EVALUATION OF THERMOELASTIC PROPERTIES OF CARBON NANOTUBE-BASED COMPOSITES USING FINITE ELEMENT METHOD

Sushen Kirtania¹ and Debabrata Chakraborty²

¹Department of Mechanical Engineering, Tezpur University, Assam, India.
²Department of Mechanical Engineering, Indian Institute of Technology Guwahati, Assam, India

ABSTRACT
This article deals with the determination of the thermoelastic properties of single-walled carbon nanotube (SWNT)-reinforced composites using finite element (FE) analysis. A full three-dimensional (3-D) FE analysis has been performed using general purpose FE software ANSYS. SOLID45 elements embodied in ANSYS have been used for modeling a square representative volume element (RVE). Both carbon nanotubes (CNTs) and matrix materials are assumed to be isotropic. Effect of different important parameters on the properties of the CNT-based composites has been studied. Present work concludes that by adding ~3% of CNT in epoxy, 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 epoxy, respectively. It is observed that axial CTE of the SWNT/EPOXY composites could be reduced to zero corresponding to a volume fraction of ~13%.

Keywords: CNT-Based Composites, Finite Element Analysis, Coefficient of Thermal Expansion.

1. INTRODUCTION
Among many potential applications of nanotechnology, nanocomposites have been one of the recent research areas. Carbon nanotubes due to their inherent advantages like high strength, stiffness, resilience along with superior thermo-electro-mechanical properties are believed to be ideal reinforcing materials for high performance structural composites. There have been good numbers of works reported in the broad area of nano-composites in recent times. One of the major difficulties in the study of CNT-based composites is experimental characterization of such materials due to their small size. On the other hand, modeling and simulation of nanocomposites can be easily analyzed by a computer. Determination of thermoelastic properties is one of the important tasks where simulation can be used advantageously. Therefore, computational approach played a significant role in the development of the CNT-based composites by providing simulation results to help in understanding, analyzing and designing of such nanocomposites.

Carbon nanotubes first discovered by Sumio Iijima in 1991 [1] and subsequently there were many papers published to determine the Young’s modulus [2-5], Poisson’s ratio [6-7] and CTE [4, 8-9] of CNTs. From the above literatures, it was found that the Young’s modulus, Poisson’s ratio, and CTE of CNTs are in the order of 1 TPa, 0.28, and $-1.5 \times 10^{-6} \text{K}^{-1}$, respectively. Due to superior mechanical, thermal and electrical properties of CNTs, they provide the ultimate reinforcing materials for the development of a new class of nanocomposites [10-11]. The mechanical load carrying capacities of carbon nanotubes in nanocomposites have been investigated in some experimental works [12-13]. Qian and Dickey [12] conducted experiments and concluded that with only 1% (by weight) addition of CNTs in polystyrene (PS), elastic modulus and breaking stress have been observed to increase by 36%-42% and ~25%, respectively.

Jia et al. [14] explained the reasons and possibility of strong (C-C) bond between the CNTs and matrix, as well as the importance of interface in CNT-based composites. Lusti and Gusev [15] performed FE analysis of Young’s modulus and CTE of CNT/epoxy composites for different orientation of CNTs in matrix, and concluded that CNTs could be more efficient as reinforcement compared to conventional glass or carbon fibers. Guo et al. [16] compared the CTE and Young’s modulus of PAN/SWNT composites by performing experiments.

The effective mechanical properties of CNT-based composites are evaluated using a 3-D nanoscale representative volume element based on the 3-D elasticity theory and solved by the FEM [17-18] and observed that with the addition of 3.6% volume fraction of the CNTs in a matrix, axial Young’s modulus of the
composites increased by 33% for the case of long CNT fibers. The tensile strength, modulus and electrical conductivity of a pitch composite fiber with 5 wt% of purified SWNTs are enhanced by ~90%, ~150%, and 340% respectively, as compared to the corresponding values in unmodified isotropic pitch fibers [19]. Han and Elliott [20] performed molecular dynamics simulation and determined axial and transverse elastic moduli using constant-strain energy minimization technique and reported that interfacial bonding effect is important.

