 CMC, vol.54, no.1, pp.1-20, 2018

Three Phase Composite Cylinder Assemblage Model for Analyzing the Elastic Behavior of MWCNT-Reinforced Polymers

Puneet Kumar[1, *] and J. Srinivas[2]

Abstract: Evolution of computational modeling and simulation has given more emphasis on the research activities related to carbon nanotube (CNT) reinforced polymer composites recently. This paper presents the composite cylinder assemblage (CCA) approach based on continuum mechanics for investigating the elastic properties of a polymer resin reinforced by multi-walled carbon nanotubes (MWCNTs). A three-phase cylindrical representative volume element (RVE) model is employed based on CCA technique to elucidate the effects of inter layers, chirality, interspacing, volume fraction of MWCNT, interphase properties and temperature conditions on the elastic modulus of the composite. The interface region between CNT and polymer matrix is modeled as the third phase with varying material properties. The constitutive relations for each material system have been derived based on solid mechanics and proper interfacial traction continuity conditions are imposed. The predicted results from the CCA approach are in well agreement with RVE-based finite element model. The outcomes reveal that temperature softening effect becomes more pronounced at higher volume fractions of CNTs.

Keywords: Multi-walled carbon nanotube, composite cylinder assemblage, continuum, representative volume element, variable interphase.

1 Introduction

Carbon nanotubes (CNTs) have been recognized as the strongest and stiffest man-made material known since their discovery [Iijima (1991)]. Some fundamental research on CNTs [Huang, Hung and Chiang (2013); Joseph and Lu (2013)] have shown that they exhibit striking mechanical, thermal, physical and electrical properties, which make them more interesting for future applications. In their synthesis, multi-walled carbon nanotubes (MWCNTs) are first obtained and can be carefully processed to single-wall carbon nanotube (SWCNTs) [Aqel, El-Nour, Ammar et al. (2012)]. In fact, MWCNTs are composed of a nested array of SWCNTs with weak interaction between inter layers and have a larger diameter compared to individual SWCNT. Although SWCNT exhibits high stiffness and strength, the main drawback is that the elongation at break of a CNT is only

[1] Research Scholar, Mechanical Engineering Department, National Institute of Technology Rourkela, Odisha-769008, India.

[2] Associate Professor, Mechanical Engineering Department, National Institute of Technology Rourkela, Odisha-769008, India.

[*] Corresponding Author: Puneet Kumar. Email: puneetahalawat2009@gmail.com

6% [Walters, Ericson, Casavant et al. (1999); Yu, Files, Arepalli et al. (2000a)]. Theoretical and experimental analysis of individual MWCNTs showed a large variation in the elastic modulus of the outermost layer of MWCNTs [Yu, Lourie, Dyer et al. (2000b); Demczyk, Wang, Cumings et al. (2002)]. It has been experimentally established that MWCNT with small outer diameters (<10 nm) have higher tensile modulus as compared to those of large outer diameter. Nevertheless, more attention should be given to their low densities and high geometry ratio which are making them promising reinforcing candidates for nanostructured materials providing very high specific stiffness and strength.

The extraordinary properties of MWCNTs can be more explored by incorporating these nanostructures into a matrix material. Polymeric matrix has been used in most of the work, but another matrix like ceramics and metals can also be used for a wide variety of applications in the area of structural, aerospace and sports appliances and communication-related applications. Chakrabarty et al. [Chakrabarty and Çagin (2008)] performed a simulation analysis to investigate the thermo-mechanical behavior of SWCNTs, bundles of SWCNTs, MWCNTs and MWCNTs based tori. They concluded that temperature effect on mechanical properties of CNTs may be neglected for low temperature operation range. Selection of the right type of MWCNTs for a specific application is crucial for designing new MWCNT based composite material. A controlled size distribution of MWCNTs and degree of dispersion are two challenging factors which control the properties of MWCNT reinforced polymer composite. Shokrieh et al. [Shokrieh, Saeedi and Chitsazzadeh (2013)] have used mechanical stirring and sonication technique to achieve good dispersion and investigation reveals the 6% and 20% improvement in tensile and flexural strength respectively, at only 0.05 wt% of MWCNTs. The small size of reinforcement leads to an exceptionally large interfacial region with different chemistry, the degree of curing of polymer, polymer chain mobility, and crystallinity. The interface controls the degree of interaction as well as load transfer mechanism between the polymer matrix and MWCNT. The concept of chemical functionalization of MWCNTs is a useful approach to improve dispersion and interfacial adhesion of CNTs in the polymer. The previous report [Ramana, Padya, Kumar et al. (2010)] indicates that significant improvement as 58% in the strength of pristine MWCNTs and 100% improvement in acid treated MWCNT reinforced epoxy at only adding 1wt% content of MWCNT. In other research work, Arun et al. [Arun, Maharana and Kanagaraj (2013)] observed that Young's modulus, compressive strength and thermal conductivity of pure epoxy were enhanced by 39.4%, 10.7% and 59.2%, respectively with addition of 0.2 wt% of MWCNTs. As agglomeration occurred at a high volume fraction of CNTs, recently few efforts have been made by Nam et al. [Nam, Goto, Yamaguchi (2016)] to develop as aligned MWCNTs/epoxy composite with 63.4% volume fraction of CNTs using hot-melt prepreg processing with a vacuum-assisted system. Few comparative experimental analysis [Cui, Wang, Xiu et al. (2013); Thostenson and Chou (2002); Wang, Song, Liu et al. (2008)] are performed to investigate the mechanical behavior of functionalized and aligned MWCNT reinforced composite. Besides experimental work, which is very explanatory but costly at the nano-scale, analytical and numerical approaches based on the continuum mechanics are more convenient. In majority of modeling works [Odegard, Gates, Nicholson et al. (2002); Liu and Chen (2003); Alavinasab, Jha and Ahmadi (2014);

Pourasghar and Kamarian (2014); Kumar and Srinivas (2014); Wang and Liew (2015)] single-walled carbon nanotubes reinforced composites have been considered to study the influence of interphase and other geometric parameters on the effective elastic properties of composite. In this regards, Matveeva et al. [Matveeva, Böhm, Kravchenko et al. (2014)] presented finite element approach to model the polymer composites reinforced wavy carbon nanotubes. The results indicated that finite element technique can provide attractive combination of accuracy, flexibility and computational cost. Hackett [Hackett (2015)] illustrated the micromechanical modeling of hollow carbon nanotube embedded in an isotropic polymer matrix, utilizing a cylindrical method of cells (CMOC). Similarly, Bhuiyan et al. [Bhuiyan, Pucha and Kalaitzidou (2016)] predicted the tensile modulus of CNT/PP composite by utilizing 3-D RVE model and demonstrated the effect of dispersion, agglomeration, and orientation of CNT within the polymer matrix. Banerjee et al. [Banerjee, Nguyen and Chuang (2016)] investigated the role of interphase between the glassy polymer and carbon nanotube on the effective property of the composite using FE method. In this analysis, CNTs are considered as a Timoshenko beam element and interphase as continuum element. A recent survey by Kundalwal [Kundalwal (2017)] illustrated the available micro and nano mechanics based modeling techniques for nanocomposites. It obvious that modeling techniques for multi-walled carbon nanotube reinforced composites are very limited [Jindal, Goyal and Kumar (2013); Joshi and Upadhyay (2014a, 2014b)] and still needed to be explored.

