Elastic behavior of CNT-reinforced polymer composites with discontinuities in CNT configurations

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Abstract: A numerical study has been made towards the effective elastic properties estimation of carbon nanotubes and carbon nanotube reinforced composite using finite element modelling (FEM). First, the elastic properties of Carbon nanotube (CNT) were predicted by considering that carbon atoms as nodes and carbon-carbon bonds as beam elements with linear and isotropic behaviour. It was observed that elastic properties of CNT predicted by FE analysis were in good agreement with previous data. Carbon atom vacancy defects were also included to investigate the adverse effect on elastic modulus of SWCNTs. To explore the macroscopic elastic behaviour of CNT in a finite densely packed polymer resin, a representative volume element (RVE) was selected instead of whole composite material in which the polymer resin was modelled as continuum material while CNT as an equivalent long fibre. FE results of RVE manifest that the CNT volume fraction and waviness have significant effect on elastic modulus of CNT reinforced polymer composite. An analytical formulation in terms of elastic properties and waviness ratio was also introduced in this study for waviness analysis. Moreover, the elastic properties of wavy CNT reinforced composite was compared with analytical outcomes. We extended present RVE model to incorporate the effects of CNTs agglomeration on the elastic behaviour of CNT-reinforced polymer composites. It was observed that anticipated elastic results not only depended on the volume fraction of CNTs, but also on the CNTs geometry, waviness and agglomeration.

Keywords: Agglomeration, elastic properties, finite element modelling, RVE, waviness

1. Introduction

Carbon nanotubes (CNT) are one of the famous reinforcing elements in several materials including polymers and hybrid matrices. Using only few weight percentage of this carbon allotrope [1], it is found the mechanical performance of the conventional composites enhances tremendously [2,3]. Over the past one decade, several investigations were carried-out for characterization of mechanical and elastic properties of confined isolated CNTs as well as CNT-reinforced polymer composites using micromechanical, molecular and experimental based approaches [4–6]. Atomistic simulation and experimental investigations stipulated Young’s modulus of CNTs 0.6 to 1 TPa [7,8] and Poisson’s ratio varying between 0.25 and 0.28 which are affected by their diameter, length, chirality, type of defects, sample synthesis, measurement techniques and computational theory. But utilization of these CNT properties as reinforcement data for polymer composites leads to several errors as there is a sharp decline in CNTs mechanical and geometrical properties during composite fabrication. In order to achieve the desired properties, recently, main focus is given on investigation of stiffening ability of CNT reinforced polymer composites considering the effects of geometric features of carbon nanotubes such as length, waviness, agglomeration and curvature. Formation of waved CNTs is mainly due to extremely high length to diameter ratio and low stiffness in transverse direction. Few studies reported in literature shows that the waviness of CNTs diminishes the overall axial stiffness of CNT-composites but has no significant change in transverse directions [9–13]. The earlier micro-mechanical models for demonstrating the waviness and agglomeration of CNTs were based on Mori Tanaka method [14,15]. Recent studies [16,17] illustrated continuum mechanics-based approach and micromechanical model to investigate the alignment and randomly oriented wavy CNT effects on effective elastic properties of composite with a parallel FE model generated for wavy CNT embedded representative volume element (RVE). Since experimental study of CNT reinforced polymers is an involved task at the nano scale, numerical modeling takes a vital part. In this line, various numerical and theoretical approaches
[18–24] outlined the combined effects of CNT distribution, dispersion, agglomeration, waviness, interfacial bonding deformation mechanisms on the elastic properties of CNT-reinforced composites.

In spite of several efforts in modeling CNT polymer composites, limited works were found related to the effect of the fiber geometric parameters on overall elastic behavior of composite using numerical modeling. The realistic molecular structure of CNT needs special focus and its integration within the polymer matrix require a careful study due to several complications like waviness, agglomeration, vacant sites etc. In present work, a finite element analysis based approach is proposed to predict the effects of CNT content, CNT waviness and agglomeration on effective elastic properties of composite. A two-dimensional representative element model is utilized for studying the waviness effect, whereas a three-dimensional representative volume element (RVE) model is developed by accounting the agglomeration effect using four CNT fibers within the matrix. The CNT fiber volume fraction and waviness factor are varied and the effects on elastic properties are reported. In this study, analytical expressions are employed to provide a better understanding of carbon nanotubes (CNTs) curvature on the overall behavior of nanocomposites. The waviness of CNT is modeled as a sine wave form and the transformed physical characteristics are applied to micromechanical framework. In addition, the predictions are compared with analytical data of the CNT-reinforced nanocomposites to assess the reliability of the proposed method.