Literature review reveals that even though number of work have been reported in the direction of characterization of CNT-based composites, especially using FE method, not many work in thermo-elastic characterization in CNT-based composites have been reported. Therefore the present work aims at FE based estimation of thermo-elastic properties of CNT-based composites and studying the effect of different important parameters on such properties which will be useful in design of such composites.

2. FORMULATION OF THERMOELASTIC PROPERTIES OF CARBON NANOTUBE-BASED COMPOSITES

In this present work, it has been assumed that the CNTs and matrix in a RVE are linear elastic, isotropic and homogeneous materials, with given Young’s modulus and Poisson’s ratios. It has also been assumed that the CNTs and matrix are perfectly bonded with no slip at the interface in the RVE to be studied. The RVE has been modeled by taking different materials like epoxy to steel and different volume fraction of SWNT in the matrix ranging from 0.5% to ~15%. The FE mesh of a cross section of the CNT-composites of the square RVE is shown in fig. 1.

![Fig 1. FE mesh of a cross section of the CNT-composites (square RVE)](image1.png)

Total number of nodes = 9,792, Total number of elements = 8,400, Total number of CNT layer = 1, Total number of matrix layers = 6, Thickness of CNT layer = 0.34 nm, Thickness of each matrix layer = 0.5 nm, Volume fraction of the CNT in the matrix i.e. \( V_{nt} = 3.056\% \)

Fig 1. FE mesh of a cross section of the CNT-composites (square RVE)

The square RVE is used for calculation of the effective Young’s modulus as well as CTE of the CNT-based composites. The diameter of CNTs has been chosen as 1.88 nm which is equal to the diameter of zigzag (24, 0) CNTs. The thickness of CNT layer \( t = 0.34 \) nm but thickness of matrix layers are different for different volume fraction of CNT in composites. The length of the CNTs has taken as 200 nm keeping the aspect ratio of the SWNT as 106. Even though it was reported in the literature [15] that the elastic modulus of CNTs does not change beyond an aspect ratio of 300, but it was observed in the present work that after an aspect ratio of 106, change in elastic modulus is insignificant.

2.1 Effective Young’s Modulus of the Nanocomposites Based on Strength of Materials Approaches

Figure 2 shows a simple strength of materials model for calculating the effective axial Young’s modulus of a long CNT reinforced inside the matrix of a square RVE. All the nodes at one end are fully restrained and the nodes at other ends are subjected to uniform tensile load (\( F \)). The axial Young’s modulus have been evaluated using

\[
E_1 = \frac{F_1}{\Delta L_a / L_a}
\]

where, \( F_1 \) (i.e. \( F \)) stands for the total axial force acting at one end, \( A_i \) is the cross sectional area, \( L_a \) (i.e. \( L \)) is the initial axial length and \( \Delta L_a \) is elongation of the nanocomposites in axial direction. In calculating the cross sectional area of the nanocomposites, the thickness \( t \) of the CNT is taken as 0.34 nm [21, 6] which is the interlayer spacing of graphite. The volume fraction of the CNT in matrix of the square RVE is defined by

\[
V_{nt} = \frac{\pi (r_i^2 - r_f^2)}{4a^2 - \pi r_i^2}
\]

where, \( r_i \) is the outer radius of the CNT, \( r_f \) is the inner radius of the CNT and \( 2a \) is the thickness (or width) of the nanocomposites model.