In most of the above studies, the interface modeling and multi-walled interlayer forces have not been considered together. In present work, a three phase composite cylinder assemblage technique is adopted based on continuum mechanics for obtaining the elastic properties of MWCNT reinforced polymer nanocomposites. The effects of interphase properties and temperature conditions, as well as geometry of multi-wall carbon nanotubes on elastic modulus of the composite are presented. A three-phase representative volume element is modeled based on CCA approach, which comprises of multi-walled carbon nanotube, interface and polymer matrix. Based on continuum mechanics and elasticity theory, displacement functions are determined, and proper stress and strain relationships are applied for each phase in composite cylindrical RVE. These relations are solved by implementing appropriate boundary conditions at the interface of each phase. The effects of interphase properties and temperature changes on the effective elastic modulus are studied. Two case studies are illustrated and results are found to be in good agreement with numerical model. The remainder of the paper is organized into the following sections. Section 2 deals the RVE model of composite along with interface considerations. Section 3 presents constitutive model of elastic modulus in polar coordinates. Section 4 gives numerical results with two case studies. Brief conclusions are presented in section 5.

2 Computational methodology

This section presents the description of modeling procedure of MWCNT, interphase and MWCNT reinforced polymer composite. Proposed continuum model based on composite cylinder assemblage approach is also illustrated here.

2.1 Modeling of MWCNT based on continuum theory

CNTs are reformed shape of single layer of graphite, which is rolled up in the form of a hollow cylindrical tube. Where-as MWCNT is a more intricate array of concentric nanotubes with diversity in structure and sequential arrangements. The simplest form of a MWCNT is when concentric tubes are identical, but different in diameter. The diameters of MWCNT are typically in the range of 1 nm to 20 nm and interlayer distance is close to the distance between graphene layers in graphite [Kumar and Srinivas (2017)]. In this case, Multiwall carbon nanotubes reinforced polymer system is selected for comprehensive investigation because of large scale production of MWCNTs is easier compare to SWCNTs. The challenges in the production of SWCNTs on large scale reflect on its cost, which is currently higher than MWCNTs. Moreover, mathematical formulation of mean radius of SWCNT *(r_{cnt})* can be presented in the form of chiral indices (*n, m*) and carbon-carbon bond length (a_{c-c}=0.1414 nm).

$$r_{cnt} = \frac{\sqrt{3(m^2 + n^2 + nm)}}{2\pi} a_{c-c} \tag{1}$$

$$r_{o,i} = r_{cnt} \pm {t_{cnt}}/{2} \tag{2}$$

Here, r_o, r_i, and t_{cnt} (=0.335 *nm*) are the outer radius, inner radius and tube thickness of SWCNT respectively. As shown in Fig. 1, modeling of molecular structure of MWCNTs is a very complex assignment. Therefore an effective cross-section area of multi-walled CNT can be calculated based on continuum model.

$$A_e = 2\pi t_{cnt}\left[N r_{cnt} + \sum_{i=1}^{N} h(i-1) \right] \tag{3}$$

where N is numbers of walls and h is interlayer spacing in MWCNT. It is observed that interlayer spacing of MWCNTs vary from 0.27 nm up to 0.42 nm [Kharissova and Kharisov (2014)], in this work interlayer spacing is considered as $1.5 \times t_{cnt}$. The effective cross-section of MWCNT can be used for calculating outermost radius (r_n) of MWCNT, and we can replace this space frame structure of multi-wall CNTs with an equivalent hollow cylinder of radius r_i and r_n (see Fig. 1). The outermost radius of MWCNT [Zhang and Wang (2005)] can be estimated as

$$r_n = r_{cnt} + h(N-1) \tag{4}$$

Polymer matrix and interphase is considered as one phase (V_1) and related with the volume fraction of CNTs in RVE.

$$V_1 = 1 - V_n = V_m + V_{\text{int}} \tag{5}$$

$$V_n = \frac{{r_n}^2}{R^2} \text{ and } V_{\text{int}} = \frac{(r_n + t_{\text{int}})^2 V_n}{{r_n}^2} - V_n \tag{6}$$

where V_n, V_{int} and V_m are the volume fractions of MWCNT, interphase and matrix in the RVE. The radius of interphase $r_{int}=r_n+t_{int}$, where t_{int} is the thickness of interphase and R is the radius of cylindrical RVE. The structure of multi-wall carbon nanotubes influences its elastic properties. Larger diameter MWCNTs behave like a graphite structure. Therefore effective elastic properties of MWCNT (E_n and G_n) can be described in structure parameters as [Wu, Zhang, Leung et al. (2006); Zhang and Wang (2005)]

$$E_n = \frac{Nt_{cnt}E_{cnt}}{(N-1)h + t_{cnt}}, \qquad G_n = \frac{Nt_{cnt}E_{cnt}}{[2(N-1)h + t_{cnt}](1+\upsilon_{cnt})} \tag{7}$$

where E_{cnt}, υ_{cnt} are the Young's modulus and Poisson's ratio of SWCNT, which may be a function of temperature change. The elastic properties of carbon nanotube and polymer can be represented in terms of temperature change (ΔT) as follows [Zhang and Wang (2005)]

$$E_{cnt} = E^0_{cnt}(1 - 0.0005 \times \Delta T)), \ E_m = E^0_m(1 - 0.0003 \times \Delta T)) \tag{8}$$

where E^0_{cnt} and E^0_m are the Young's modulus of CNT and polymer matrix at room temperature.

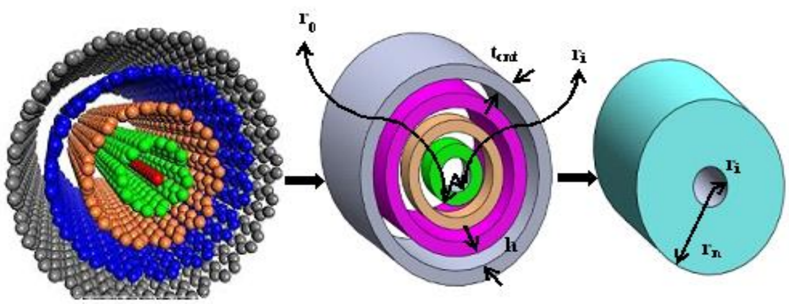

Figure 1: Equivalent model of Multi-wall Carbon Nanotube

2.2 Interphase modeling

In a real scenario, a small region arises around the CNT embedded in a polymer matrix which can alter the overall mechanical behavior of composite. Most of the studies considered the homogenous behavior of interphase adopting the linear isotropic properties but experimental studies in the literature have shown that CNT surface interacts with its surrounding polymer matrix to create a three-dimensional region with gradient properties. The interphase region between CNT and polymer matrix behaves as the buffer medium, and selection of its properties are challenging task to investigate the overall performance of the composite. A simple theoretical model is employed here to analyze the interphase effect on elastic properties of MWCNT reinforced polymer composite. The interphase region is considered as a layer developed around the multi-walled carbon nanotube with varying properties along the interphase thickness (see Fig. 2). Young's modulus of interphase (E_{int}) can be calculated as follows [Hu, Arefin, Yan et al. (2014)]

