Estimation of Effective Directional Strength of Single Walled Wavy CNT Reinforced Nanocomposite

Krishnendu Bhowmik, Pranav Kumar, Niloy Khutia and Amit Roy Chowdhury

Department of Aerospace Engineering and Applied Mechanics, Indian Institute of Engineering Science and Technology, Shibpur, Howrah 711103, India

E-mail: krishnendub@aero.iiests.ac.in

Abstract. In this present work, single walled wavy carbon nanotube reinforced into composite has been studied to predict the effective directional strength of the nanocomposite. The effect of waviness on the overall Young’s modulus of the composite has been analysed using three dimensional finite element model. Waviness pattern of carbon nanotube is considered as periodic cosine function. Both long (continuous) and short (discontinuous) carbon nanotubes are being idealized as solid annular tube. Short carbon nanotube is modelled with hemispherical cap at its both ends. Representative Volume Element models have been developed with different waviness, height fractions, volume fractions and modulus ratios of carbon nanotubes. Consequently a micromechanics based analytical model has been formulated to derive the effective reinforcing modulus of wavy carbon nanotubes. In these models wavy single walled wavy carbon nanotubes are considered to be aligned along the longitudinal axis of the Representative Volume Element model. Results obtained from finite element analyses are compared with analytical model and they are found in good agreement.

1. Introduction

Carbon nanotube (CNT) brought a new interest to use as reinforcement as Iijima [1] found a needle tube like structure made of carbon atoms. High specific strength of CNT is the potential candidate for application in industries like aerospace, automotive, electronics and infrastructure [2]. It has been reported that addition of only 1% weight of straight CNT in the matrix enhances the stiffness of composite by 36-42% [3]. Feng et al. [4] conducted several experiments with single walled carbon nanotube (SWCNT) reinforced in epoxy matrix with maximum weight fraction of 39.1%. It is observed from their experiments that the tensile strength and Young’s modulus are increased by 183% and 408%, respectively compared to the epoxy. Fisher et al. [5] investigated the behaviour of waviness of nanotubes inside polymers in the form of wavy sinusoidal long nanotube with high aspect ratio using both experimental and numerical approaches. Three dimensional (3-D) finite element (FE) analysis of wavy particle is modelled into infinite matrix to numerically compute the dilute strain concentration tensor using Mori–Tanaka approach for aligned or randomly oriented particles. They observed that wavy characteristic reduces effective tensile modulus of the composite. Shao et al. [6] observed that the waviness of CNTs and interfacial bond between CNT and matrix are the major parameters that affect the efficiency of reinforcement. Joshi et al. [7] investigated the effect of wavy carbon nanotubes on elasticity and strength for nanocomposites using a 3-D representative volume element (RVE) for long as well as short wavy carbon nanotubes. Carbon nanotube is modelled as a continuous hollow tube with curvature in its geometry. It is being observed that the waviness significantly reduces the effectiveness of reinforced composite. Tsai et al. [8] investigated the effects of randomly distributed or partially aligned inclusion of wavy reinforced composite. Different configurations of waviness, aspect ratio are considered in their analyses. It is being concluded that the waviness of the inclusion has a greater effect on tensile modulus as well as shear modulus of the nanocomposite. Yazdchi and Salehi [9] used 3-D RVE model for a wavy CNT to visualize the stress
transfer mechanism of SWCNT reinforced polymer composite and to predict the axial and interfacial shear stresses along wavy CNTs. Dastgerdi et al. [10] developed a micro mechanical model for wavy CNT based composite to investigate the overall stiffness of the composite. The nanotubes are taken as bow shaped solid short fibers with a circular cross-section. Paunikar and Kumar [11] studied the effect of waviness of nanotube in the form of cosine function using micromechanics approach and 3-D finite element analysis (FEA). Nanotubes are taken as solid cylindrical shape without any end cap. Alian et al. [12] reported a multiscale model to predict the effect of waviness and agglomeration of CNTs on the elastic properties of nanotube epoxy composites. Free vibration and bending behaviour of CNT reinforced composite plate under hygroscopic environment are investigated using shear deformation theory by Mehar and Panda [13]. Similarly, the bending behaviours of functionally graded sandwich spherical panel are studied under hygroscopic environment using first order shear deformation theory by Mahapatra et al. [14]. Kumar and Srinivas developed an analytical model for wavy CNT reinforced polymer composites to show that the elastic parameters are not only depending on the volume fraction of CNT but also on geometry and agglomeration of CNTs [15].

