Numerical Estimation of the Mechanical Properties of CNT-reinforcing Composites

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ABSTRACT: Carbon nanotubes (CNTs) possess excellent mechanical properties, such as high stiffness, strength, resilience etc., and may become an ideal reinforcing material for the development of nanocomposites. In this paper, we establish a finite element model of the volume representative element (RVE) for CNT-reinforcing composites and evaluate their mechanical properties based on the Equivalent Homogeneous material concept. Cases considered in this study include two different CNT-reinforcing types, i.e. long and short CNTs embedded in a matrix as well as in a carbon fiber (CF) composite. For verification, the obtained results are compared with those provided by the other approaches, such as Rule of Mixture and Eshelby’s Equivalent Inclusion Theory, and good agreement in most cases shows that the present approach is an effective tool to characterize CNT-reinforcing composites. Moreover, we investigate the obtained mechanical properties and find that the axial Young’s modulus of a matrix can increase as large as 2.3 times and 45% with only 1% weight fraction of long and short CNT addition respectively. However, for adding CNTs to CF composite, the reinforcement in axial Young’s modulus is not as good as in the matrix, but the transverse Young’s modulus and shear modulus can still increase significantly with a small amount of CNT addition. Especially for random and uniform distribution type of the adding CNTs, which demonstrate the best reinforcement effect in the transverse Young’s modulus and shear modulus among the present studied cases, the two moduli can be raised by about 33% and 39% respectively.

KEYWORDS: carbon nanotubes, nanocomposites, mechanical properties, finite element method

INTRODUCTION

Carbon nanotubes (CNTs), discovered by Iijima [1] in 1991, possess exceptionally high stiffness, strength, low density, excellent electrical and thermal properties etc., and attract extensive research activities devoted to their application in many engineering fields. Among the wide range of application, CNTs are expected to be an ideal reinforcing material for the development of nanocomposites due to their outstanding mechanical properties, and therefore
the effective elastic moduli of the reinforced nanocomposites have been investigated by many researchers to give a deeper understanding of the reinforcing effect of CNTs.

The difficulty in analytically evaluating the effective mechanical properties of CNT-reinforcing nanocomposites is their multi-scale essence: host material in macro-scale and CNTs nano-scale. Methods to solve this so-called meso-scale problem are in general divided into two major approaches: Molecular Dynamics (MD) and Continuum Mechanics (CM). The MD approach can provide abundant information about the mechanical behavior of nanocomposites, but currently are limited to small size and short time scale due to its computational expense for convergence requirement. Frankland et al. [2] employed this approach to estimate the effective mechanical properties of polymer matrices embedded with continuous and discontinuous CNTs, and reported that the former has better reinforcing effect. Zhu et al. [3] have also used MD approach to establish the model of a polymer matrix reinforced by singled-walled CNTs and obtained the Young’s modulus and stress-strain curve of the nanocomposite. On the other hand, the CM approach has been employed by many researchers in the study of simulating individual CNT, and it seems to be the only feasible approach at present to obtain preliminary results for characterizing CNT-reinforcing nanocomposites. However, the validity and practical skills of this approach still need to be fully established for some kinds of problems. Liu and Chen [4, 5] use CM approach and the concept of Representative Volume Element (RVE) to evaluate the effective mechanical properties of a matrix reinforced by aligned CNTs, and their results show good agreement with those obtained by the other methods such as Rule of Mixture [6] and Boundary Element Method. Song and Youn [7] utilize RVE and the concept of equivalent homogeneous material proposed by Sun and Vaidya [8] to investigate the cases of aligned and random orientation of CNTs embedded in a polymer matrix, and find that the values of elastic moduli evaluated from the random distribution type is closer to those experimental ones.

In this paper, we establish a finite element model of the RVE for CNT-reinforcing nanocomposites and evaluate their elastic moduli based on the concept of equivalent homogeneous material. Two different CNT-reinforcing types, i.e. long and short CNTs embedded in a matrix as well as in a carbon fiber composite are studied. For verification, the obtained results will be compared with those provided by the other methods, such as Rule of Mixture and Eshelby’s Equivalent Inclusion Theory [9]. The reinforcing effect by different CNTs adding types are also discussed from the obtained elastic moduli.