$$E_{\text{int}}(r) = E_m\left(\frac{r_{\text{int}}}{r}\right) + \left[\frac{r_{\text{int}} - r}{t_{\text{int}}}\right]^k \left[E_n - E_m\left(\frac{r_{\text{int}}}{r_n}\right)\right] \tag{9}$$

where $r_n \le r \le r_{\text{int}}$ and $k(\ge 1)$ is the interphase enhancement index that depends on the morphology, chemistry and surface treatment between the polymer matrix and MWCNT in the nanocomposite. The average value of interphase elastic modulus, E_{int}, can be derived based on the cross-sectional area of interphase region:

$$E_{\text{int}} = \frac{2}{r_{\text{int}}^2 - r_n^2} \int_{r_n}^{r_{\text{int}}} E_{\text{int}}(r) r dr \tag{10}$$

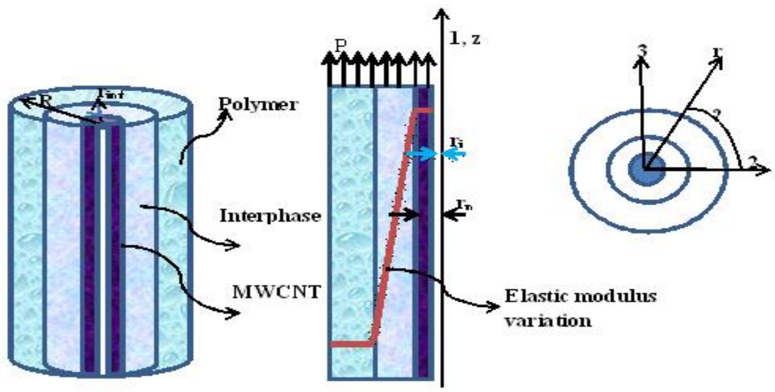

Figure 2: RVE of MWCNT reinforced polymer composite

3 Constitutive model for effective elastic modulus

The MWCNT reinforced polymer composite is assumed to be statistically homogeneous and periodic, i.e. CNTs are uniformly dispersed within the polymer matrix. The polymer matrix is considered as a continuum isotropic material. Furthermore, CNTs in the polymer matrix are assumed to be aligned axially but practically it is very difficult to align CNTs perfectly. The size of CNTs and interphase region strongly depends on the synthesis method and process parameters. A mathematical model (*CCA*) is developed for determining the effective elastic modulus of MWCNT reinforced polymer composite in the axial direction using 3-D elasticity theory. In this approach, a small portion of the nanocomposite system can be modeled using a Representative Volume Element (*RVE*). In carbon nanotube reinforced composites, stress transfer takes place through the interphase region that evolves during the interaction of polymer and CNT in the synthesis process of the composite. Interphase is considered here as the third phase with functionally graded properties, and perfect bonding exists at interphase and CNT interface, interphase and polymer interface. A cylindrical RVE of radius (R) consist of polymer embedded with MWCNT (r_i innermost radius and r_n outermost radius) is selected for present investigation. The typical view of all phases in cylindrical coordinate system is shown in Fig. 2. RVE is considered under an axial load (P) to determine the effective elastic modulus of the nanocomposite in the axial direction. Applied load is in the range of elasticity, hence average stress σ_z can be written as

$$\sigma_z = \frac{P}{\pi\left(R^2 - r_i^2\right)} \tag{11}$$

According to theory of elasticity,

$$\sigma_z = E_z \varepsilon_z \tag{12}$$

where E_z is the effective elastic modulus of nanocomposite and ε_z is a strain in the axial direction. Thus

$$E_z = \frac{P}{\pi\left(R^2 - r_i^2\right)\varepsilon_z} \tag{13}$$

The effective strain (ε_z) in nancomposite is evaluated using displacement function. The basic derivation of displacement function is illustrated [Kaw (1997)]. As the MWCNT and RVE are considered a cylindrical volume, the radial displacement of each phase given by

$$u^n = A_c r + \frac{B_c}{r}, r_i \le r \le r_n \tag{14}$$

$$u^{\text{int}} = A_i r + \frac{B_i}{r}, r_n \le r \le r_{\text{int}} \tag{15}$$

$$u^m = A_m r + \frac{B_m}{r}, r_{\text{int}} \le r \le r_m \tag{16}$$

where u^n u^{int} and u^m indicates the displacement functions for nanotube, surrounding interphase and polymer matrix respectively. A_c, B_c, A_i, B_i, A_m, B_m, ε_z are the seven unknown parameters need to be estimated to solve the elastic problem. In this line, strains in each phase are to be calculated using displacement function from Eqs. (14-16). Then, stiffness matrices are computed from the elastic properties of respective phase. Substituting the stiffness matrix and strain values of each phase, we can get stress developed in particular phase according to $\{\sigma^i\} = [C^i]\{\varepsilon^i\}$, where $[C^i]$ represents the i^{th} phase stiffness. Following seven boundary and interface traction continuity conditions can be used to solve this boundary value problem.

The radial displacement is continuous at the interface of MWCNT and interphase

$$u^n(r = r_n) = u^{\text{int}}(r = r_n) \tag{17}$$

The radial displacement is continuous at the interface of interphase and polymer matrix

$$u^{\text{int}}(r = r_{\text{int}}) = u^m(r = r_{\text{int}}) \tag{18}$$

The radial stress is continuous at $r=r_n$ and $r=r_{int}$

$$\sigma_r^n(r = r_n) = \sigma_r^{\text{int}}(r = r_n), \quad \sigma_r^{\text{int}}(r = r_{\text{int}}) = \sigma_r^m(r = r_{\text{int}}) \tag{19}$$

Surface at $r=r_i$ and $r=R$ is traction free, therefore

$$\sigma_r^n(r=r_i)=0,\ \sigma_r^m(r=R)=0 \tag{20}$$

The overall force on the MWCNT reinforced polymer composite cross-section in longitudinal direction is equal to applied load.

$$\int_0^R \sigma_z 2\pi r dr=P,\ \ \sigma_z=\begin{cases}\sigma_z^n, r_i\le r\le r_n\\ \sigma_z^{\text{int}}, r_n\le r\le r_{\text{int}}\\ \sigma_z^m, r_{\text{int}}\le r\le R\end{cases} \tag{21}$$

Solving the Eqs. (17-21), we can obtain the values of parameters A_c, B_c, A_i, B_i, A_m, B_m, ε_z and substituting ε_z in Eq. (13), yields the elastic modulus of MWCNT reinforced polymer composite.