![Fig 2. A simple strength of materials model for calculating effective axial Young’s modulus of a long CNT reinforced inside the matrix of a square RVE](image2.png)

For a fiber composite under uniaxial loading, the dependence of the effective Young’s modulus in terms of the modulus and the volume fraction of each constituent can be estimated by the rule of mixture (ROM) [22]. The same equations of the ROM are used to predict the effective Young’s modulus of the CNT-based composites. The longitudinal elastic modulus or effective axial modulus \( E_1 \), of the nanocomposites with long CNT is

\[
E_1 = E_{nt} V_{nt} + E_m V_m
\]

where \( E_{nt} \) and \( E_m \) are the elastic modulus of the CNT and matrix, respectively, and \( V_{nt} \) and \( V_m \) are the volume fractions of the CNT and matrix, respectively. Where

\[
V_{nt} + V_m = 1
\]

These ROM formulae are applied to verify the computational results of the effective Young’s modulus.
of the CNT-based composite materials.

2.2 The Effective Coefficient of Thermal Expansion of the CNT-Reinforced Composites

The thermal expansion of a solid can be anisotropic if the coefficients of thermal expansion are direction dependent. This situation occurs in composite or nanocomposites materials with a directional reinforcement. In the present study, the axial and transverse linear CTE of the nanocomposites have been evaluated using finite element method (FEM). The uniform temperature is applied on each node by fixing the nodes at one end (zero displacement). The axial CTE of the composites in the axial direction is given by

\[ \alpha_1 = \frac{1}{E_m} \frac{\Delta L}{L_0} \Delta T \]

where, \(\Delta T\) is the change in temperature. Similarly, the coefficient of thermal expansion of the nanocomposites in the transverse direction is given by

\[ \alpha_2 = \frac{1}{E_m} \frac{\Delta L}{L_0} \Delta T \]

To verify the computed CTE of the CNT-based composite materials, following are the expressions developed for the two thermal expansion coefficients using the thermoelastic extremum principle [23].

\[ \alpha_1 = \frac{\alpha_n V_n E_n + \alpha_m V_m E_m}{E_n V_n + E_m V_m} \] \hspace{1cm} (7)

\[ \alpha_2 = (1 + \nu_n)\alpha_n V_n + (1 + \nu_m)\alpha_m V_m - \alpha_{12} \]

where, \(\alpha_1\) and \(\alpha_2\) are the linear CTE in axial and transverse direction, \(\alpha_n\) and \(\alpha_m\) are the CTE for the CNT and matrix, and \(\nu_n\) and \(\nu_m\) are the Poisson’s ratio for the CNT and matrix, respectively. The effective axial Poisson’s ratio, \(\nu_{12}\), is

\[ \nu_{12} = \nu_n V_n + \nu_m V_m \]

which is approximated by the ROM expression [22], as in axial effective Young’s modulus of the nanocomposites.

3. RESULTS AND DISCUSSION

The effective Young’s modulus as well as the CTE of the CNT-reinforced composite has been evaluated considering a square RVE using FEM. The computed Young’s modulus and CTE are compared to the Young’s modulus and CTE of the matrix, respectively. To get a clear idea on the variation of the Young’s modulus and CTE of the different types of nanocomposites, four types of matrix materials have been chosen. The matrix materials are epoxy, lead, titanium and steel i.e. from low strength to high strength materials. Effect of volume fraction on the variation of the Young’s modulus as well as the CTE of the nanocomposites has also been studied.

SOLID45 elements embodied in ANSYS10 have been used for modeling the RVE. Properties of epoxy have been chosen from literature [24] and densities of epoxy and SWNT are chosen from books [22, 25], respectively. Properties of the matrices materials and the SWNT [2-7] are as follows

- Epoxy: \(E_n = 3.89\ \text{GPa}, \ \nu_n = 0.37, \ \rho_n = 1380\ \text{kg/m}^3\)
- Lead: \(E_n = 16\ \text{GPa}, \ \nu_n = 0.44, \ \rho_n = 11340\ \text{kg/m}^3\)
- Titanium: \(E_n = 116\ \text{GPa}, \ \nu_n = 0.32, \ \rho_n = 4500\ \text{kg/m}^3\)
- Steel: \(E_n = 210\ \text{GPa}, \ \nu_n = 0.29, \ \rho_n = 7800\ \text{kg/m}^3\)

