Research Article

Atomistic Multiscale Modeling of SWCNT Reinforced Polymer Nanocomposites: Effects of Waviness, Volufraction and Interface Material

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ABSTRACT

Carbon nanotube (CNT) is a multifunctional nanostructured material with exceptional mechanical, thermal and electrical properties and one of the strongest materials known to men. CNTs are frequently used as reinforcements in composites. However, process induced defects like vacancies and curvature in CNT are common. Such defects are known to have detrimental effects on the overall properties of the composites. In an approach to quantify the effects of CNT waviness on mechanical properties of CNTs and their composites, a multiscale analysis is performed. At the nanoscale analysis, an atomistic model of wavy single walled CNT (Armchair and Zigzag) is developed and the effect of waviness ratio and wavelength ratio on Elastic modulus is studied. Then a finite element model is developed where fibers are oriented in two different process-induced patterns, aligned and random orientation. In each case, elastic modulus and shear modulus are determined in both longitudinal and transverse directions and the variation of their values with the change of waviness ratio as well as volume fraction are studied by finite element method where the dilute strain concentration tensor is obtained directly from a finite element solution. It was observed that the Elastic modulus decreases with increasing waviness of CNT, but after a certain value of waviness ratio, the decreasing rate becomes insignificant. Additionally, the modulus of the CNT decreases with diameter, while having drastic change in the larger diameter region. Though composite reinforced with CNTs follow similar trend with the atomic model, it was observed that at higher waviness ratio, alignments of CNTs have less impact on the modulus of the composite. Furthermore, it was observed that the overall strength of the composite increases non-linearly with the increment of volume fraction,and as expected, interface material reinforces the mechanical properties of the composite.

Keywords: *CNT, SWCNT, Single Walled Carbon Nanotube, Advanced Material, Wavy CNT, Composite, Atomistic Modeling*

1. INTRODUCTION

The discovery of Carbon Nanotubes (CNTs) only a couple of decades ago [1] have opened up a new era of multifunctional nanostructured materials. CNTs are hollow cylindrical shells of carbon atoms laid in a honeycomb pattern. Their modulus values have been shown on the order of 1 TPa, with strength several times that of graphite fibers [2-5]. Despite the prohibitive cost of manufacturing, carbon nanotubes are already being used in a wide range of applications including airplane and vehicle components, in bulletproof clothing and electronics [6].

Properties of multi and single-walled nanotubes (MWNTs or SWNTs) have been studied using both experiments and modeling. Molecular dynamics (MD) and elastic continuum modeling approaches have been used to estimate the characteristics of CNTs. However, a wide scatter can be seen in experimental and simulation data for moduli of CNTs. For example, experiments conducted by Treacy et al. [7], using Transmission Electron Microscopy (TEM) to measure the Young's modulus of MWNTs, found a mean value of 1.8 TPa with a variation from 0.40 to
4.15 TPa; while similar experiments by Krishnam et al. [8] observed Young's modulus ranging from 0.90 to 1.70 TPa. Wang et al. [9] conducted bending tests on cantilevered tubes of CNTs using atomic force microscopy and estimated the Young's modulus of 1.28 TPa. Poncharal et al. [10] observed the static and dynamic mechanical deflections of cantilevered MWNTs, which is induced by an electric field, and reported a modulus of about 1.0 TPa for small- diameter tubes.

Among the numerical and theoretical studies, molecular modeling in particular, which is based on the force field and total potential energy for CNTs in a macroscopic sense has been used most extensively (Iijima et al. [11]; Gau et al. [12]; Zhou et al. [13]; Belytschko et al. [14]). However, the computational expense for convergence requirements in MD simulations limits the size of CNTs that can be studied by this technique.