4 Numerical results and discussion

The homogenization process is employed to the periodic structure of uniformly reinforced MWCNT nanocomposite to evaluate the effective elastic modulus. Here an effective solid fiber is considered, which replaces a MWCNT as the filler phase in the representative volume element. Further, composite cylinder assemblage approach is employed to the RVE for predicting the effective elastic modulus of the nanocomposite. A mathematical model is developed for three phase RVE based on 3-D elasticity theory, and proper boundary conditions are imposed to determine the effective elastic modulus of MWCNT nanocomposite. A MATLAB program with computer configuration [Intel (R) core (TM) i7 CPU @ 3.40 GHz with 2 GM RAM and 64-bit operating system] is implemented for solving the model equations of unknown parameters. Deformation and stresses are computed for different load cases to extract effective elastic modulus of the nanocomposite. It took approximately 30 seconds to run the code every time. Applied load (*P*) and Young's modulus values are considered in *nN* and nN/nm^2 respectively to introduce nano-scale effect in RVE model. Interphase thickness varies from 0.5 to 4 times of the CNT thickness, which play a major role in influencing the effective elastic modulus of the nanocomposite. In present study interphase thickness is considered 0.754 nm [Hu, Arefin, Yan et al. (2014)]. A (10, 5) armchair CNT is considered for investigation and according to the volume fraction of CNTs in the polymer, the outer diameter of RVE is calculated using CNT diameter. The results obtain from the present model are compared with finite element method [Hu, Arefin, Yan et al. (2014)] and analytical results (rule of mixture). The results shown in Fig. 3 are for MWCNT inside cylindrical RVE, for a range of volume fraction 1% to 5% considering single layer ($N=1$) and $P=1000\ nN$. The CCA model results are found to be in good agreement with FEM results. One more case study is performed to determine the accuracy of the present approach for different composite system (CNT/PMMA) with properties as given in [Montazeri and Naghdabadi (2010)], E_{cnt}=1000 nN/nm^2, E_m=2.5 nN/nm^2, E_i=93.67 nN/nm^2, t_{int}=0.42 nm $\upsilon_i=\upsilon_m$=0.35, and (10,10) armchair CNT. A computer-based simulation study has been carried out to estimate the elastic results, which are presented in Tab. 1. Predicted results show good agreement at higher volume fraction also.

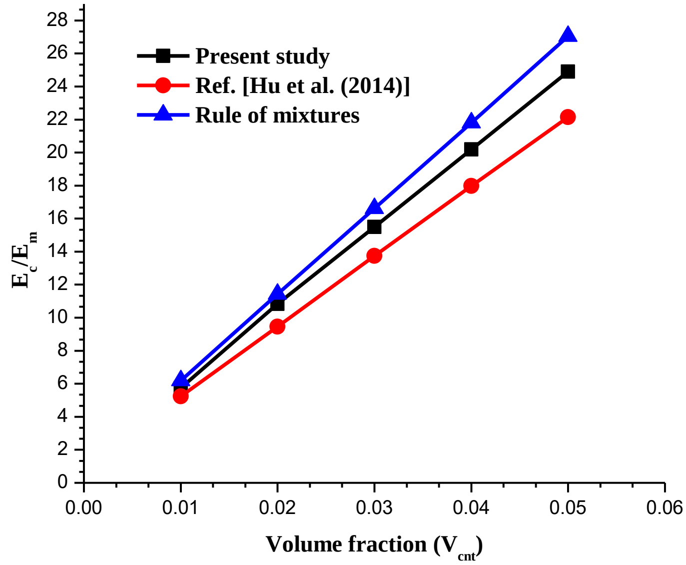

Figure 3: Comparison of the elastic modulus ratio (E_c/E_m) of MWCNT reinforced composite for (N=1)

Table 1: Case study for validation of present model

V_{cnt} (%)	MD [(Han and Elliott (2007)]	2-Phase model [(Montazeri and Naghdabadi (2010)]		3-phase model (Present work)	
		Result	Deviation	Result	Deviation
12	94.6	81.2	14.2%	98.95	4.39%
17	138.9	114.0	17.9%	141.45	1.8%
28	224.2	186.1	17.0%	231.57	3.18%

Tab. 2 shows the elastic and geometric properties of single wall CNT, polymer, and interphase. Elastic properties of MWCNTs are calculated from the SWCNT properties and geometric parameters as described in Eq. 7 and Eq. 8. The sets of analysis are conducted for RVEs for different volume fraction, a number of layers, types of chirality, interphase property, and temperature conditions. Following studies are made considering the data as shown in Tab. 2. Fig. 4 shows the relationship between stress and strain for three different volume fraction of MWCNT ($N=1$). It can be seen from results that stress in the composite is increasing as the volume fraction of CNT increases, which can be understood that high concentration of CNT leads to more stiffness. The decreasing trend of E_c/E_m values for different MWCNTs is observed in Fig. 5. It can be noticed that addition of number walls in SWCNT tends to lower the effective modulus of composite because complete load can not be transferred from innermost wall to outermost wall in MWCNTs. Results are obtained for the different volume fraction of MWCNTs at constant interspacing ($h=1.5\times t_{cnt}$) between layers. Fig. 6 shows the variation of effective elastic modulus of the composite with interspacing between layers (tubes) of MWCNT (at 1% volume fraction of MWCNT). It is observed that the elastic modulus of the composite decreases as interspacing increases, it is because of load transfer mechanism affected by the interspacing of tubes. It is also observed that elastic modulus decreases with the increase in number of walls in MWCNT. This phenomenon can be explained as the number of was an increase, load transfer from matrix to MWCNT innermost tube decreases and overall elastic modulus decreases. Also for *N=1* (SWCNT case), there is no effect of interspacing on effective elastic modulus which shows that model predicts accurate results. In Fig. 7 effective elastic modulus of MWCNT reinforced polymer composite are plotted for a different type of CNTs to observe the effect of CNT chirality. It can be seen from the figure that (10, 0) CNT configuration shows a drastic decrement in elastic modulus as compared to (10, 5). It is also observed from results that the elastic modulus of composite reinforced with (10, 10) and (10, 20) CNT configuration shows enhancement as a number of walls in MWCNT increases.