2. Methodology

In this current study, waviness pattern of CNT is being considered as $y=\text{Acos}(2\pi x/\lambda)$; a periodic cosine function (Fig. 1), where $A$ is the amplitude of a cosine function, $x$ is the axial direction of the RVE, $\lambda$ is the wavelength. Both long (continuous) and short (discontinuous) CNTs are being considered and idealized as solid annular tube. Short CNT is modelled with hemispherical cap at its both ends. In present study, parameters considered for the FE analysis are; waviness ratio, $w$ (ratio of amplitude and wavelength, $A/\lambda$); modulus ratio, $\lambda_1$ (ratio of Young’s modulus of CNT and matrix); particle aspect ratio, $\lambda_2$ (ratio of CNT height and diameter); particle height fraction, $\lambda_3$ (ratio of CNT height and RVE length); particle volume fraction, $V_{\text{CNT}}$ (ratio of CNT volume and RVE volume).

![Figure 1. Schematic of typical rectangular RVE with wavy long CNT [11].](image)

The orientation of the CNT with respect to the global co-ordinate system ($x, y, z$) varies throughout the length of the RVE. The principal (local) coordinate system at any location along the length of the RVE is assumed as $(x_0, y_0, z_0)$, where axis $x_0$ is along the central path of the CNT. A general coordinate transformation from the principal to global axes can be described by Euler angles [11].

The angle of rotation $\gamma$, at any location along the length of RVE is calculated as

$$\gamma = -\tan^{-1}\left(\frac{dy}{dx}\right) = -\tan^{-1}\left(\frac{2\pi A}{\lambda} \sin\left(\frac{2\pi x}{\lambda}\right)\right)$$

(1)

The stress and strain vectors in the global and principal co-ordinate systems are

$$\{\sigma\}' = [T_2]\{\sigma\}$$

(2)

$$\{\varepsilon\}' = [T_1]\{\varepsilon\}$$

(3)

where, $\sigma$, $\varepsilon$ are stress and strain in global and $\sigma'$, $\varepsilon'$ are stress and strain in principal co-ordinate systems; $[T_1]$ and $[T_2]$ are the transformation matrix given by
where, $m = \cos \gamma$ and $n = \sin \gamma$

The stress-strain relation in the principal coordinate direction at any point in the RVE

\[
\{\epsilon'\} = [S'] \{\sigma\}
\]

where, $S'$ is the compliance matrix in principal coordinate system and their values are calculated as

\[
[S'] = \begin{bmatrix}
1/E_1 & -\nu_{12}/E_1 & -\nu_{23}/E_1 & 0 & 0 & 0 \\
-\nu_{12}/E_1 & 1/E_2 & -\nu_{23}/E_1 & 0 & 0 & 0 \\
-\nu_{23}/E_1 & -\nu_{12}/E_1 & 1/E_2 & 0 & 0 & 0 \\
0 & 0 & 0 & 1/G_{23} & 0 & 0 \\
0 & 0 & 0 & 0 & 1/G_{12} & 0 \\
0 & 0 & 0 & 0 & 0 & 1/G_{12}
\end{bmatrix}
\]

The components of the compliance matrix of the composite are calculated using rule of mixture

\[
E_1 = v_f E_f + (1 - v_f)E_m
\]

\[
E_2 = \left(\frac{v_f}{E_f} + \frac{1-v_f}{E_m}\right)^{-1}
\]

\[
G_{12} = \left(\frac{v_f}{G_f} + \frac{1-v_f}{G_m}\right)^{-1}
\]

\[
\nu_{12} = v_f v_f + (1 - v_f)\nu_m
\]

\[
\nu_{23} = v_f v_f + (1 - v_f)\left(2\nu_m - \frac{\nu_{12} E_2}{E_1}\right)
\]

\[
G_{23} = \frac{E_2}{2(1+\nu_{23})}
\]

Similarly, using principle of complimentary energy, the effective compliance matrix of composite is calculated as

\[
[S_{RVE}] = \frac{1}{L} \int_0^L [T_2] [S'] [T_1]^{-1} dx
\]

For Short CNT, RVE can be considered as two parts (Fig. 2). Central part is composed of CNTs/matrix connected in parallel; end part consists of matrix only. Equivalent longitudinal Young’s modulus of central part can be estimated using eqn. (12). The effective Young’s modulus ($E_{\text{Effective}}$) of the composite in the longitudinal direction can be obtained using inverse Rule of Mixtures considering the compatibility of strains and equilibrium of stresses as given by eqn. (13).