The other approach is the continuum/finite element method (Zhang et al. [15, 16]; Jin and Yuan [17]; Li and Chou [18, 19]). Since a nanotube closely resembles a continuum solid beam or shell on macro-scale, it is reasonable to model the nanotube as a frame or shell-like structure. Using this approach, the mechanical properties of such a structure can be obtained by classical continuum mechanics or finite element method. However, due to the uncertainty of the CNT wall thickness for both of the above modeling techniques, the obtained mechanical properties of SWNTs or MWNTs have scattered values; for example, the results of axial Young's modulus ranged from about 1.0 to 5.5 TPa can be found in the existing literature [20].

Carbon nanotubes are stronger than most conventional reinforcements [2-5]. Not surprisingly, CNTs have been incorporated into various bulk materials to enhance the properties of the parent materials. Significant improvements have been reported for nanotube-reinforced polymers with regard to mechanical, electrical and thermal properties [21-23]. Such composites take advantage of the extraordinary electrical and thermal conductivity of CNTs to create multifunctional composites with improved electrical and thermal properties [24].

Although at the beginning, CNTs were thought to be cylindrical shells that consisted of regular hexagonal arrays of carbon atoms, it is now widely accepted that defects and morphological variations are common. Researchers have only started to look at the effects of these structural variations on the properties of CNTs as well as their composites [25, 26].

Another feature characteristic of nanocomposites is that the embedded CNTs are not straight but rather have significant curvature or waviness that varies throughout the composite [27]. While it is reasonable to surmise that this waviness reduces the effectiveness of the CNT reinforcement of the polymer, the degree to which this is the case is unclear. The goal of this work is to develop a micromechanics-based model that can be used to assess the effect of nanotube waviness on the properties of composites. In the studies of Fisher, Bradshaw, and Brinson [28, 29], the problem was simplified by modeling the wavy CNTs as infinitely long straight NTs; the effect of waviness was incorporated using a reduced effective nanotube modulus determined via finite element (FE) modeling. The wavy CNT was modeled by using a straight CNT with a reduced modulus to determine the dilute strain concentration tensor analytically via Eshelby's solution [30]. In this work, an alternate approach is used. The NT is modeled as single wavelength long sinusoidal fiber and the dilute strain concentration tensor is obtained directly from a finite element solution. This approximates the NT and the surrounding matrix as a continuum; once the NT and surrounding matrix are modeled as a continuum, the length scale of the NT is no longer material to the analysis. Thus, the model developed in this article applies equally well to larger inclusions such as graphite fibers. As such, in this article the term fiber is used interchangeably with the term nanotube when speaking of the reinforcement phase of the composite material.

In this study, a finite element model of SWNTs was developed and their modulus of elasticity (longitudinal and transverse direction) with variation of the diameter and waviness of the CNT were consequently estimated. The key concept of the modeling is that the carbon nanotube can be treated as a frame like structure, and the primary bonds between two nearest neighboring atoms can be simulated as beam elements.

After developing a model for straight CNT, an elastic modulus was estimated and the tube thickness was adjusted to get relevant value as done in the past studies. Then waviness was applied to the CNT and the values of elastic modulus were calculated for different waviness as well as different diameters of the CNT. These values were used in this study in the Composite model to estimate the modulus of elasticity and shear modulus (both in the longitudinal and transverse direction) and six finite element solutions were performed to determine the constants by which a transversely isotropic material can be described. The study was carried out for aligned CNTs and randomly orientated of the CNTs to observe the effect of random orientation of CNTs in the composite (Figure 1).The variation of elastic modulus with volume fraction was studied and compared with the modified rule of mixture [31].