Table 2: Material properties and geometric parameters for each phase at room temperature [Hu, Arefin, Yan et al. (2014)]

Parameter	CNT	Polymer	Interphase
Young's modulus E (nN/nm^2)	1054	2.026	16.10 (k=50)
Poisson's ratio (υ)	0.25	0.40	0.40
Geometric parameters	n=10, m=5, t_{cnt}=0.335 nm		t_{int}=0.754 nm

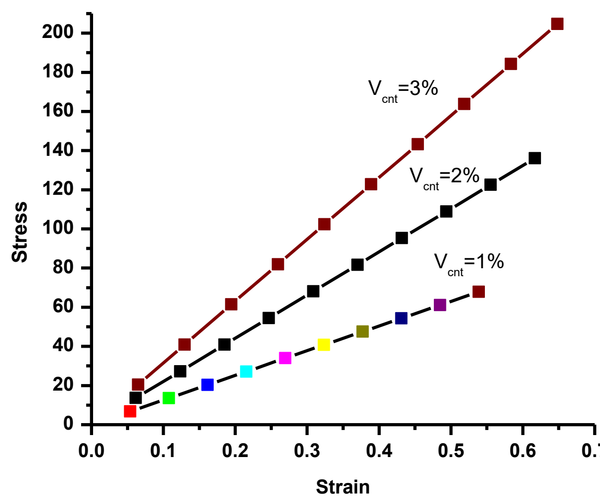

Figure 4: Stress v/s strain plot for different volume fraction of (10, 5) MWCNT (N=1)

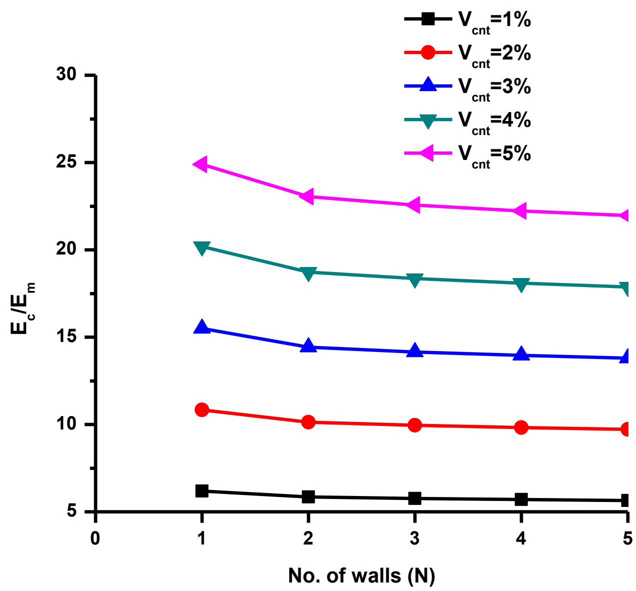

Figure 5: Effect of number of walls in MWCNT on effective elastic modulus of composite for different volume fraction (*h=1.5×tcnt*)

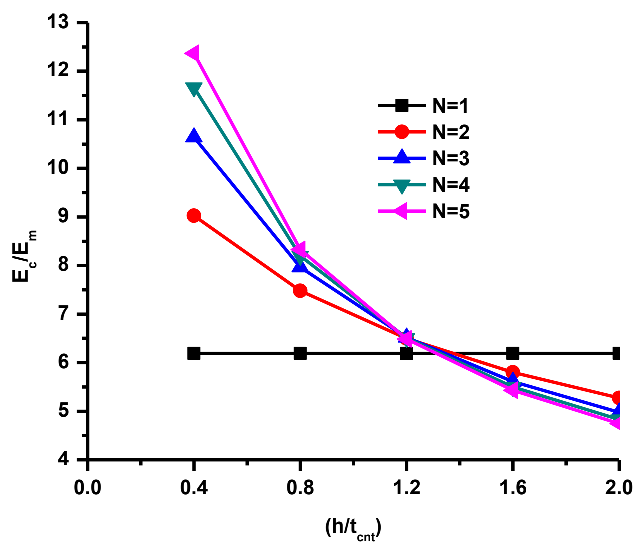

Figure 6: Effect of interlayer spacing in MWCNT on effective elastic modulus of composite for (10, 5) configuration

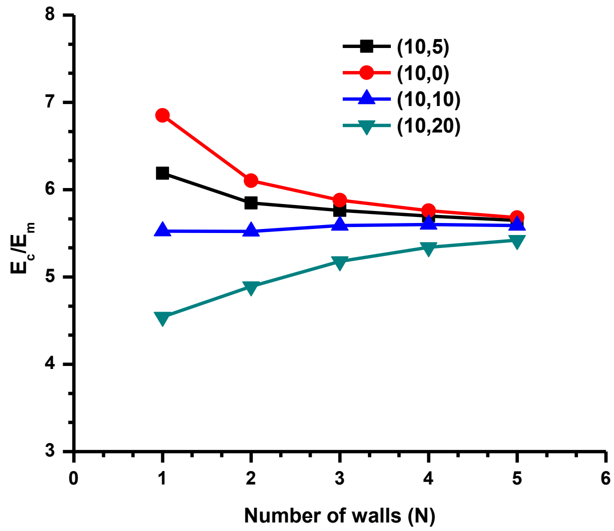

Figure 7: Effect of CNT chirality on effective elastic modulus of MWCNT reinforced composite ($h=1.5\times t_{cnt}$)

4.1 Effect of interphase property

Interphase plays a significant role in the evaluation of elastic properties of the nanocomposite. It provides the bridge to load transfer mechanism from polymer matrix to nano-fiber. As carbon nanotubes have a large surface area which leads to a very large interphase region around CNT. This region possesses special properties, varies between polymer and CNT properties (as shown in Fig. 8). Therefore, in the present analysis interphase region is considered as the third phase with functionally graded properties and at particular interphase index (k) value, the average value of interphase elastic modulus is determined. As shown in mathematical modeling section, temperature affects the elastic properties of the polymer matrix, and MWCNT, similarly interphase properties will also be affected by the temperature change because interphase modulus depends on the polymer and CNT. Fig. 9 shows the effect of temperature change on elastic modulus of interphase for the interphase index, $k=2$. It is observed that temperature change lowered the elastic modulus of interphase and finally effective modulus of the composite will also be affected. Fig. 10 shows the relationship between effective elastic modulus and interphase index at various volume fractions of CNTs. It can be observed from the results effective elastic modulus decreases as interphase index increases. The reason behind this cause is a decrement in interphase modulus as interphase index increases. Fig. 11 describes a relationship between effective elastic modulus and interphase index for different CNT chirality at 1% CNT volume fraction. It can be observed from the results that (10, 0) type CNT shows the sudden decrement in elastic modulus in comparison to other configuration.