HOMOGENIZATION METHOD

A composite is usually composed of fibers and matrix with quite different properties, and will demonstrate non-uniform response when even subjected to a uniform loading in a micro-mechanical view. However, for convenience to study and describe the macro-mechanical behavior, the composite is always treated as a homogeneous medium in classical composite theory. Therefore, a homogenization process has to be established to link the actual heterogeneous composite medium and the simplified homogeneous model. In the general homogenization process, a RVE is firstly constructed under the assumption that the reinforcing material is in a periodic arrangement, and the RVE has the same elastic moduli and volume fraction as those of the composite. Then, the RVE is considered as a homogeneous orthotropic medium, and its macro-mechanical behavior is described in terms of average stress $\bar{\sigma}_y$ and strain $\bar{\varepsilon}_y$ which are defined as

$$\bar{\sigma}_y = \frac{1}{V} \int_V \sigma_y(x, y, z) dV ,$$

(1)
\[
\bar{\varepsilon}_g = \frac{1}{V} \int \varepsilon_g(x,y,z) dV ,
\]
where \( V \) is the RVE volume. In such a way, the effective moduli can then be evaluated by various homogeneous elastic theories.

In the present approach, we utilize the theory of equivalent homogeneous material proposed by Sun and Vaidya [8] as a basis to compute the effective moduli of the nanocomposites. This theory states that the total strain energy stored in an actual heterogeneous RVE volume is equal to that in its simplified homogeneous model when appropriate boundary conditions are applied to the RVE. In addition, we set up the appropriate boundary conditions to achieve a pure tension or pure shear condition as close as possible for the RVE model, then the effective moduli can be extracted from the equations of classical elastic theory.

For example, consider the square RVE model shown in Fig. 1, in order to evaluate the axial Young’s modulus \( E_3 \), the boundary conditions which simulate a pure tension are set up as

\[
u_3(x, y, -\frac{z_0}{2}) = 0, \quad \nu_3(x, y, \frac{z_0}{2}) = \nu_3^*,
\]

where \( x_0, y_0, z_0 \) and \( \nu_1, \nu_2, \nu_3 \) are respectively the lengths of the RVE model and the displacement in the \( x-, y-, z- \) direction, \( \nu_3^* \) is an applied constant displacement along the \( z- \) direction.

![Fig.1. Pure tension loading case for the RVE model](image)

Similarly, to acquire the shear modulus \( G_{12} \), the boundary conditions which make the RVE model under pure shear condition (Fig. 2) are represented as

\[
\begin{align*}
u_i(x, -\frac{y_0}{2}, z) &= 0, & \nu_i(x, \frac{y_0}{2}, z) &= \nu_i^*, \\
\nu_i(x, -\frac{y_0}{2}, z) &= 0, & \nu_i(x, \frac{y_0}{2}, z) &= 0, \\
\nu_i(x, -\frac{y_0}{2}, z) &= 0, & \nu_i(x, \frac{y_0}{2}, z) &= 0
\end{align*}
\]

where \( \nu_i^* \) is an applied constant displacement along the \( x- \) direction.
Fig. 2. Pure shear loading case for the RVE model

As for computing the other moduli, the associated boundary conditions can be easily set up by modifying Eqs. (3) and (4).

With the appropriate boundary conditions applied to the RVE model, a finite element analysis can be performed to provide the required numerical results by which the effective mechanical properties can be computed from Hooke’s law and the strain energy equation, i.e.

\[
E_1 = \frac{2U_1}{V(\varepsilon_{11})^2}, \quad E_2 = \frac{2U_2}{V(\varepsilon_{22})^2}, \quad E_3 = \frac{2U_3}{V(\varepsilon_{33})^2},
\]

\[
\nu_{12} = \frac{-2\Delta y}{y_0\varepsilon_1}, \quad \nu_{32} = \frac{-2\Delta y}{y_0\varepsilon_3}, \quad \nu_{31} = \frac{-2\Delta x}{x_0\varepsilon_3},
\]

where \( \varepsilon_{11} = \frac{u_1^*}{x_0}, \quad \varepsilon_{22} = \frac{u_2^*}{y_0}, \quad \varepsilon_{33} = \frac{u_3^*}{z_0} \) and \( U_1, U_2, U_3 \) are respectively the normal strain and the total strain energy calculated for the different loading conditions of pure tension cases. \( \nu_{ij} \) are the Poisson’s ratio.