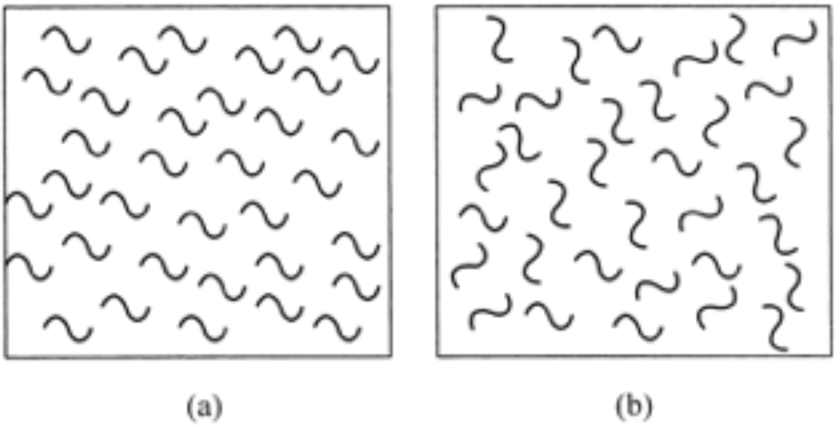

Figure 1. Wavy NT orientations: (a) similarly oriented wavy NTs with common axis directions and waviness planes; (b) wavy NTs randomly oriented in all directions with randomly oriented planes of waviness.

1.1. FE modeling

CNTs carbon atoms are bonded together with covalent bonds forming a hexagonal lattice. These bonds have a characteristic bond length αC-C and bond angle in the 3D space. The displacement of individual atoms under an external force is constrained by the bonds. Therefore, the total deformation of the nanotube is the result of the interactions between the bonds. By considering the bonds as connecting load-carrying elements, and the atoms as joints of the connecting elements, CNTs may be simulated as space-frame structures.

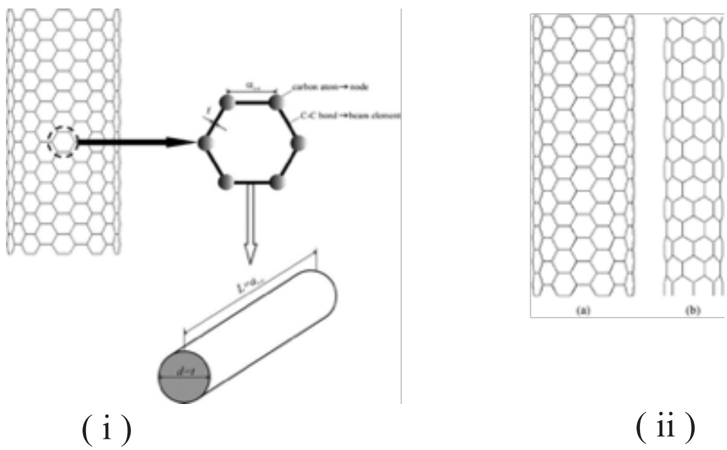

Figure 2. i) Schematic of a SWCNT as a space-frame structure.
ii) Side views of the FE meshes of the (a) (8,8) and (b) (8,0) SWCNTs. [32]

By treating CNTs as space-frame structures, their mechanical behavior can be analyzed using classical structural mechanics methods. Figure 2 depicts how the hexagon, which is the constitutional element of CNTs nanostructure, is simulated as structural element of a space- frame. In the same way, the entire nanotube lattice is simulated. The simulation leads to the correspondence of the bond length αC-C with the element length L as well as the wall thickness t with the element thickness. In the study, size of nanotube varied from zigzag (10,0) to (14,0) and armchair (6,6) to (10,10).

1.2. Elastic moduli of beam elements

According to classical structural mechanics, the strain energy of a uniform beam of length L and cross-section A under pure axial force N is,

$$U_A = \frac{1}{2}\int_0^L \frac{N^2}{EA} dL = \frac{1}{2}\frac{N^2 L}{EA} = \frac{1}{2}\frac{EA}{L}(\Delta L)^2$$

$$U_M = \frac{1}{2}\int_0^L \frac{M^2}{EA} dL = \frac{1}{2}\frac{EI}{L} = \frac{1}{2}\frac{EI}{L}(2\alpha)^2$$

Where ΔL = the axial stretching deformation. The strain energy of a uniform beam under pure bending moment M is,

Where α denotes the rotational angle at the ends of the beam. The strain energy of a uniform
beam under pure torsion T is,

Where, $\Delta\beta$ is the relative rotation between the ends of the beam and J the polar moment of inertia.