\[
E_{\text{Effective}} = \left[\frac{1}{E_m} \left(\frac{L_e}{L}\right) + \frac{1}{E_{\text{center}}} \left(\frac{L_c}{L}\right)\right]^{-1}
\]

where, $L_e$, $L_c$ and $L$ are the length of central part, end part and total length ($L_e + L_c$), respectively. $E_{\text{center}}$ is taken as $S_{RVE}$ in eqn. (13) and $E_m$ is the Young’s modulus of matrix.

![Figure 2. Typical representation of short CNT inside RVE model.](image)
3. Finite Element Analysis

In this current study, rectangular based RVE is being considered for 3-D finite element (FE) analyses (ANSYS 14.0) for the composite. Both long (continuous) and short (discontinuous) CNTs are being idealized as solid annular tube. Nominal diameter and thickness of CNT (24,0) are being taken as 1.88 nm and 0.34 nm, respectively. Short CNT is modelled with hemispherical cap at its both ends. Five wavy CNTs are modelled with equal spacing of 15 nm in transverse direction (Fig. 3). Wavy CNTs are reinforced centrally inside the full RVE. Due to symmetry, 1/4th of the full RVE is being considered in FEA. Figures 3a and 3b represent typical schematic diagrams of full RVE and 1/4th RVE models, respectively. Two symmetry boundary conditions are imposed on two respective faces of RVE where out of plane translational degrees of freedom (DOF) are being restricted. Uniform displacement corresponding to 1% longitudinal strain is being applied in the FE model. Young’s modulus and Poisson’s ratio of CNT are taken as 1000 GPa and 0.3, respectively. Young’s modulus of matrix is being varied to produce a wide range of modulus ratios (\(\lambda\)). However, Poisson’s ratio of matrix is being taken as 0.3 for the entire analyses. Both particle and matrix are considered as linear and isotropic in nature. Wavy CNT is assumed to be perfectly bonded to the surrounding matrix. CNTs and Matrix are modelled using second order tetrahedron (solid186) elements with reduced integration. Typical number of nodes and elements are taken as 216270 and 131952 (waviness ratio, \(w=0.1\) and CNT volume fraction of 2.00%), respectively. Longitudinal Young’s modulus (\(E_c\)) of composite under axial load can be estimated using equation, \(E_c = \frac{F}{AE}\), where \(F\) is the longitudinal reaction force at support obtained from FEA, \(A\) is the cross-sectional area of RVE and \(\varepsilon\) is the average strain.

![Figure 3. Typical rectangular RVE for short CNTs (\(w=0.1, \lambda_s=0.8\)) (a) full model and (b) quarter model.](image)