Similar for the pure shear loading cases, the shear moduli can be obtained by the following equations,

\[
G_{23} = \frac{2U_4}{V(\varepsilon_{23})^2}, \quad G_{13} = \frac{2U_5}{V(\varepsilon_{13})^2}, \quad G_{12} = \frac{2U_6}{V(\varepsilon_{12})^2},
\]

where \( \varepsilon_{23} = \frac{u_3^*}{y_0}, \quad \varepsilon_{13} = \frac{u_1^*}{x_0}, \quad \varepsilon_{12} = \frac{u_2^*}{y_0} \) and \( U_4, U_5, U_6 \) are respectively the shear strain and the total strain energy calculated for the different loading cases.

**CLASSICAL THEORIES OF EQUIVALENT MECHANICAL PROPERTIES**

For verification, the results obtained by the procedure described in the previous section will be compared with those analytical solutions provided by classical theories of equivalent mechanical properties. For convenience of referring, a brief description of these theories is given in the following.

**Rule of Mixture (RM):** Following the strength of material theory, RM can be applied to give a quick and primary solution of the axial Young’s modulus for a composite with aligned
reinforcing material. For the present case that a matrix is reinforced by a continuous (long) CNT (shown in Fig.3), the effective axial Young’s modulus $E_c$ can be calculated by RM as

$$E_c = E_{cnt}V_{cnt} + E_m(1-V_{cnt}),$$

(7)

where $E_{cnt}$ and $E_m$ are respectively the Young’s modulus of CNT and matrix, $V_{cnt}$ is the volume fraction of CNT.

As for the case that a matrix is reinforced by a discontinuous (short) CNTs (shown in Fig.4), the effective axial Young’s modulus $E_s$ can be represented by modifying Eq.(7) as

$$\frac{1}{E_s} = \frac{V_f}{E_c} + \frac{V_m}{E_m} = \frac{L_{cnt}}{E_c(L_{cnt} + L_m)} + \frac{L_m}{E_m(L_{cnt} + L_m)},$$

(8)

where $L_{cnt}$ and $L_m$ are respectively the lengths of CNT and matrix.

Eshelby’s Equivalent Inclusion Theory (EI): Consider a plane strain condition of a host material embedded with an elliptical inclusion, Eshelby’s theory assumes that the stress and strain fields between the entire simplified homogeneous domain and the actual heterogeneous domain are equivalent by introducing the so called ‘eigen-strain’, and leads to an equation of the equivalent stiffness matrix $\bar{c}$ as follows

$$\bar{c} = c_m - V_I c_m ((c_m - c_1)^t c_m - S_e)^t,$$

(9)

where $c_m$ and $c_1$ are respectively the stiffness matrices of the host material and the inclusion, $V_I$ the volume fraction of the inclusion, and $S_e$ is the Eshelby’s tensor which is related to the
shape of inclusion and the stiffness matrix of the host material. Then, one can easily extract the effective engineering constants from the equivalent stiffness matrix $\overline{\mathbf{c}}$.

**Halpin-Tsai Equation [10]:** When the reinforcing materials are discontinuous short CNTs distributed randomly in a matrix, Halpin and Tsai proposed an equation to estimate the effective Young’s modulus $E_c$ of the composite which is treated as an isotropic medium, i.e.

$$
E_c = \left( \frac{3}{8} \frac{1 + 2\left( \frac{l_{cnt}}{d_{cnt}} \eta_L V_{cnt} \right)}{1 - \eta_L V_{cnt}} + \frac{5}{8} \frac{1 + 2\eta_T V_{cnt}}{1 - \eta_T V_{cnt}} \right) E_m ,
$$

(10)

where

$$
\eta_L = \frac{E_{cnt}}{E_m} - 1, \quad \frac{E_{cnt}}{E_m} + 2\left( \frac{l_{cnt}}{d_{cnt}} \right),
$$

and

$$
\eta_T = \frac{E_{cnt}}{E_m} - 1, \quad \frac{E_{cnt}}{E_m} + 2.
$$

d_{cnt}$ is the diameter of CNT.

**NUMERICAL RESULTS FOR POLYMER / CNTs**

In the numerical simulation process, we employ the SOLID45 element which is a built-in element type in the commercial software ANSYS to establish a 3D finite element model of the RVE. Then, the effective elastic moduli can be calculated by substituting the total strain energy acquired from the finite element analysis into Eqs. (5) and (6).