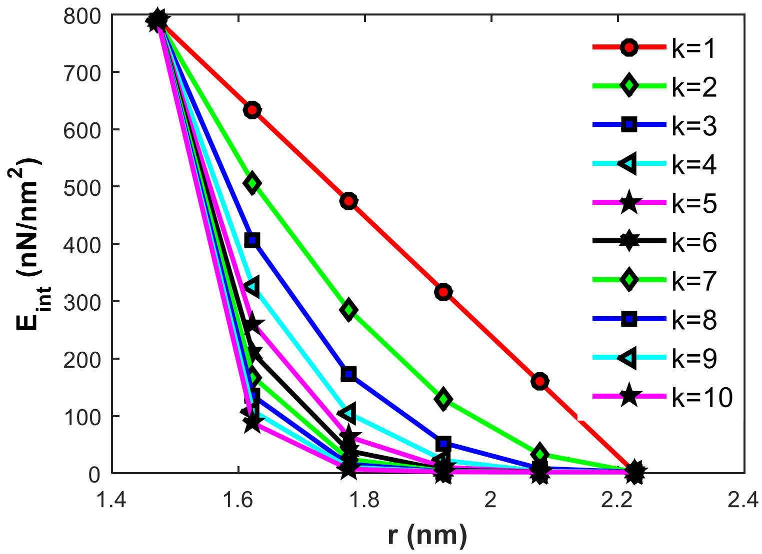

Figure 8: Variation of elastic modulus of interphase along the interphase radius ($\Delta T=0$, $N=3$)

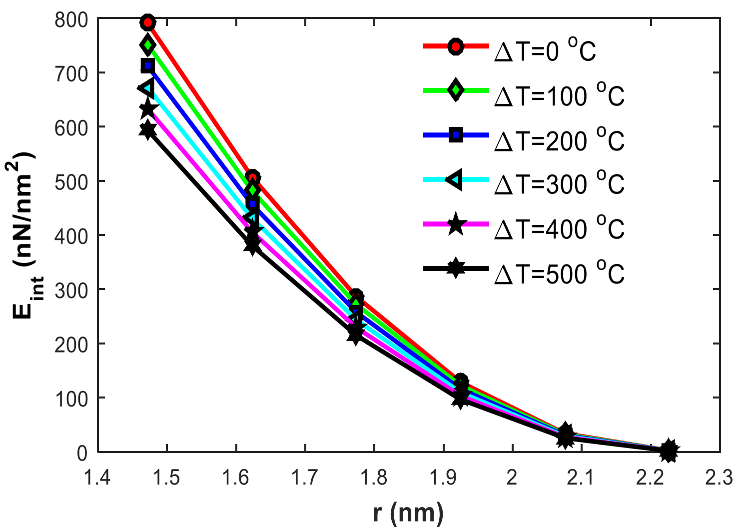

Figure 9: Variation of elastic modulus of interphase along the interphase radius for different temperature change ($k=2$, $N=3$)

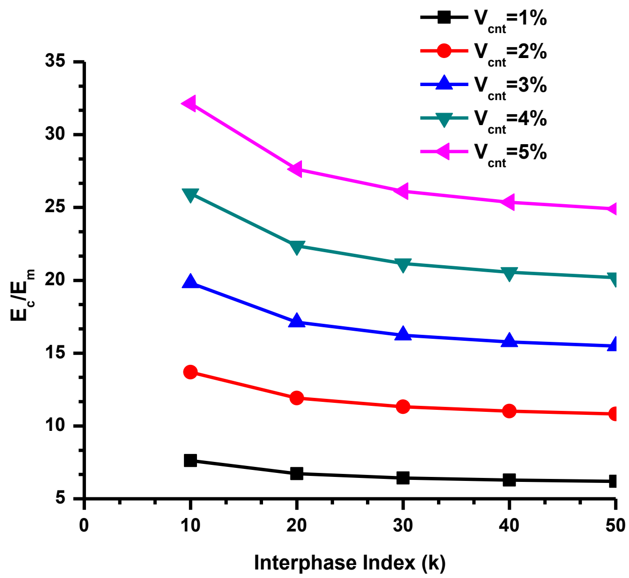

Figure 10: Effect of interphase index on effective elastic modulus of composite at different volume fraction of CNT (*N=3*)

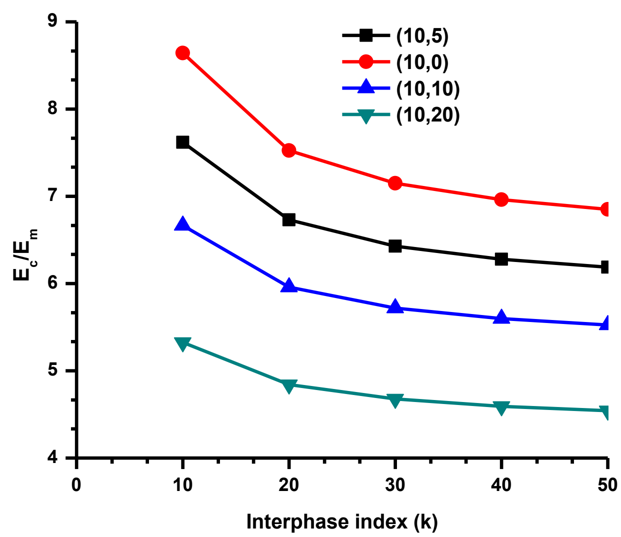

Figure 11: Effect of interphase index on effective elastic modulus of composite for different configuration type of CNT (*N=3*)

4.2 Effect of temperature change

CNTs make the polymers highly conductive, mechanically stronger and less susceptible to thermal degradation. Thermal stability may be affected by the incorporation of CNTs in the polymer composite. To ensuring the high-temperature applications of CNT-reinforced polymer composite temperature effect of temperature change on the elastic modulus of MWCNT reinforced polymer composite is to be studied. In this regards, a mathematical formulation is employed to investigate the effect of temperature on the elastic modulus of the polymer composite, and computer results are presented in this section. Figs. 12 and 13 show the effect of temperature change on effective elastic modulus for different volume fraction and different CNT configurations (*V_n=1%).* It can be observed from results that effective elastic modulus of CNT reinforced composite become lower at high temperature as compared to low temperature condition. Also, temperature effect seems more influencing at high volume fraction. As at high-temperature bonding between carbon and carbon atoms in CNT and bonding between polymer and CNT at interface becomes less stable, this diminishes the advantages of CNT reinforcement. Fig. 13 reveals that (10, 0) configuration of CNT provides more stability against temperature change in comparison to other configurations. Fig. 14 shows the relationship between temperature change and effective elastic modulus of MWCNT reinforced polymer composite. It is observed that sudden drops in the effective elastic modulus between SWCNT and DWCNT reinforced polymer composite. It is also observed that elastic modulus goes on decreasing as number of walls increase in MWCNT.