It can be concluded that *U c*,Æ represent the stretching energies in the two systems (molecular and structural), U_θ, U_M,the bending energies, and U_c, U_T the torsional energies. It can be assumed that the rotation angle 2α is equivalent to the total change Δθ of the bond angle, ΔL is equivalent to Δr, and $\Delta\beta$ is equivalent to $\Delta\varphi$. Therefore, by comparing Eqn. (3)–(5) with Eqn. (6)–(8), the following direct relationships between the structural mechanics parameters EA, EI and GJ and the molecular mechanics parameters k_r, k_θ and k_c are obtained, Given the force constants , k_θ and, k_c the bond diameter and elastic moduli can be obtained from Eqn. (10).

Tserpes, K. and P. Papanikos [32] demonstrated a method for evaluating the diameter, elastic modulus and bulk modulus, and found the values to be d = 0.147, E = 5.49 TPa and G = 0.871 TPa. The procedure provides a unique value of bond diameter (= wall thickness). In order to compare the evaluated elastic moduli of the SWCNTs with the literature results, the FE model was implemented using various values of wall thickness and finally a fixed value of wall thickness (d = 0.13 nm) and $a_{c\text{-}c} = 0.1452\ nm$ was used throughout the study.

1.3. Numerical Homogenization

The study used the mathematical model where the composite material is considered to have cylindrical fibers of infinite length, embedded in an elastic matrix. Because of the periodicity, the three dimensional representative volume element (RVE) can be used for FE analysis [33]. A transversely isotropic material is described by five constants. When the axis of symmetry is the fiber direction, 3D Hooke's law reduces to,

Once the components of the transversely isotropic tensor C are known, the five elastic properties of the homogenized material can be computed by Eqn. (13) – (17), i.e. the longitudinal and transversal Young's moduli E_1 and E_2, the longitudinal and transversal Poisson's ratios V_{12} and V_{23}, and the longitudinal shear modulus G_{12}, as follows,

2. COMPUTATIONAL METHOD

2.1. Elastic Modulus of Single-walled Carbon Nanotube

Polymer nanocomposites containing wavy CNTs were characterized in a two-step micromechanical approach. Firstly, individual CNTs were studied for effects of change of
waviness ratios (a/λ) using an atomistic structure. The resulting nanostructure was studied in FEM and the complete 3D material constitutive matrix was populated by data generated through six different stress boundary conditions applied to the CNT.

2.2. Atomic modeling of Carbon nanotubes

The coordinates of carbon atoms in nanotubes of varying chirality were generated using a GNU code. These coordinates will be exported to commercial FE software using an in-house code that will generate the hexagonal lattice of the selected CNT and represent the lattice using link elements.

2.3. Carbon Nanotube

One end of the CNT was defined as fixed and force was applied at the other end. The value of displacement was collected from the horizontal parts of the CNT for calculating the average value of the strain. The horizontal part close to the application of the force shows negative displacement when the waviness increases, so values of displacement was taken at the horizontal part closest to the fixed end of the CNT (Figure 3 and Figure 4). Elastic modulus was calculated from the strain and stress determined from the applied force.

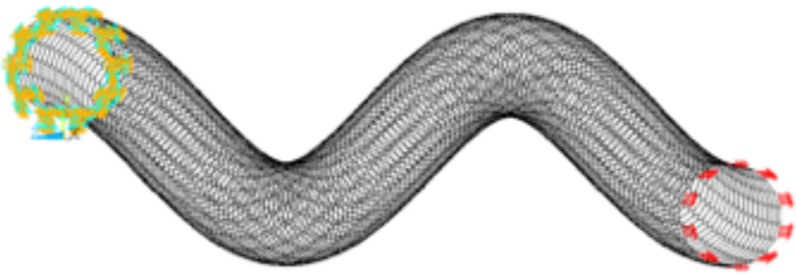

Figure 3. Atomic Structure of a (10, 10) CNT with boundary conditions at waviness ratio = 0.04 and Wavelength ratio =18.13