Two different CNT reinforcing types: continuous (long) and discontinuous (short) type are considered here. The CNT type used in all of the illustrating examples throughout this paper is the single-walled armchair (9,9) type, its tube thickness and diameter are respectively 0.34 nm and 1.22 nm, and the Young’s modulus and Poisson’s ratio which are needed to be fed into the ANSYS program for CNT and matrix are chosen as

CNT: $E_{cnt}=1000\text{nN/nm}^2\text{(GPa)}, \nu_{cnt}=0.3,$

Matrix: $E_m=6.46\text{nN/nm}^2\text{(GPa)}, \nu_m=0.3.$

The adding quantity of CNTs is represented in terms of weight fraction wt% which is defined as wt% = (weight of CNTs)/(sum of CNTs and matrix weight), and 1wt% which is equivalent to 0.86% volume fraction for the present armchair (9,9) type is selected for the following examples. In this section, CNTs are assumed to be added uniformly and aligned with the axial direction of the RVE. The simulating result for each case will be presented in the following subsections.

**Continuous CNT / Polymer:** The RVE model shown in Fig.3 is composed of a continuous CNT and a polymer matrix, and the sizes of this model are set as

Matrix: $L_m=100\text{nm}, \ 2a=10.47\text{nm},$

CNT: $L_{cnt}=100\text{nm}.$

From the result of finite element analysis and the formula described in Eqs. (5) and (6), the estimating values of the effective mechanical properties are obtained as shown in Table.1. For verification, these results of Young’s and shear moduli are compared with the analytical solutions provided by RM and EI theory, which is shown in Table.2.
Table 1. The effective mechanical properties for Continuous CNT / Polymer

<table>
<thead>
<tr>
<th>Property</th>
<th>Continuous type (GPa)</th>
<th>EI (GPa)</th>
<th>*Deviations</th>
<th>RM (GPa)</th>
<th>*Deviations</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_z$</td>
<td>15.00</td>
<td>15.00</td>
<td>0%</td>
<td>15.00</td>
<td>0%</td>
</tr>
<tr>
<td>$E_x = E_y$</td>
<td>6.88</td>
<td>6.83</td>
<td>-0.73%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$G_{yx}$</td>
<td>2.54</td>
<td>2.57</td>
<td>1.2%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$G_{xz}$</td>
<td>2.54</td>
<td>2.57</td>
<td>1.2%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$G_{xy}$</td>
<td>2.53</td>
<td>2.55</td>
<td>0.8%</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*Deviations = (analytical value - numerical value) / numerical value

From Table 2, we can observe that the values of the axial Young’s modulus meet very well for all of the three different approaches, while the deviation for the other moduli are also under 1.2%. This comparison indicates that the present approach is quite effective and accurate for the case of continuous CNT adding type.

**Discontinuous CNT / Polymer:** The RVE model for this case contains a short CNT located in the central part of a polymer matrix, as shown in Fig.4. To retain the same volume fraction of 0.86% as in the former case, the sizes of this RVE are adjusted as

Matrix: $L_m = 100nm$, $2a = 7.4nm$

CNT: $L_{cnt} = 50nm$.

Therefore, the slenderness ration of the CNT which is defined as (length of CNT)/(diameter of CNT) will be about 41. The estimating values of the effective mechanical properties and the comparison with those given by RM and EI theory are respectively listed in Table 3 and 4.

Table 3. The effective mechanical properties for Discontinuous CNT / Polymer

<table>
<thead>
<tr>
<th>Property</th>
<th>Continuous type (GPa)</th>
<th>EI (GPa)</th>
<th>*Deviations</th>
<th>RM (GPa)</th>
<th>*Deviations</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_z$</td>
<td>15.00</td>
<td>15.00</td>
<td>0%</td>
<td>15.00</td>
<td>0%</td>
</tr>
<tr>
<td>$E_x = E_y$</td>
<td>6.88</td>
<td>6.83</td>
<td>-0.73%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$G_{yx}$</td>
<td>2.54</td>
<td>2.57</td>
<td>1.2%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$G_{xz}$</td>
<td>2.54</td>
<td>2.57</td>
<td>1.2%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$G_{xy}$</td>
<td>2.53</td>
<td>2.55</td>
<td>0.8%</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Table 4. Comparison of the effective mechanical properties for Discontinuous CNT / Polymer with those obtained by EI and RM theory

