hexagonal, square and cylindrical RVE models, respectively.

Table 3: Ratio of axial Young's modulus (E_1/E_m) of CNT-based composites and matrix.

Nanocomposites	Hexagonal RVE	Square RVE	Cylindrical RVE	ROM
CNT/epoxy	8.763	8.752	8.739	8.825
CNT/Mg	1.649	1.645	1.634	1.648
CNT/Al	1.405	1.405	1.394	1.406
CNT/Ti	1.234	1.234	1.222	1.233
CNT/Al_2O_3	1.053	1.053	1.046	1.051

It could be concluded from the Table 3 that the increase in axial Young's modulus for CNT/epoxy composites is maximum compared to other CNT-based composites for a constant volume fraction. This is due to the fact that the differences in relative stiffness among the CNT-based composites. It can also be observed from Table 3 that as the relative stiffness of the composites increased, the differences of present computed axial Young's modulus and theoretical axial Young's modulus based on ROM decreases. Table 3 also show that the results obtained considering hexagonal and square RVEs are not so significant compared to the theoretical results based on ROM, but in case of cylindrical RVE it has been observed to be underestimated. Therefore, the rest of the analysis in the following sections will be carried out by considering hexagonal and square RVE models.

5.3 Effective axial Young's modulus for different volume fraction of CNT.

5.3.1 *CNT/epoxy composites*

In the present analysis, the effect of volume fraction on the axial Young's modulus of CNT/epoxy composites has been observed. The computed axial Young's modulus considering square and hexagonal RVE models have been compared with the theoretical results based on ROM for different volume fractions. Figure 5 shows the variation of axial Young's modulus *(E_1/E_m)* of CNT/epoxy composites at different volume fractions.It can also be seen from the Fig. 5 that the axial Young's modulus of composites increases linearly with the increase in volume fraction of CNT for both the RVE models. It is cleared from the Fig. 5 that the present computed axial Young's modulus for both the RVE models are in good agreement with the theoretical values obtained based on ROM.

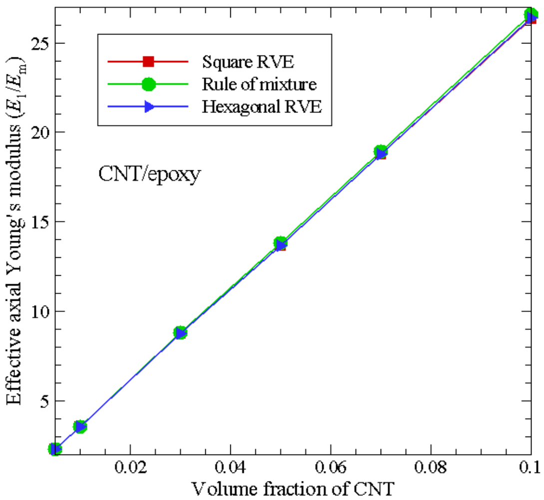

Figure 5: Variation of axial Young's modulus of CNT/epoxy composites with volume fraction.

5.3.2 *CNT/metal (Al, Mg and Ti) composites*

The axial Young's modulus of CNT/metal (Al, Mg and Ti) composites has been computed for different volume fractions considering hexagonal and square RVE models. Figure 6 shows the variation of axial Young's modulus (E_1/E_m) of the CNT/metal matrix composites for both the RVE models.

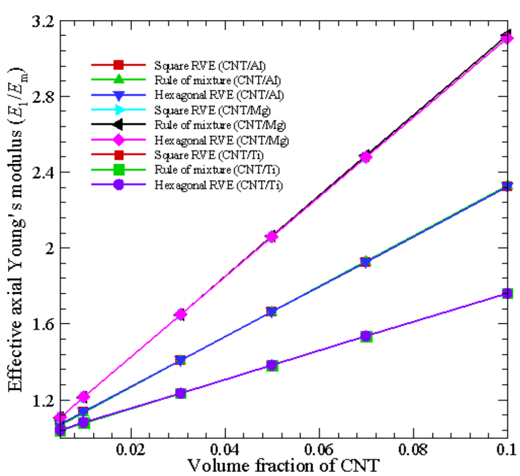

Figure 6: Variation of axial Young's modulus of CNT/metal matrix composites with volume fraction.

5.3.3 *CNT/alumina composites*

Figure 7 shows the variation of axial Young's modulus of CNT/Al_2O_3 composites for different volume fraction ranging from 0.5% to 10% considering hexagonal and square RVE models.

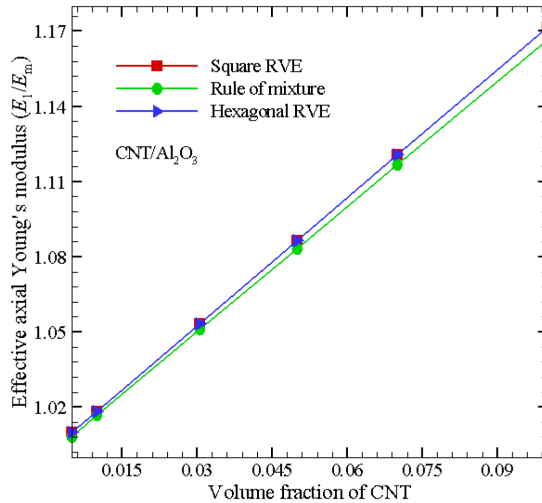

Figure 7: Variation of axial Young's modulus of CNT/alumina composites with volume fraction.

It has been observed from the Fig. 7 that the axial Young's modulus of CNT/Al_2O_3 composites increases with the increase in volume fractions for both the RVE models.It is observed from Fig. 7 that there is a deviation between the computed axial Young's modulus and the theoretical axial Young's modulus calculated based on ROM. The deviation increases as the volume fraction of CNT increases. This is again may be due to the high relative stiffness of CNT/alumina composites.

From the above study, overall it could be concluded that the square and hexagonal RVE gives better values of axial Young's modulus compared to the cylindrical RVE when compared with theoretical value based on ROM. Therefore, the present study will provide a direction on the selection of RVE to determine axial Young's modulus of CNT-reinforced composite.

6. Conclusions

Finite element analysis has been carried out of CNT-based composites considering threetypes of RVEs to estimate the effective axial Young's modulus. Effect of matrix materials and volume fraction on effective axial Young's modulus has also been determined. Some of the important conclusions drawn from the above study are given below:

Axial Young's modulus of CNT-based composites increased due to the addition of CNT in matrix materials. By the addition of only 3.06% volume fraction of the CNT in matrix,the axial Young's modulus could be increased by 8.825 times and 1.051 times compared to the Young's modulus of the pure epoxy and alumina, respectively.Axial Young's modulus increases with the increase in volume fraction for all the RVE models as well as for all types of CNT-reinforced composites.Among the three RVE models, the axial Young's modulus obtained using cylindrical RVE are less than those obtained using other two RVE models.Hexagonal and square RVEs are found to be conferring closer value of axial Young's modulus with the theoretical value calculated based on ROM.The present computed results are in good agreement with earlier published literatures.

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