2. Numerical Modeling
Analysis is divided into two parts. In the first part CNT modelling is presented using finite element discretization, followed by modelling of reinforced polymer composite by considering waviness and agglomeration.

2.1 Modeling of CNT geometry
Three types of CNTs are observed during experimental analysis: SWCNTs, DWCNTs and MWCNTs. A SWCNT can be viewed as a rolling up form of graphene sheet, which is composed of hexagonal carbon rings. The chiral vector \((C_h)\) and chiral angle \((\theta)\) are two main influencing factors for atomic structure of carbon nanotubes. The chiral vector can be represented in terms of chiral indices and diameter of CNT and can be estimated as \([25]\)

\[
D_{cnt} = \frac{\sqrt{3}}{\pi} d_{cc} \sqrt{n^2 + m^2 + nm}
\]

where \((n, m)\) is the chiral indices and is the \(d_{cc}\) carbon-carbon bond length. Further CNTs are classified based on chiral indices: \((n, n)\) armchair and \((n, 0)\) zigzag respectively. In this section, modeling of SWCNTs, DWCNTs and MWCNTs is presented using finite element approach. First, a MATLAB code was developed to generate the coordinates of each carbon atom present in tube. Zigzag and armchair CNTs are considered in this analysis and corresponding atoms coordinates are generated shown in Figure 1. The carbon atom coordinates generated in MATLAB are imported in the commercial available software ANSYS and copied in axial direction to get desire length of CNTs. A finite element model of CNT is developed by considering the carbon atoms as nodes and carbon-carbon bond as beam element (Beam 188). In Figure 2 a finite element model of \((50, 50)\) SWCNT is represented.

![Carbon atom coordinates generated in MATLAB for (50, 50) and (50, 0) CNT](attachment:image.png)

Fig. 1 Carbon atom coordinates generated in MATLAB for (50, 50) and (50, 0) CNT

In order to define the material model of beam elements, previous studies \([26–28]\) results are employed in present modeling approach. Based on molecular mechanics and continuum theories,
materials properties are obtained from equivalency theorem of molecular and structure energy. The material and geometric properties utilized in ANSYS APDL model are adopted from literature [26]. Figure 2 depicts the typical FE model of armchair (50, 50) and zigzag (50, 0) nanotube with and without vacancy defects for calculating the Young’s modulus and shear modulus. The Young’s modulus of a material is the ratio of normal stress to normal strain as obtained from a uniaxial tension test. In this regards, one end of the tube is remaining to be fixed in all directions while a small finite displacement is applied on other end. Then, following equation can be used to calculate the elastic modulus of CNT.

\[
E_{\text{cnt}} = \frac{\sigma}{\varepsilon} = \frac{FL_{\text{cnt}}}{\pi D_{\text{cnt}}^4 t \Delta L}
\]

where \( t = 0.34 \text{ nm} \) is the wall thickness and \( D_{\text{cnt}} \) is the diameter of the SWCNT, \( L_{\text{cnt}} \) and \( \Delta L \) are the initial tube length and elongation in axial direction. \( F \) is the reaction force estimated from ANSYS results. Similarly, shear modulus of CNT can be estimated by applying the initial small rotation at one end and keeping other end fixed. The following relation is used

\[
G_{\text{cnt}} = \frac{T_{\theta}}{\theta}
\]