2.4. RVE of polymer composite reinforced with SWCNT

A continuum approach was utilized to model the wavy CNT as a curved solid beam in a representative volume element (RVE) of a polymer matrix (Figure 4). Consequently, the analysis at this macro-level incorporated the changes associated with CNT waviness, providing a more accurate prediction of the effective material properties of the nanocomposite. The polymer that was used for the composite matrix was Polystyrene with elastic modulus of 3.12 GPa. A volume fraction of 2.5% has been used in all the nanocomposites.

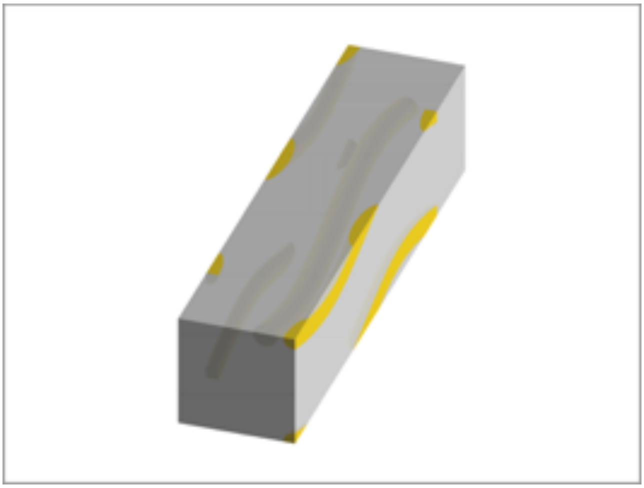

Figure 4. RVE of Composite reinforced with 2.5% aligned (14, 0) Carbon Nanotube at Waviness ratio = 0.024with the fiber direction

3. RESULT AND DISCUSSION

For each type of CNT Waviness ratio ( ) was varied from 0 to 0.08, where waviness of 0 stands for straight tube.

3.1. Elastic modulus of Single Walled armchair CNT with variation of Waviness

Three types of armchair CNTs ((6, 6), (8,8) and (10,10)) were studied and their moduli of elasticity were compared for same variation of waviness ratio (from straight tube to 8% waviness ratio). Waviness ratio is the ratio of amplitude to wavelength.

Elastic Modulus vs Waviness Ratio for Armchair SWCNT

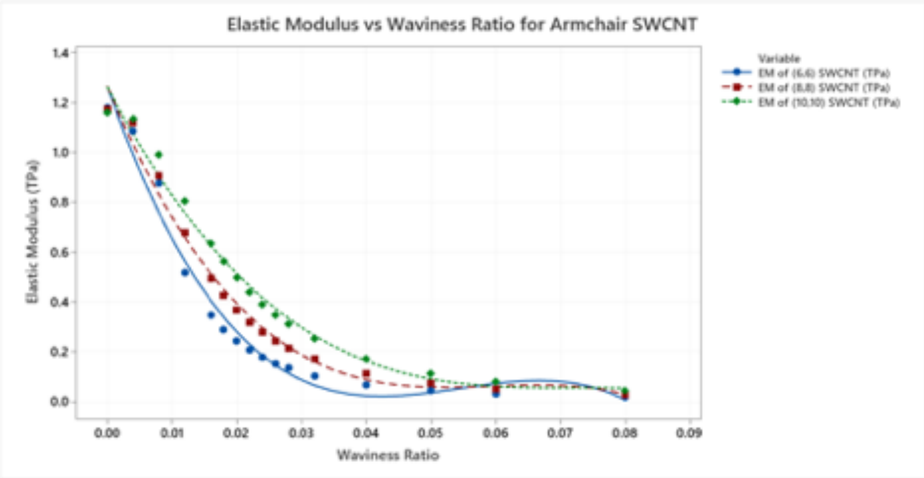

Figure 5. Elastic modulus vs. Waviness Ratio of armchair carbon nanotube

Effect of waviness on elastic modulus of Single walled armchair Carbon Nanotube is illustrated in Figure 5. Elastic modulus decreases with increasing waviness. After a certain value of waviness ratio (approximately 0.04) the curve seems to be flattened and the decreasing rate of elastic modulus become insignificant. For a waviness ratio of 3.2%, elastic modulus decreases by around 85% of that of the straight nanotube.