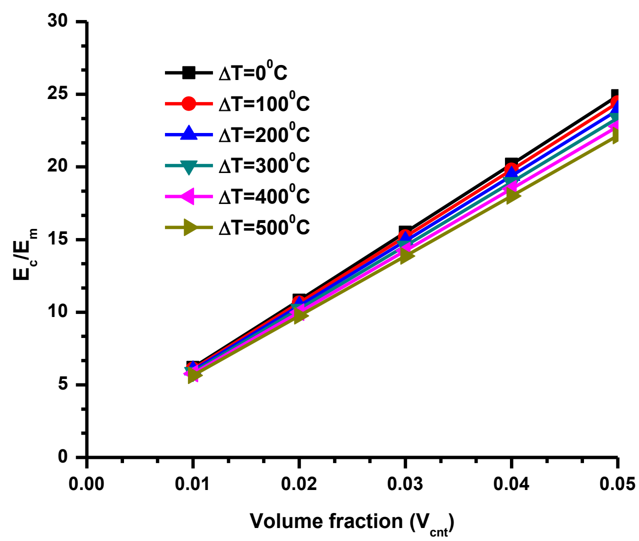

Figure 12: Effect of temperature change on effective elastic modulus of composite (*N=3*)

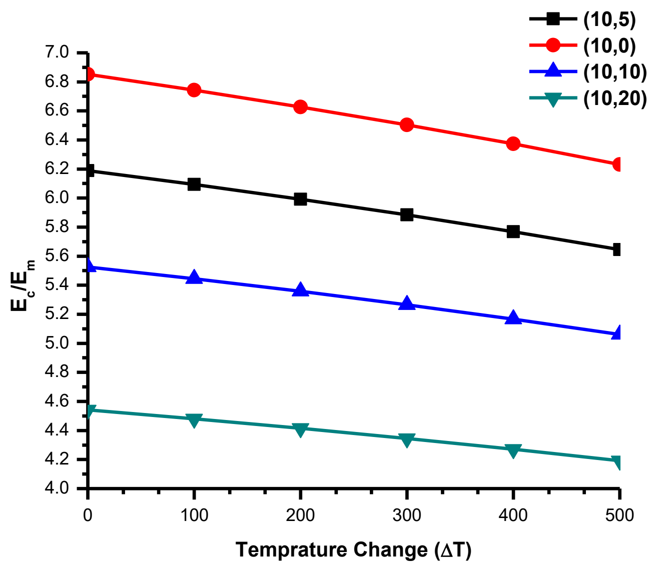

Figure 13: Effect of temperature change on effective elastic modulus for different CNT configuration (*N=3*)

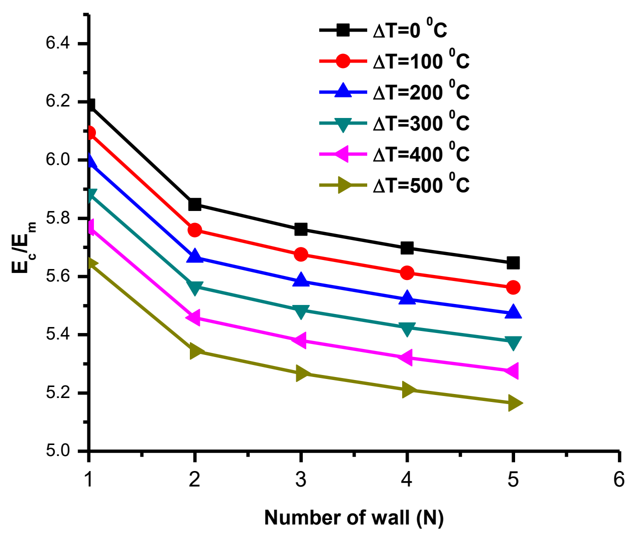

Figure 14: Effect of temperature change on effective elastic modulus with number of walls

5 Conclusion

A continuum modeling approach was employed to demonstrate the elastic behavior of MWCNT reinforced polymer composite. Nanocomposite materials have complex reinforcement phenomenon, so homogenization technique was considered for selecting a representative volume element instead of composite periodic structure. A three phase cylindrical representative volume element (RVE) based on composite cylinder assemblage (CCA) approach was adopted to elaborate the effect of MWCNT on elastic properties of composites. Based on continuum mechanics and theory of elasticity, displacement functions were determined, and proper stress and strain relationships were employed for each phase in composite cylindrical RVE. These stress-strain relations were solved by implementing appropriate boundary conditions at the interface of each phase and the boundary value problem was solved. An equivalent hollow cylindrical tube model of MWCNT was developed based on geometric and elastic properties of SWCNT. The main objective of this analysis is to apply this CCA approach to investigate the influence of MWCNT with different geometric parameters and temperature change. The results obtained from RVE model were compared with the analytical results and also validated with results available in the literature for single wall CNT (for $N=1$) case. A decrease in composite elastic modulus was found to be remarkable in the case of more number of layers in MWCNT with small interspacing between the layers. The outcomes also reveal that temperature effect has been found more pronounced at higher volume fractions. As a future scope, the work can be extended to the debonding condition of CNT inside the polymer.

Acknowledgement: The authors are thankful to National Institute of Technology Rourkela for providing computational facilities and infrastructure to carry out the research work.

References

Alavinasab, A.; Jha, R.; Ahmadi, G. (2014): Modeling of Carbon Nanotube Composites Based on Nonlocal Elasticity Approach. *International Journal for Computational Methods in Engineering Science and Mechanics*, vol. 15, no. 1, pp. 17-25.

Aqel, A.; El-Nour, K. M. M. A.; Ammar, R. A. A.; Al-Warthan, A. (2012): Carbon nanotubes, science and technology part (I) structure, synthesis and characterisation. *Arabian Journal of Chemistry*, vol. 5, no. 1, pp. 1-23.

Arun, S.; Maharana, M.; Kanagaraj, S. (2013): Optimizing the Processing Conditions for the Reinforcement of Epoxy Resin by Multiwalled Carbon Nanotubes. *Journal of Nanotechnology*, vol. 2013, pp. e634726.

Banerjee, D.; Nguyen, T.; Chuang, T. J. (2016): Mechanical properties of single-walled carbon nanotube reinforced polymer composites with varied interphase's modulus and thickness: A finite element analysis study. *Computational Materials Science*, vol. 114, pp. 209-218.

Bhuiyan, M. A.; Pucha, R. V.; Kalaitzidou, K. (2016): 3D RVE Models Able to Capture and Quantify the Dispersion, Agglomeration, and Orientation State of CNT in CNT/PP Nanocomposites. *Polymeric and Composite Materials*, vol. 3, pp. 1-13.

Chakrabarty, A.; Çagin, T. (2008): Computational Studies on Mechanical and Thermal Properties of Carbon Nanotube Based Nanostructures. *Computers, Materials & Continua*, vol.7, no.3, pp.167-189.

Cui, L. J.; Wang, Y. B.; Xiu, W. J.; Wang, W. Y.; Xu, L. H. et al. (2013): Effect of functionalization of multi-walled carbon nanotube on the curing behavior and mechanical property of multi-walled carbon nanotube/epoxy composites. *Materials & Design*, vol. 49, pp. 279-284.

Demczyk, B. G.; Wang, Y. M.; Cumings, J.; Hetman, M.; Han, W. et al. (2002): Direct mechanical measurement of the tensile strength and elastic modulus of multiwalled carbon nanotubes. *Materials Science and Engineering: A*, vol. 334, no. 1-2, pp. 173-178.

Hackett, R. M. (2015): Modeling carbon nanotube reinforced composite materials with the cylindrical method of cells. *International Journal for Numerical Methods in Engineering*, vol. 103, no. 6, pp. 413-429.

Han, Y.; Elliott, J. (2007): Molecular dynamics simulations of the elastic properties of polymer/carbon nanotube composites. *Computational Materials Science*, vol. 39, no. 2, pp. 315-323.