where \( \theta \) is the initial torsional angle applied at one end of the tube, \( J_{\theta} \) is the polar moment inertia of the cross-section area calculated as \( J_{\theta} = \frac{\pi}{32} [(D_{\text{cnt}} + t)^4 - (D_{\text{cnt}} - t)^4] \). \( T \) represents the torque estimated from the ANSYS results. Double walled CNTs are modeled as two concentric SWCNTs connected with weak Vander Waals interactions. In multi walled CNTs case, three concentric tubes are considered. Similar analysis was carried for DWCNTs and MWCNTs as described in case of SWCNTs. Additionally, the interaction between two tubes is modeled using LINK 180 element with stiffness and cross-sectional area equal to \( 3.7 \times 10^{-9} \text{ N/nm} \) and \( 0.433 \text{ nm}^2 \) respectively [29]. A three walled CNT [(5, 5) (10, 10) (20, 20)] and LINK elements between the tubes are represented in Figure 3.

![Fig.2 Finite element models of SWCNTs](image)

![Fig.3 Inter atomic interaction between CNTs through link elements in 3 walled CNT](image)

Agglomeration and waviness are responsible for the absence of homogeneous dispersion inside the polymers and bring about insufficient stress transfer leading to poor overall mechanical properties. In order to investigate the effect of these parameters, finite element analysis is employed to discretize a representative region of the composite in next section.

### 2.2 Modeling of CNT reinforced polymer

Naturally, interaction between reinforced CNT and its surrounding polymer resin takes place through Vander Waals bonds. Some investigators attempted to improve the load transfer efficiency between CNT and its surrounding polymer by utilizing functionalization technique which provides covalent bonds between and polymer and CNT. Functionalization has a main drawback that it distorted the structure of CNT which can diminish the overall mechanical properties of CNTs significantly. So Vander Waal’s (vdW) interaction can be consider for including interphase effect in modeling and
represented using Lennard-Jones potential. Furthermore, vdW interaction can be ignored when the inter-atomic separation is equal or greater than 0.85 nm. For simplicity, CNT and the interphase can be modeled as an equivalent long fiber, a solid cylinder with diameter 1.424 nm. In previous literature [30,31] equivalent properties of long fiber have been investigation using inverse rule of mixture. An armchair SWCNT with chiral index of (10, 10) is picked here for both instances of RVE with waviness and agglomeration, thickness of CNT is chosen as 0.34 nm. Till to date lots of investigation have been made considering interphase effect but waviness and agglomeration effect is less in consideration, in this particular study waviness agglomeration phenomenon is described with a perfect bonding between CNT fiber and polymer matrix.

2.2.1 Simulation of CNT waviness

Two-dimensional representative model is employed for CNT/polymer composites as it has already been used by many researchers [32], for obtaining the effective elastic properties of wavy CNTs reinforced composites. A CNT of length \( L_{\text{cnt}} \) is embedded inside a polymer matrix and forms a RVE of length \( L_{\text{rve}} \), where \( L_{\text{rve}} = L_{\text{cnt}} \). RVE dimensions used were fixed to \( W_{\text{rve}} = 120 \text{ nm} \) and \( L_{\text{rve}} = 100 \text{ nm} \), based on amplitude of wavy CNT. It is important to mention that for a selected volume faction of CNT as 5%, the developed equivalent fiber has 7.5% volume fraction. This difference is due to the hollow shape of CNT and interphase thickness while equivalent long fiber has a solid shape as shown in Figure 4. Simulating polymers chain at atomic scale obliges a huge measure of elements and calculations. Since atomic chains of polymer are significantly tighter than atomistic structure of CNT, it can be displayed as a continuum medium as a satisfactory simplification in modeling method. The Young’s modulus of the simulated isotropic resin is considered 10 GPa and Poisson’s ratio 0.3 [30].