3.2. Elastic modulus of Single Walled zigzag CNT with variation of Waviness

Three types of zigzag CNTs ((10, 0), (12, 0) and (14, 0)) were studied and their moduli of elasticity were compared for same variation of waviness ratio (from straight tube to 8% waviness ratio). Zigzag CNTs were chosen such that they have similar range of wavelength ratio as that of armchair CNTs.

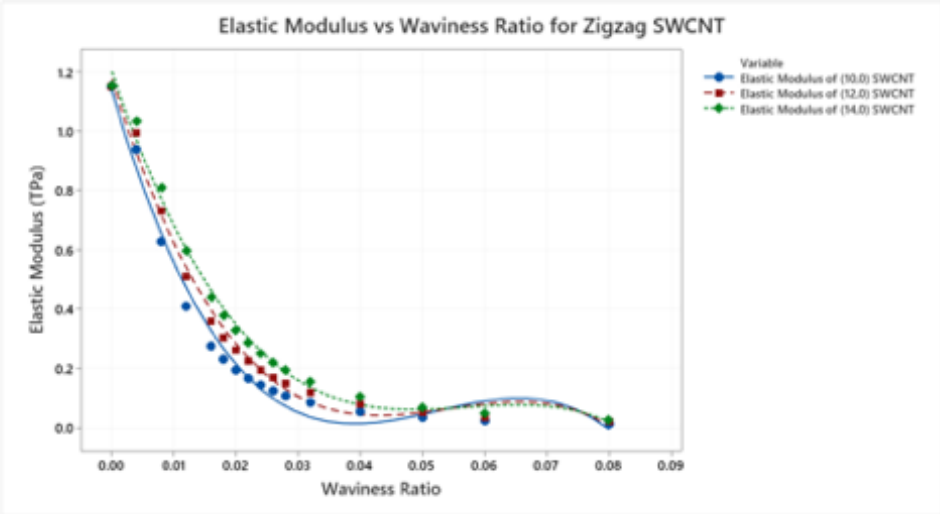

Figure 6. Elastic modulus vs. Waviness Ratio of zigzag carbon

Effect of waviness on elastic modulus of Single walled zigzag Carbon Nanotube is illustrated in Figure 6. Elastic modulus decreases with increasing waviness. After a certain value of waviness ratio (approximately 0.04) the curve seems to be flattened and the decreasing rate of elastic modulus becomes insignificant. For a waviness ratio of 3.2%, elastic modulus decreases by around 90% of that of the straight nanotube. The reduction in the values of elastic modulus is similar to the findings of Marino Brcic et al. [34] for straight CNTs. According to their study, in a (5, 5) CNT, longitudinal elastic modulus decreased by around 82.5% for an increment of waviness ratio of 3.5%.

It can be assumed that waviness imposes instability on the CNTs. As a result, with the increasing waviness it requires less stress to impose strain than that of a straight tube which is the most stable form. In the atomic scale, carbon atoms in the cusps of the wavy CNTs are deviated from the ideal location for optimum stiffness. Axial elongations tend to be favored by such CNTs, in order to achieve this optimum atomic distance, resulting in lower stiffness. The greater the wavelength ratio of a CNT, the greater the deviation of atomic positions from the optimum locations, and the easier it is for an atom to move relative to its closest neighbor. This explanation is found to be consistent with the sharp drop in stiffness of CNTs with high wavelength ratios. However, to explain this feature in the