### Table 1: Computed axial effective Young’s modulus of the CNT-based composites of RVE by using volume fraction = 3.056%

<table>
<thead>
<tr>
<th>Types of nanocomposites</th>
<th>(\frac{E_n}{E_m})</th>
<th>% of increased (E_n) w.r.t (E_n) (Comp.)</th>
<th>% of increased (E_n) w.r.t (E_n) (RO M)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SWNT/EPOXY</td>
<td>257</td>
<td>776.61</td>
<td>782.66</td>
</tr>
<tr>
<td>SWNT/LEAD</td>
<td>62.5</td>
<td>186.93</td>
<td>187.98</td>
</tr>
<tr>
<td>SWNT/TITANIUM</td>
<td>8.6</td>
<td>23.47</td>
<td>23.29</td>
</tr>
<tr>
<td>SWNT/STEEL</td>
<td>4.76</td>
<td>11.75</td>
<td>11.49</td>
</tr>
</tbody>
</table>

Based on the formulation described in section 2, effective axial Young’s modulus of the CNT-based composites have been determined from the present FEA of the RVE. Table 1 shows the axial Young’s modulus of the CNT-based composites compared with that of the matrix for a constant volume fraction 3.056%. For comparison the strength of materials solution based on ROM is calculated using Eq. (2) and also listed in Table 1.

Results in Table 1 show that by adding 3.056% CNT
in a matrix, the axial Young’s modulus \( (E_a) \) of CNT-based composites could be increased by 11.75% compared to the Young’s modulus of the matrix, when the ratio of the Young’s modulus of CNT and matrix i.e. \( E_a / E_m = 4.76 \). In the case of \( E_a / E_m = 257 \), the Young’s modulus of the composites in the axial direction \( (E_a) \) has been observed to have increased by about nine times compared to that of the matrix. Fig. 4 shows that percentage increase of effective axial Young’s modulus of different nanocomposites at a constant volume fraction of 3.056%.

Fig 4. The variation of the percentage of increase of effective axial Young’s modulus of different nanocomposites at a constant volume fraction (3.056%)

In practice the weight fraction of CNT in CNT-based composites is limited to 10% [25] and hence in the present analysis the range of the volume fraction is taken between 0.5%-10.3%. Table 2 shows the variation of \( E_a \) with increasing volume fraction in a CNT/Titanium composite. Results in table 2 show that there is a very high percentage increase of \( E_a \) as the volume fraction is increase from 0.5% to 10.3%. Same trend has also been observed for CNT/Epoxy composite.

Table 2: Computed effective axial Young’s moduli of the CNT-Titanium nanocomposites taking volume fraction 0.5% to 10.3%

<table>
<thead>
<tr>
<th>( V_m )</th>
<th>% of increased ( E_a ) w.r.t ( E_m ) (computed)</th>
<th>% of increased ( E_a ) w.r.t ( E_m ) (ROM)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5%</td>
<td>4.1044</td>
<td>3.76</td>
</tr>
<tr>
<td>1%</td>
<td>7.91</td>
<td>7.64</td>
</tr>
<tr>
<td>3%</td>
<td>23.475</td>
<td>23.29</td>
</tr>
<tr>
<td>5.45%</td>
<td>41.6865</td>
<td>41.56</td>
</tr>
<tr>
<td>7.9%</td>
<td>60.34</td>
<td>60.29</td>
</tr>
<tr>
<td>10.3%</td>
<td>78.544</td>
<td>78.5548</td>
</tr>
</tbody>
</table>

From the results shown in Table 1 and Table 2 it could be observed that the effective axial Young’s modulus of composites calculated from the present study appear very close to those obtained from ROM. Fig. 5. shows that by taking 0.5% to 10.3% volume fraction of CNT in Titanium matrix, the percentage of increase in effective axial Young’s modulus of nanocomposites vary from 4.1% to 78.54% with respect to the Young’s modulus of Titanium.