![Fig.4. A 3-D and 2-D rectangle RVE with wavy CNT](image)

A 2-D model is adopted to simulate the behavior of nanocomposites consist of waved carbon nanotube. Polymer matrix is treated as linear elastic and isotropic and perfect bonding is assumed between the nanotube and matrix along with consideration of equivalent fiber approach instead of nanotube and interphase. FEA is used to compute Elastic properties of CNT reinforced polymer composite. Commercial simulation software (ANSYS 15.0) was utilized for the analysis. Both CNT and polymer resin were modeled utilizing two-dimensional structural solid elements (“PLANE 83”) with 8-node elements (one at middle and one at each corner node) and two degrees of freedom at every node (translational in \( x \) and \( y \)-direction) configured in plane strain. The RVE was developed utilizing model of around 2000 elements, with 600 elements being connected with the CNT and the rest of the polymer matrix. In view of the equivalent fiber model representation which takes into account the CNT hollow structure with interphase as equivalent solid structure. To compute the longitudinal and transverse components of elastic modulus, the RVE was subjected to a strain in the \( x \) or \( y \)-direction as shown in Figure 5, depending on the component of interest. For computing longitudinal modulus, the nodes at the left side edge of the RVE (\( x = 0 \)) were constrained to have zero displacement in the \( x \)-direction while small strain was applied to the right side edge (\( x = L_{\text{rve}} \)). An analogous procedure was performed for the calculation of transverse modulus, but constraining now nodes at \( y = 0 \) to have a zero displacement condition in the \( y \)-direction and imposing a uniform displacement in the \( y \)-direction on the nodes located at \( y = W_{\text{rve}} \). Thus, a pure tensile testing is performed in both cases and bending was excluded by the applied displacement boundary conditions.
In linear elastic range, effective Young’s modulus of CNTs reinforced composite is defined as follows:
\[ E_i = \frac{\sum F_i \times L_{RVE}}{A \times \Delta L} \quad (i=x,y) \]  

where \( \sum F_i \) is the summation of reaction force on the constrained edge, \( A \) is the edge area of the RVE \( (A=W_{rve} \times 1) \) and \( \Delta L \) is a very small displacement. Since wavy amplitude has direct effect on Young’s modulus majorly depends on a parameter called waviness factor \( (w=A/\lambda) \).

In this investigation wavelength of wavy CNT \( (\lambda) \) kept constant and is equal to the length of RVE and waviness factor varied from 0.01 to 0.1 with help of the amplitude of Wavy CNT. As result point of view first we varied the waviness and then secondly volume fraction of CNTs (as area fraction in 2-D RVE model) varied by varying the width of RVE \( (W_{rve}) \).

A two-dimensional micromechanical model [16] is employed here for predicting effective elastic properties of CNTRC with aligned wavy CNT. An appropriate RVE is considered and upper and lower bounds for effective stiffness properties are calculated using energy principles. Upper bound is calculated using the minimum potential energy principle and iso-strain assumption while lower bound is calculated using the minimum complementary energy principle and iso-stress assumption. The direction vector of the CNT with respect to the global co-ordinate system \( (x, y, z) \) varies throughout the length of the RVE. We selected the principal (material) coordinate system at any location along the length of the RVE to be \( (x_0, y_0, z_0) \), where \( x \) axis is along the central line of the CNT. In the present case, co-ordinate transformation matrix is simply given by:
\[ [\Omega] = \begin{bmatrix} \cos \gamma & -\sin \gamma & 0 \\ \sin \gamma & \cos \gamma & 0 \\ 0 & 0 & 1 \end{bmatrix} \]  

The angle of rotation \( \gamma \) at any location along the length of RVE can be calculated as
\[ \gamma = -\tan^{-1}\left(\frac{dy}{dx}\right) = -\left(\frac{2\pi A \sin(2\pi / \lambda)}{\lambda}\right) \]  

The stress and strain vectors in the global and principal co-ordinate systems are dependent by the following equations:
\[ \{\sigma\}' = [T]{\sigma} \]
\[ \{\varepsilon\}' = [T]\varepsilon \]  

where the strain transformation matrix \([T]\) is given by
\[ [T] = \begin{bmatrix} p^2 & q^2 & 0 \\ p^2 & q^2 & 0 \\ 0 & 0 & p^2 - q^2 \end{bmatrix} \]
with \( p = \cos \gamma; q = \sin \gamma \). The stress–strain relation in the principal material direction at any point in the RVE is given by

\[
\varepsilon' = [S'][\sigma']
\]

\[
\sigma' = [C'][\epsilon']
\]