4. Results and Discussions

4.1. Effective Young’s modulus versus CNT volume fraction

The variations of normalised Young’s modulus (ratio of Young’s modulus of nanocomposite and matrix; \(E/E_m\)) versus CNT volume fraction (\(V_{CNT}\)) are shown in Figs. 4-5. CNT volume fractions are taken as 0.5%, 0.75%, 1.0%, 1.25%, 1.5%, 1.75% and 2.0%. The variations of the strength of the composite with the volume fraction for long CNTs (\(\lambda_s=1\)) are shown in Figs. 4a and 4b. Figure 4a shows the variation of \(E/E_m\) versus \(V_{CNT}\) for modulus ratio (\(\lambda_s\)) of 50 with different waviness ratios (\(w\)) of 0.1, 0.2, 0.3, 0.4 and 0.5. Values of \(E/E_m\) increase linearly with \(V_{CNT}\). Further, Fig. 4a indicates that for same volume fraction and modulus ratio, higher waviness exhibits lower effective modulus of composite. It can be noted from Fig. 4a that the slope of curve is highest in case of \(w=0.1\) compared with \(w=0.2, 0.3, 0.4\) and 0.5. In case of \(V_{CNT}=0.5\%), values of \(E/E_m\) are 1.120, 1.049, 1.030, 1.026 and 1.022 for \(w=0.1, 0.2, 0.3, 0.4\) and 0.5, respectively. Corresponding values are 1.464, 1.186, 1.108, 1.088 and 1.081 in case of \(V_{CNT}=2.0\%). Sensitivities on overall directional elastic modulus of composites are less when waviness ratio (\(w\))>0.3 and values are close to each other for \(w=0.4\) and 0.5. Figure 4b illustrates the variation of \(E/E_m\) versus \(V_{CNT}\) with \(w=0.1\) for modulus ratios (\(\lambda_s\)) of 5, 10, 20, 50, 100 and 200. Rate of change of \(E/E_m\) is more with higher value of modulus ratio. Minimum and
maximum values of $E_c/E_m$ obtained from FEA are 1.011 and 1.976, respectively, for $V_{CNT}=0.5\%$, $\lambda_1=5$ and $V_{CNT}=2.0\%$, $\lambda_1=200$. Figure 5a exhibits variation of $E_c/E_m$ versus $V_{CNT}$ for short CNT with height fraction ($\lambda_3$) of 0.8 and $\lambda_1=50$. Results for different waviness ratios ($w$) of 0.1, 0.2, 0.3, 0.4 and 0.5 are also plotted in Fig. 5a. The variations of $E_c/E_m$ with $V_{CNT}$ shown in Fig. 5a are similar to Fig. 4a, except the values are lower in case of short CNTs for same waviness and volume fraction. Effect of height fractions on overall elastic response of composite are shown in Fig. 5b. Considering $w=0.1$ and $\lambda_1=200$, height fractions ($\lambda_3$) are taken as 0.6, 0.7, 0.8 and 0.9. Rate of enhancement of effective Young’s modulus with $V_{CNT}$ slightly decreases in case of $\lambda_3=0.6$. However, the slope of $E_c/E_m$ with $V_{CNT}$ remains almost constant for $\lambda_3=0.9$. Values of $E_c/E_m$ for $V_{CNT}=0.5\%$ are 1.138 and 1.181 for $\lambda_3=0.6$ and 0.9, respectively. Corresponding values for $V_{CNT}=2.0\%$ are 1.448 and 1.679, respectively.

![Figure 4](image_url) Young’s modulus versus volume fraction for long CNTs (a) $\lambda_1=50$ and (b) $w=0.1$.

![Figure 5](image_url) Young’s modulus versus volume fraction for short CNTs (a) $\lambda_1=50$, $\lambda_3=0.8$ and (b) $w=0.1$ $\lambda_1=200$.

4.2. Effective Young’s modulus versus CNT waviness

The effect of waviness is being illustrated in Figs. 6a and 6b, considering volume fraction of CNT as 2.0\%. Results obtained from FEA and analytical solution based on micromechanics approach for different modulus ratios of 10, 20, 50 and 200 are also plotted in Figs. 6a and 6b. In case of long CNTs (Fig. 6a), with increase of waviness, the strength of the composite decreases sharply between $w=0.1$ and 0.2 but when $w>0.3$ (can be considered as critical value) $E_c/E_m$ variation remains almost constant for same modulus ratio. Figure 6b shows $E_c/E_m$ variation with waviness for short CNTs ($\lambda_3=0.8$). In case of analytical model, the overall modulus are being calculated using eqn. (12) for long CNTs; and using both eqn. (12) and eqn. (13) for short CNTs. FEA results under predicts the analytical solution for all cases. The maximum variations of FEA and analytical results for long and short CNTs are 7.2\% and 11.6\%, respectively in case of $w=0.1$ and $\lambda_1=200$. However, finite element results and analytical solutions are very close to each other when $w>0.2$. Figures 6a and 6b show similar trend in variation of
normalized Young’s modulus with waviness. The rate of reduction of $E_c/E_m$ is more with higher modulus ratio as demonstrated in Figs. 6a and 6b. However, the results obtained from the analytical approach are comparatively closer to FEA solution in case of long CNTs than short CNTs.

Figure 6. Young’s modulus versus waviness with $V_{CNT}=2.0\%$ (a) long CNTs (b) short CNTs, $\lambda_c=0.8$.

5. Conclusions

Following conclusions can be drawn from the present analyses:

- Straight CNTs are more efficient than wavy CNTs.
- Effective Young’s modulus of composite decreases with CNT waviness. However, sensitivity of modulus of composite becomes less significant with higher waviness.
- Long CNTs are more effective in enhancement of overall modulus of composite than short CNTs.
- Enhancement of overall elastic response of the composite increases with higher modulus ratios.
- Finite element analysis results are in good agreement with the results obtained from micromechanics approach.

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