<table>
<thead>
<tr>
<th></th>
<th>Discontinuous type (Gpa)</th>
<th>EI (Gpa)</th>
<th>*Deviation</th>
<th>RM (Gpa)</th>
<th>*Deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_z$</td>
<td>9.40</td>
<td>11.56</td>
<td>23%</td>
<td>9.02</td>
<td>-4%</td>
</tr>
<tr>
<td>$E_x = E_y$</td>
<td>6.78</td>
<td>6.81</td>
<td>0.44%</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>$G_{yz}$</td>
<td>2.54</td>
<td>2.57</td>
<td>1.2%</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>$G_{xz}$</td>
<td>2.54</td>
<td>2.57</td>
<td>1.2%</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>$G_{xy}$</td>
<td>2.53</td>
<td>2.55</td>
<td>0.8%</td>
<td>N/A</td>
<td>N/A</td>
</tr>
</tbody>
</table>

*Deviation = (analytical value-numerical value)/ numerical value

From Table 4, we see that the deviation of the axial Young’s modulus is as high as 23% between the results obtained by the present approach and EI theory. The possible reason may be that the arrangement type and geometric shape of fibers are not considered in EI theory. As for the other moduli, all the deviations are still at a reasonable range as in the former case.

**NUMERICAL RESULTS FOR CNTs / CARBON FIBER / POLYMER**

In this section, we consider the problem that the reinforcing CNTs add into a composite composed of carbon fibers (CFs) and a polymer matrix. For adapting to the real condition, an assumption is made that the CF is continuous through an entire RVE, and the CNTs are uniformly distributed in a discontinuous type. A typical RVE model of this composite system is shown in Fig. 5. Since all the components of this composite are in quite different scale to form a multi-scale problem, it is difficult to construct a suitable RVE model to be dealt with. Instead of modeling this CNTs/CF/Polymer system directly, we first combine the polymer and the CNTs into an equivalent homogeneous matrix by the homogenization process stated in the
above, then construct the RVE model of this homogeneous matrix and CF to perform the subsequent analysis procedure.

![Fig.5. Typical RVE model for aligned CNTs/CF/Polymer system](image)

For the illustrating examples below, the material properties of the CF are given as

\[ E_x = E_y = 6\text{GPa}, \quad E_z = 379\text{GPa}, \quad G_{yz} = G_{xz} = 4.83\text{GPa}, \quad G_{xy} = 7.58\text{GPa} \]

\[ \nu_{yz} = \nu_{xz} = 0.00327, \quad \nu_{xy} = 0.2 \]

while the type of the CNTs is selected as same as that used in the previous sections, and the length of each individual CNT is set to be 50 nm. Moreover, the weight fraction of CNTs is raised up to 2.64\% (equal to a volume fraction of 2.274\%), which is the general level in associated experiments. Two different CNTs distribution types are studied in the following: one is aligned type and the other is random type.

**Aligned CNTs/CF/Polymer:** In this case, the CNTs and the CF are arranged in alignment with the axial direction of the RVE model, as shown in Fig.5. The material properties of the equivalent homogeneous matrix, which can be obtained by the procedure and data described in the above, are listed in Table.5. The sizes of the RVE composed of the equivalent matrix and CF are set as

- Equivalent matrix: \( L_m = 1000\mu m, \quad 2\alpha = 123.3\mu m \)
- CF: \( L_{CF} = 1000\mu m, \quad \text{diameter } D_{CF} = 76.2\mu m, \quad \text{volume fraction } V_{CF} = 30\% \)

**Table.5. The mechanical properties of the equivalent homogeneous matrix**

<table>
<thead>
<tr>
<th>( \frac{E_{cnt}}{E_m} )</th>
<th>155, CNT volume fraction = 2.274%, slenderness ratio = 41</th>
</tr>
</thead>
<tbody>
<tr>
<td>( E_z )</td>
<td>10.95GPa</td>
</tr>
<tr>
<td>( E_x = E_y )</td>
<td>7.07GPa</td>
</tr>
<tr>
<td>( \nu_{xy} )</td>
<td>0.34</td>
</tr>
<tr>
<td>( \nu_{xz} = \nu_{yz} )</td>
<td>0.35</td>
</tr>
</tbody>
</table>

\[ E_y = 10.95\text{GPa}, \quad G_{xy} = 2.61\text{GPa} \]

\[ G_{xz} = 7.07\text{GPa}, \quad G_{xy} = 2.65\text{GPa} \]

By a similar way, the estimating values of the effective mechanical properties of the present Aligned CNTs/CF/Polymer composite system can be obtained as shown in Table.6. The results show that the reinforcing effect by adding CNTs into the CF/Polymer composite is
not as obvious as adding CNTs into a pure polymer matrix. For example, the axial Young’s modulus grows up to only 2.7% which is calculated from the data of Table.6. This may result from the fact that the modulus of CNT is only about 3 times as large as that of CF in this case, and the 2.64 wt% of adding CNT is not large enough to raise the modulus significantly. However, the increase of the transverse Young’s moduli and shear moduli are evident to illustrate the reinforcing effect of CNTs.