Fig 5. The variation of the percentage of increase of effective axial Young’s modulus of CNT-Titanium composites in different volume fraction (0.5% to 10.3%)

### 3.2 Effective Coefficient of Thermal Expansion of CNT-Reinforced Composites

The effective CTE of CNT-based composites have been evaluated by using FEM. The effective axial CTE of the composites have been calculated by taking a constant volume fraction as well as by varying the volume fraction of the CNT in matrix. The same 3-D FE model for the square RVE with a long CNT is used which was used for the calculation of the effective Young’s modulus of composites. The CTE s of SWNT, epoxy, lead, titanium, and steel are \(-1.5\times10^{-4} K^{-1}\), \(58\times10^{-6} K^{-1}\), \(29\times10^{-6} K^{-1}\), \(8.6\times10^{-6} K^{-1}\), and \(12\times10^{-6} K^{-1}\), respectively.

#### 3.2.1 Effective CTE of CNT-Reinforced Composites at a Constant Volume Fraction

The effective axial as well as transverse CTE of the composite are calculated by taking a constant volume fraction 3.056%. All the nodes at \( z = 0 \) are fully restrained and a uniform temperature, \( AT = 10^0\text{C} \) is applied on all nodes. The effective axial CTE are calculated using equation (5). The calculated effective axial CTE of the CNT-based composites by using FEM are listed in Table 3 and compared with the theoretical values using equation (7).

Table 3: Computed axial CTE of the CNT-based composites of RVE by using a constant volume fraction = 3.056%

<table>
<thead>
<tr>
<th>Types of nanocomposites</th>
<th>% reduction of ( \alpha_t ) w.r.t ( \alpha_m ) (Computational)</th>
<th>% reduction of ( \alpha_t ) w.r.t ( \alpha_m ) (Theoretical)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SWNT/EPOXY</td>
<td>-91.2</td>
<td>-91.32</td>
</tr>
<tr>
<td>SWNT/LEAD</td>
<td>-69.23</td>
<td>-69.7669</td>
</tr>
<tr>
<td>SWNT/TITANIUM</td>
<td>-25.33</td>
<td>-25.1</td>
</tr>
<tr>
<td>SWNT/STEEL</td>
<td>-15.0833</td>
<td>-14.6858</td>
</tr>
</tbody>
</table>

For all the four composite materials the axial CTE have
been observed to have decreased and the percentage of reduction of axial CTE of nanocomposites is maximum for SWNT/EPOXY (~91%) and minimum for SWNT/STEEL (~15%) is shown in Fig. 6.

![Graph showing the variation of the percentage of axial CTE for different types of nanocomposites by taking a constant volume fraction ~3%](image)

**3.2.2 Effect on Volume Fraction on the Effective CTE of CNT-Reinforced Composites**

Effective axial and transverse CTE are calculated using Eq. (5) and (6), respectively. For comparison of the calculated values with the theoretical values, equations (7) and (8) have been used. The calculated effective axial and transverse CTE of the CNT/EPOXY composites by using FEM for different volume fractions are listed in Table 4.

![Table 4: Computed effective axial and transverse CTE of the CNT/EPOXY nanocomposites taking volume fraction from 0.5% to 15.77%](image)

In this study, the axial as well as transverse CTE of the SWNT/EPOXY composites are calculated by varying volume fraction from 0.5% to 15.77%. The variation of the axial CTE of SWNT/EPOXY with volume fraction of CNT is plotted in Fig. 7. It can be seen that the axial CTE of the nanocomposites are 6125.2 $10^{-6}$ K$^{-1}$ and 610.32 $10^{-6}$ K$^{-1}$ corresponding to its volume fractions of 0.5% and 15.77%, respectively. Another important observation from Fig. 7 is that the axial CTE of the composites is zero at a volume fraction ~13%. The same reduction trend of axial CTE with CNT volume fraction is also observed for CNT/Titanium composites. The computed effective CTE using FE results are very close to the computational [15] and experimental [16] results.