(9)

where \([S']\) is the compliance matrix and \([C']\) is the stiffness matrix in a principal coordinate system. These matrices are same as the corresponding matrices for a unidirectional nanocomposite in which the CNT is straight and aligned along the principal axis. These are given by

\[
[S'] = \begin{bmatrix}
1/E_1 & -v_{12}/E_1 & 0 \\
-v_{12}/E_1 & 1/E_2 & 0 \\
0 & 0 & 1/G_{12}
\end{bmatrix}
\]

(10)

\[
[C'] = [S']^{-1}
\]

(11)

The engineering constants of unidirectional nanocomposite, appearing in the matrix can be determined either by different micromechanical models or by using finite element simulation. Rules of mixture provide the following relations:

\[
E_1 = \nu_{cm} E_{cnt} + (1 - \nu_{cm}) E_m
\]

\[
E_2 = \left( \frac{\nu_{cm}}{E_{cnt}} + \frac{1 - \nu_{cm}}{E_m} \right)^{-1}
\]

\[
G_{12} = \left( \frac{\nu_{cm}}{G_{cnt}} + \frac{1 - \nu_{cm}}{G_m} \right)^{-1}
\]

\[
v_{12} = \nu_{cm} \nu_{cnt} + (1 - \nu_{cm}) \nu_m
\]

(12)

Utilizing the minimum potential energy principle with iso-strain assumption, the following form of average (effective) stiffness matrix of the RVE can be employed:

\[
[C_{rve}] = \frac{1}{L_{rve}} \int_T [T]^T [C'] [T] dx
\]

(13)

where \( L_{rve} \) is the length of the RVE. The average compliance matrix is given as \([S_{rve}] = [C_{rve}]^{-1}\) and from the average compliance matrix, the effective engineering constants of the RVE can be calculated. The values of the elastic constants thus calculated give the upper bound of the values. Similarly, from the principle of minimum complimentary energy with iso-stress assumption, effective compliance matrix of the RVE is obtained as

\[
[S_{rve}] = \frac{1}{V_{rve}} \int_T [T]^T [S'] [T] dx
\]

(14)

From the effective compliance matrix \([S_{rve}]\), the lower bounds of effective engineering constants of the RVE can be estimated.

### 2.2.2 Simulation of agglomerated CNT

To some extent, continuum mechanics is a useful tool to describe the relationship between nanomechanics parameters and micromechanical properties of CNT based composites. An effective method to evaluate the macroscopic properties of nanocomposite is construction of RVE from a sample of the polymer matrix with embedded CNT. A square RVE is selected here (Figure 6 (a)) as the square and hexagonal RVEs are already accepted to yield the best outcomes due to their capacity to fill the space as contrasted with the cylindrical shaped RVE.
Agglomeration of CNTs is represented using a four CNT based RVE (see Figure 6 (b)), which touch each other. Agglomerates are expected to result in lower overall modulus than individual CNTs. Due to agglomeration, maximum shear stress is generated in RVE at inter-touching face of CNTs. A 4-CNT based finite element model is employed by considering uniform distribution and agglomeration respectively. The elastic properties of CNT/polymer composites is measured as a function of inter-tube spacing and compared with uniformly distributed CNT reinforced composite. A square RVE consisting of 4 agglomerated CNT and Polymer matrix is modeled using FEM. A three-dimensional (3D) RVE along with appropriate boundary conditions is explored under uniform extension to focus the effective elastic modulus of CNT/Polymer composites. Higher order brick structure element (quadratic element SOLID186-20-node with three degrees of freedom per node – ANSYS 15) is used for discretization. RVE is constrained at $z = 0$ in the displacement direction ($z$ direction) and free to move in the transverse directions. The four free edges are also constrained to their respective perpendicular directions in order to permit contraction of the RVE because of extension. An extension with in elastic region, approximately 5% of the total experimental strain, is applied to all nodes on the end surface ($z = L_{rve}$). A very fine mesh is used for mesh the RVE and glue operation is performed at the interface of polymer and fiber, which gives better converged results. Firstly, uniform dispersion of four CNTs within the PP matrix is considered for the modeling and then distance between CNTs is varied to take account of agglomeration. The CNT content is varied by changing the cross-sectional area of RVE. The effective elastic modulus of the composite is computed as the ratio of the average stress to the applied strain. The average stress is computed taking the average of elemental stresses obtained from the FEA reaction forces generated at fixed end of RVE.