<table>
<thead>
<tr>
<th></th>
<th>Original CF/Polymer</th>
<th>Aligned CNTs/CF/Polymer</th>
<th>Random CNTs/CF/Polymer</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_z$</td>
<td>118.2 GPa</td>
<td>121.40 GPa</td>
<td>120.52 GPa</td>
</tr>
<tr>
<td>$E_y$</td>
<td>6.7 GPa</td>
<td>7.35 GPa</td>
<td>8.92 GPa</td>
</tr>
<tr>
<td>$E_x$</td>
<td>6.7 GPa</td>
<td>7.35 GPa</td>
<td>8.92 GPa</td>
</tr>
<tr>
<td>$G_{xy}$</td>
<td>3.254 GPa</td>
<td>3.4 GPa</td>
<td>4.53 GPa</td>
</tr>
<tr>
<td>$G_{yz}$</td>
<td>3.0 GPa</td>
<td>3.12 GPa</td>
<td>4.05 GPa</td>
</tr>
<tr>
<td>$G_{xz}$</td>
<td>3.0 GPa</td>
<td>3.12 Gpa</td>
<td>4.05 GPa</td>
</tr>
</tbody>
</table>

Random CNTs/CF/Polymer: In this case, the CNTs of the same volume fraction as in the previous case are assumed to be uniformly distributed with random directions in a polymer matrix, while the CF still stays aligned with the axial direction. A typical RVE model for this composite system is depicted in Fig.6. Since the reinforcing CNTs are randomly distributed, the equivalent homogeneous matrix which combines the CNTs and polymer in prior is assumed to be an isotropic medium, and its equivalent Young’s modulus $\tilde{E}_m$ can be calculated by Halpin-Tsai equation introduced above. Thereafter, the numerical process for estimating the effective mechanical properties of the equivalent homogeneous matrix/CF composite system can then be performed in a way similar to that described in the previous sections.

Fig.6. Typical RVE model for random CNTs/CF/Polymer system

The parameters and sizes of the RVE model for the case are given as
Equivalent matrix: Young’s modulus $\tilde{E}_m = 18.7$ GPa, Poisson’s ratio $\tilde{\nu}_m = 0.3$, $L_m = 1000 \mu$m, $2a = 123.3 \mu$m.
CF: $L_{CF} = 1000 \mu m$, diameter $D_{CF} = 76.2 \mu m$, volume fraction $V_{CF} = 30\%$.

The results of the effective moduli of the Random CNTs/CF/Polymer system are also listed in Table.6. From the table, one can observe that the reinforcing effect on the axial Young’s modulus by this CNTs adding type is also unobvious as in the previous case. However, the values of the transverse Young’s moduli and shear moduli are increased as high as up to 33% and 39% respectively. This seems to imply that the random CNTs adding type has significant reinforcing effect on these moduli even with a small amount of CNTs addition.

CONCLUSION

For estimating the effective mechanical properties of a multi-scale heterogeneous medium such as a composite added by CNTs, we utilize a homogenization method to establish a RVE model of the simplified homogeneous medium for subsequent finite element analysis. Several cases including continuous/discontinuous CNTs adding into a polymer matrix and aligned/random distribution type of CNTs adding into a CF/Polymer composite are studied. The results of the estimating effective mechanical properties show that the continuous CNTs demonstrate better reinforcing effect than the discontinuous ones in view of the axial Young’s modulus. However, for the case of adding CNTs into a CF/Polymer composite, the increase of the axial Young’s modulus is not so significant as that in the former case. Instead, the transverse Young’s moduli and shear moduli are found to be raised obviously, especially for the random distribution type of adding CNTs. From these results, we can have a better insight into the reinforcing effect of CNTs, and this will help the further development of new nanocomposites.

REFERENCES