FE analysis, where bond stiffness is independent of atomic distances, bond lines orientations are considered. Atomic bonds at the inner edge of a cusp are subjected to a greater amount of the axial load due to the alignment of such lines with the loading direction. While bond lines in the straight portions of the CNT, located in an inclined orientation due to the structure of the CNT, receive much lower portions of the boundary load component. As a result, only a small portion of the bonds, within the cusp zones in particular, support a major portion of the applied load in case of wavy CNTs, resulting in a lower overall stiffness for wavy CNTs.
Moreover, this effect is diminished beyond a wavelength ratio of approximately 0.4. Again, this is related to the atomic bonds within the cusp zones. Beyond a critical waviness ratio ($^{a}/\lambda$), atomic bond alignment change with increasing waviness becomes insignificant, so no change in stiffness can be observed beyond this critical wavelength ratio. This concept should be equally relevant for the atomic scale and the RVE.

3.3. Elastic modulus of Single Walled armchair CNT with variation of Diameter

In the current study, diameter has been represented by wavelength ratio, which is the ratio of wavelength to diameter ($^{\lambda}/d$). In the case of CNT, diameter changes with the change of indices (m, n). To study the effect of diameters of wavy CNTs on their modulus, armchair CNT from (6, 6) to (12, 12) were used with a resultant variation of diameter between 0.8193 nm to 1.6575
nm.

Elastic Modulus vs Wavelength Ratio for Armchair SWCNT

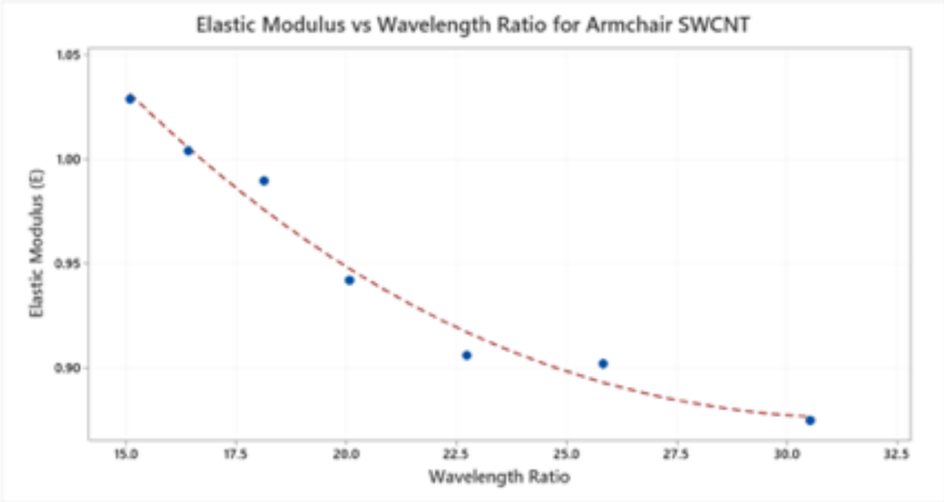

Figure 7. Variation of elastic modulus with varying diameter for (8, 8) CNTs with waviness ratio = 0.008

The change of diameter is represented by wavelength ratio, which is a dimensionless number and determined by the ratio of wavelength to diameter. In Figure 7, the elastic modulus decreases as the diameter of a Single walled armchair CNT is decreasing. Within the range of analysis, for a decrease in diameter by 50.57%, the modulus of elasticity decreases by 14.88%. It is also observed that CNT with higher wavelength ratio (ratio of wavelength to diameter; more the wavelength ratio smaller the tube diameter) has less strength than the CNT of lower wavelength ratio. Furthermore, the modulus of the CNT with lower wavelength ratio (larger diameter) decreases more drastically than that of higher wavelength ratio.