Hu, Z.; Arefin, M. R. H.; Yan, X.; Fan, Q. H. (2014): Mechanical property characterization of carbon nanotube modified polymeric nanocomposites by computer modeling. *Composites Part B: Engineering*, vol. 56, pp. 100-108.

Huang, C. J.; Hung, T. Y.; Chiang, K. N. (2013): Estimation of the Mechanical Property of CNT Ropes Using Atomistic-Continuum Mechanics and the Equivalent Methods. *Computers, Materials & Continua*, vol. 36, no. 2, pp. 99-133.

Iijima, S. (1991): Helical microtubules of graphitic carbon. *Nature*, vol. 354, no. 6348, pp. 56-58.

Jindal, P.; Goyal, M.; Kumar, N. (2013): Modeling Composites of Multi-Walled Carbon Nanotubes in Polycarbonate. *International Journal for Computational Methods in Engineering Science and Mechanics*, vol. 14, no. 6, pp. 542-551.

Joseph, J.; Lu, Y. C. (2013): Design of Aligned Carbon Nanotubes Structures Using Structural Mechanics Modeling Part 1: Theory and Individual Carbon Nanotube Modeling. *Computers, Materials & Continua*, vol. 37, no.1, pp. 39-57.

Joshi, P.; Upadhyay, S. H. (2014a): Effect of interphase on elastic behavior of multiwalled carbon nanotube reinforced composite. *Computational Materials Science*, vol. 87, pp. 267-273.

Joshi, P.; Upadhyay, S. H. (2014b): Evaluation of elastic properties of multi walled carbon nanotube reinforced composite. *Computational Materials Science*, vol. 81, pp. 332-338.

Kaw, A. K. (1997): Micromechanical Analysis of a Lamina, *Mechanics of Composite Materials*, Second., CRC Press, New York, pp. 241-248.

Kharissova, O. V.; Kharisov, B. I. (2014): Variations of interlayer spacing in carbon nanotubes. *RSC Advances*, vol. 4, no. 58, pp. 30807-30815.

Kumar, P.; Srinivas, J. (2014): Numerical evaluation of effective elastic properties of CNT-reinforced polymers for interphase effects. *Computational Materials Science*, vol. 88, pp. 139-144.

Kumar, P.; Srinivas, J. (2017): Elastic behavior of CNT-reinforced polymer composites with discontinuities in CNT configurations. *IOP Conference Series: Materials Science* *and Engineering*, IOP Publishing, vol. 178, no. 1, pp. 12016.

Kundalwal, S. I. (2017): *Review on Micromechanics of Nano- and Micro-Fiber Reinforced Composites*. Https://doi.org/10.1002/pc.

Liu, Y. J.; Chen, X. L. (2003): Evaluations of the effective material properties of carbon nanotube-based composites using a nanoscale representative volume element. *Mechanics of Materials*, vol. 35, no. 1-2, pp. 69-81.

Matveeva, A. Y.; Böhm, H. J.; Kravchenko, G.; Hattum, F. W. J. V. (2014): Investigation of the Embedded Element Technique for Modelling Wavy CNT Composites. *Computers, Materials & Continua*, vol. 42, no. 1, pp. 1-23.

Montazeri, A.; Naghdabadi, R. (2010): Investigation of the interphase effects on the mechanical behavior of carbon nanotube polymer composites by multiscale modeling. *Journal of Applied Polymer Science*, vol. 117, no. 1, pp. 361-367.

Nam, T. H.; Goto, K.; Yamaguchi, Y.; Premalal, E. V. A.; Shimamura, Y. et al. (2016): Improving mechanical properties of high volume fraction aligned multi-walled carbon nanotube/epoxy composites by stretching and pressing. *Composites Part B: Engineering*, vol. 85, pp. 15-23.

Odegard, G. M.; Gates, T. S.; Nicholson, L. M.; Wise, K. E. (2002): Equivalent-continuum modeling of nano-structured materials. *Composites Science and Technology*, vol. 62, no. 14, pp. 1869-1880.

Pourasghar, A.; Kamarian, S. (2014): Mechanical material characterization of an embedded Carbon nanotube in polymer matrix by employing an equivalent fiber. *International Journal of Nano Dimension*, vol. 6, no. 2, pp. 167-175.

Ramana, G. V.; Padya, B.; Kumar, R. N.; Prabhakar, K. V. P.; Jain, P. K. (2010): Mechanical properties of multi-walled carbon nanotubes reinforced polymer nanocomposites. *Indian Journal of Engineering and Materials Sciences*, vol. 17, no. 5, pp. 331-337.

Shokrieh, M. M.; Saeedi, A.; Chitsazzadeh, M. (2013): Mechanical properties of multi-walled carbon nanotube/polyester nanocomposites. *Journal of Nanostructure in Chemistry*, vol. 3, no. 1, pp. 1-5.

Thostenson, E. T.; Chou, T. W. (2002): Aligned multi-walled carbon nanotube-reinforced composites: processing and mechanical characterization. *Journal of Physics D: Applied Physics*, vol. 35, no. 16, pp. L77-L80.

Walters, D. A.; Ericson, L. M.; Casavant, M. J.; Liu, J.; Colbert, D. T. et al. (1999): Elastic strain of freely suspended single-wall carbon nanotube ropes. *Applied Physics Letters*, vol. 74, no. 25, pp. 3803-3805.

Wang, D.; Song, P.; Liu, C.; Wu, W.; Fan, S. (2008): Highly oriented carbon nanotube papers made of aligned carbon nanotubes. *Nanotechnology*, vol. 19, no. 7, pp. 75609.

Wang, J. F.; Liew, K. M. (2015): On the study of elastic properties of CNT-reinforced composites based on element-free MLS method with nanoscale cylindrical representative volume element. *Composite Structures*, vol. 124, pp. 1-9.

Wu, Y.; Zhang, X.; Leung, A. Y. T.; Zhong, W. (2006): An energy-equivalent model on studying the mechanical properties of single-walled carbon nanotubes. *Thin-Walled Structures*, vol. 44, no. 6, pp. 667-676.

Yu, M. F.; Files, B. S.; Arepalli, S.;Ruoff, R. S. (2000a): Tensile Loading of Ropes of Single Wall Carbon Nanotubes and their Mechanical Properties. *Physical Review Letters*, vol. 84, no. 24, pp. 5552-5555**.**

Yu, M. F.; Lourie, O.; Dyer, M. J.; Moloni, K.; Kelly, T. F. et al. (2000b): Strength and Breaking Mechanism of Multiwalled Carbon Nanotubes Under Tensile Load. *Science*, vol. 287, no. 5453, pp. 637-640.

Zhang, Y. C.; Wang, X. (2005): Thermal effects on interfacial stress transfer characteristics of carbon nanotubes/polymer composites. *International Journal of Solids and Structures*, vol. 42, no. 20, pp. 5399-5412.