3. Results and discussion

In this section numerical result of effective elastic properties of CNTs and CNT reinforced polymer composite are presented. Carbon nanotube was considered as space frame structure and its analogous finite element structure was developed in ANSYS environment. A numerical study was performed to simulate the elastic behavior of different configuration of CNTs. In addition, the elastic behavior of DWCNTs and MWCNTs were also investigated using same approach. Further, an investigation was made to determine the effect of waviness and agglomeration of CNTs on elastic behavior composite material.

3.1 Properties of CNTs

Carbon nanotube is having a complex structure with hexagonal array. In present study a finite element analysis was carried out to evaluate the elastic and shear modulus of SWCNTs. The deformation of SWCNT and MWCNTs under axial stretch is shown in Figure 7. Maximum deformation can be seen at free end and its vary as function of length of CNT. In table 1, a comparison study is tabulated to validate the present analysis of (50, 50) armchair CNT with previous work outcomes and it shows the good agreement. Moreover, elastic modulus of DWCNT and MWCNT was also estimated using finite element approach. The predicted elastic modulus of DWCNT and MWCNT are 0.625 TPa and 0.520 TPa respectively, which are lower than corresponding SWCNT.
| Study                              | Elastic modulus ($E_{cnt}$) TPa | Shear modulus ($G_{cnt}$) TPa |
|-----------------------------------|---------------------------------|------------------------------|
| Present study                     | 0.715                           | 0.381                        |
| Natsuki et al (Ref. [33])         | 0.48-0.61                       | 0.27-0.3                     |
| Zhou et al. (Ref.)                | 0.764                           | -                            |
| Guo et al (Ref. [34])             | 0.69                            | -                            |
| Chandraseker and Mukherjee (Ref.[35]) | 0.46-0.68                  | 0.186-0.236                  |
| Agarwal et al. (Ref. [36])        | 0.73-0.82                       | -                            |

The shear deformation of SWCNT under torsional loading and effect of vacancy defect in carbon nanotube are shown in Figure 8. It is observed that elastic modulus is continuously decreasing as more carbon atoms are missing in carbon nanotube. A comprehensive analysis was carried out to investigate the shear and elastic modulus of different configuration of SWCNTs. Table 2 provides the elastic and shear modulus values of zigzag and armchair CNTs.

![Image](image.png)

(a) Shear deformation of SWCNT                                           (b) vacancy defects

Fig. 8 (a) Shear deformation and (b) effect of vacancy defects on elastic modulus of SWCNT

Table 2 Estimated elastic and shear modulus of different configuration of CNTs

| Configuration | $E_{cnt}$ (TPa) | $G_{cnt}$ (TPa) | Configuration | $E_{cnt}$ (TPa) | $G_{cnt}$ (TPa) |
|---------------|-----------------|-----------------|---------------|-----------------|-----------------|
| (5,5)         | 0.711           | 0.364           | (5,0)         | 0.676           | 0.354           |
| (10,10)       | 0.712           | 0.375           | (10,0)        | 0.708           | 0.366           |
| (15,15)       | 0.713           | 0.377           | (15,0)        | 0.716           | 0.371           |
| (20,20)       | 0.714           | 0.378           | (20,0)        | 0.720           | 0.374           |
| (25,25)       | 0.714           | 0.379           | (25,0)        | 0.723           | 0.380           |
| (50,50)       | 0.715           | 0.381           | (50,0)        | 0.728           | 0.384           |