![Graph showing the variation of the axial CTE with respect to the volume fraction of the CNT in epoxy matrix](image)

**4. CONCLUSIONS**

- In general, the load carrying capacity is enhanced and CTE is reduced due to addition of CNTs in matrices.
- By adding ~3% of CNT in a particular matrix, the axial Young’s modulus of CNT-based composites could be increased between 1.11 times to 8.76 times that of the matrix, depending upon the ratio of the Young’s moduli of CNT and matrix.
- The increase in effective CTE in transverse direction is very less compared to the increase in effective CTE in axial direction.
- By adding 3% of CNT in epoxy matrix, the axial CTE of CNT-based composites could be reduced by 91% compared to the CTE of the matrix.
- Increase in volume fractions of CNT in matrix lead to decrease in CTE and the axial CTE of the SWNT/EPOXY could be reduced to zero corresponding to a volume fraction of ~13%.

**5. REFERENCES**


6. NOMENCLATURE

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Meaning</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A_c$</td>
<td>Cross sectional area</td>
<td>$\text{nm}^2$</td>
</tr>
<tr>
<td>$E_i$</td>
<td>Young’s modulus</td>
<td>$\text{GPa}$</td>
</tr>
<tr>
<td>$E_m$</td>
<td>Young’s modulus of Matrix</td>
<td>$\text{GPa}$</td>
</tr>
<tr>
<td>$E_{nt}$</td>
<td>Young’s modulus of CNT</td>
<td>$\text{GPa}$</td>
</tr>
<tr>
<td>$L_a$</td>
<td>Initial axial length</td>
<td>$\text{nm}$</td>
</tr>
<tr>
<td>$L_t$</td>
<td>Initial transverse length</td>
<td>$\text{nm}$</td>
</tr>
<tr>
<td>$\Delta L_a$</td>
<td>Change in axial length</td>
<td>$\text{nm}$</td>
</tr>
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<td>$\text{nm}$</td>
</tr>
<tr>
<td>$r_i$</td>
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<td>$\text{nm}$</td>
</tr>
<tr>
<td>$r_o$</td>
<td>Outer radius of CNT</td>
<td>$\text{nm}$</td>
</tr>
<tr>
<td>$T$</td>
<td>Temperature</td>
<td>$\text{K}$</td>
</tr>
<tr>
<td>$\Delta T$</td>
<td>Change in temperature</td>
<td>$\text{K}$</td>
</tr>
<tr>
<td>$V_m$</td>
<td>Volume fraction of Matrix</td>
<td>$\text{V}_m$</td>
</tr>
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<td>$\text{V}_{nt}$</td>
</tr>
<tr>
<td>$\alpha_1$</td>
<td>Axial CTE of Nanocomposites</td>
<td>$\text{K}^{-1}$</td>
</tr>
<tr>
<td>$\alpha_2$</td>
<td>Transverse CTE of Nanocomposites</td>
<td>$\text{K}^{-1}$</td>
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<tr>
<td>$\alpha_m$</td>
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<td>$\text{K}^{-1}$</td>
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<td>Poisson’s ratio of CNT</td>
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<tr>
<td>$\nu_m$</td>
<td>Poisson’s ratio of Matrix</td>
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</table>

7. MAILING ADDRESS

Assistant Prof. Sushen Kirtania
Department of Mechanical Engineering,
Tezpur University
P.O.- Napaam, Tezpur-784028, Assam, India
Phone : +91-3712-267007/8/9 (Extn 5857)
Fax: 091-3712-267005/06
E-mail: sushen.kirtania@gmail.com