3.2 Effect of CNTs waviness

Waviness of CNT was modelled sine wave form and 2 D RVE model was employed to estimate the effective elastic properties. Results are computed for small displacement along the CNT direction at a 1.2 % volume fraction. Figure 9 shows the dependency of longitudinal modulus of CNT reinforced polymer composite over the CNTs waviness ratio. It can be observed from figure that longitudinal elastic modulus is strongly dependent over the curvature and drastically decreases as the CNTs waviness increases. Therefore, it can be concluded that waviness of CNTs deceases the stiffening ability of CNTs inside the polymer resin. Figure 10 shows that transverse modulus variation with the CNTs waviness and it can be seen that transverse elastic modulus is almost unchanged. But it shows significant increment at higher waviness ratio ($w=0.1$). So, longitudinal modulus shows remarkable change as compared to transverse modulus with waviness ratio.
Figure 11 shows the Poisson’s ratio variation with the increase in waviness ratio of CNTs. It can be seen from results, Poisson’s ratio of CNT reinforced polymer composite remains unchanged. So it can be concluded that waviness of CNTs have very less effect over the Poisson’s ratio of composite.

3.3 Effect of CNTs agglomeration

The approach presented here to give the fundamental idea of agglomeration (or clustering) of CNTs by a numerical technique. In this analysis square RVE with side edge dimension, $a = 24$ nm and length $L=50$ nm was employed. As an initial step we have tried to investigate the effect of agglomeration on the longitudinal strain and stress distribution as shown in Figure 12. It is clear from figure that maximum longitudinal strain developed in a small region as compared to uniform distribution case of CNTs that may cause fracture or separation between CNT and polymer matrix. It can be seen from Fig. 13, that the effective elastic modulus varies with inter tube distance. There is no significant increment but it is having minimum effective elastic modulus when CNTs touch each other or inter tube distance is equal to zero.

The stress concentration region is clearly seen in agglomerated case. To investigate the effect of CNTs clusters on longitudinal elastic modulus we have varied the width of RVE and the elastic modulus values are listed in Table 3. These results give interesting information that the effective elastic
modulus decreases as width of RVE increases, but RVE with agglomerated CNTs having low elastic modulus than RVE without agglomeration.

Table 3 Effective elastic modulus with and without agglomeration

| Side of RVE (a in nm) | Volume fraction of CNT (V_{cnt}) in % | Effective Elastic Modulus without agglomeration | With agglomeration |
|-----------------------|--------------------------------------|-----------------------------------------------|-------------------|
| 24                    | 1.11                                 | 13.3213                                       | 13.2914           |
| 22                    | 1.31                                 | 15.2261                                       | 15.190            |
| 20                    | 1.59                                 | 17.7367                                       | 17.6938           |
| 18                    | 1.96                                 | 21.1411                                       | 21.0875           |
| 16                    | 2.48                                 | 25.9216                                       | 25.8544           |
| 14                    | 3.25                                 | 32.9411                                       | 32.8543           |

4. Conclusion

Effective elastic properties of CNTs and CNT reinforced polymer composite were investigated by using finite element Modelling. FE analysis of SWCNTs have shown that nanotube chirality and diameter influence the effective elastic property of SWCNTs. Additionally, effect of carbon atom vacancy in SWCNT was also investigated and it was observed that elastic modulus of CNT decreases with increase in number of carbon atom vacancy. It was also found that MWCNTs have lower modulus as compared to SWCNTs. Further, an attempt was made to predict the effect of waviness and agglomeration on over all elastic properties of CNT reinforced composite. By selecting optimal mesh size in simulation process, FEA results were compared with micromechanics wherever possible. Predicted results show that CNTs curvature was responsible for decrement in longitudinal modulus whereas transverse modulus was almost constant for small waviness. Transverse elastic modulus showed the sudden improvement at waviness ratio order of 0.1, while Poisson’s ratio was not affected by the waviness. In addition, agglomerations of CNTs in polymer matrix was elaborated using 3-D RVE and it was observed that effective elastic modulus of 4 CNT based RVE with inter-tube spacing zero was less as compared to RVE with uniform inter-tube spacing. Maximum increase in elastic modulus of composite was observed when inter-tube spacing change zero to a/16. Present work can be extended further to include the effect of orientation, reinforcing effect of MWCNTs with interatomic Van der Waal forces and also a similar thermal analysis of CNT reinforced polymer composite material may be carried out.

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