3.4. CNTs reinforced composites with aligned and random orientation: For studying the composite, (8,8) armchair CNT and (14,0) zigzag CNT were selected as their diameters are almost same. This study considered two orientations: (1) aligned orientation and

(2) cross direction, which is the direction normal to the wave propagation represented the random orientation. The waviness of the CNTs cause them to be spaced apart which reduces the van der Waals forces and does not allow the CNTs to all be loaded at the same time, thus reducing the

strength of the composite. In the previous section it was explained how in FE analysis, CNT stiffness is reduced by the effect of waviness. In a similar fashion, the composite material with a wavy CNT exhibits reduced stiffness. It is to be noted that the scale of the analysis for an individual CNT was atomistic, while the composite analysis is conducted using the continuum approach. In the continuum analysis, it was assumed that the effect of CNT waviness was carried over from the atomistic simulation data, and interfacial interaction between the bulk matrix and a curved nanotube would further influence the overall stiffness of the composite.

3.5. Polymer composite reinforced with (8, 8) CNT

For (8, 8) CNT reinforced composite, a wavelength ratio = 22.73 and volume fraction = 2.5% were considered. From the simulation software, the values of the constants in stiffness matrix have been determined. Then Eqn. (12-17) were used to determine the values of elastic and shear modulus.

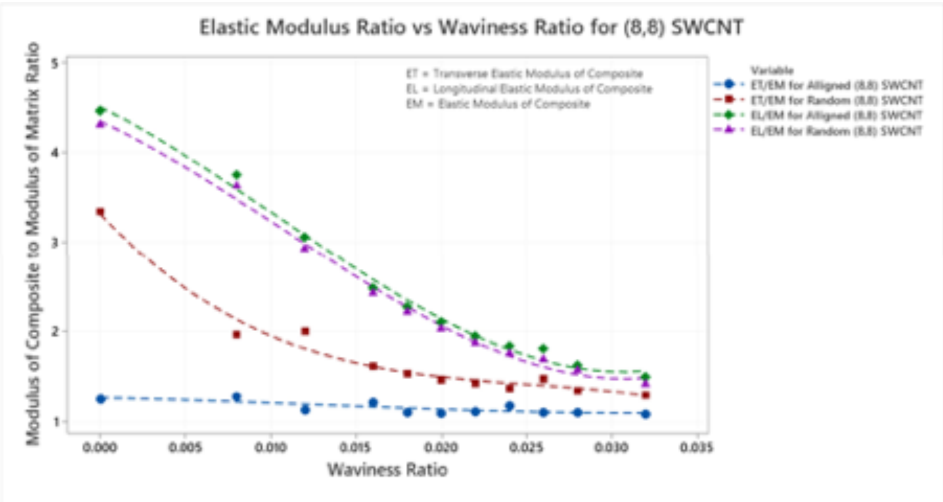

Figure 8. Elastic Modulus Ratio vs Waviness Ratio for (8,8) SWCNT with 2.5% volume fraction and wavelength ratio = 22.73

In Figure 3.4 variation of elastic modulus of nanocomposite reinforced with (8,8) CNTs with the increasing waviness ratio has been illustrated for both aligned and random orientations. The Elastic modulus of both orientations demonstrate downward trends with increasing waviness.

The longitudinal elastic modulus (Figure 8) follows almost the same trend as the (8, 8) CNT (Figure 5) and for aligned CNT, decreases by 66.7% as the waviness is increases to 3.2%. On the other hand, transverse elastic modulus (Figure 8) decreases with increasing waviness ratio in an irregular way and decreases by 13.6% as the waviness varies up to 3.2%. For random orientation, the longitudinal elastic modulus decreases by 67.2% as the waviness increases up to 3.2%, and decreases with a few fluctuating values to around 61.25%. Paunikar et al. also observed similar phenomenon in 2014 [35].

Composite with aligned orientation of CNT shows higher Longitudinal modulus than that of the random orientation, whereas the transverse elastic modulus increases significantly as the orientation is changed from aligned too random. Moreover, the variation due to alignment decreases with increasing waviness, which implies that at higher waviness ratio, alignments of CNTs have less impact on the modulus of the composite.

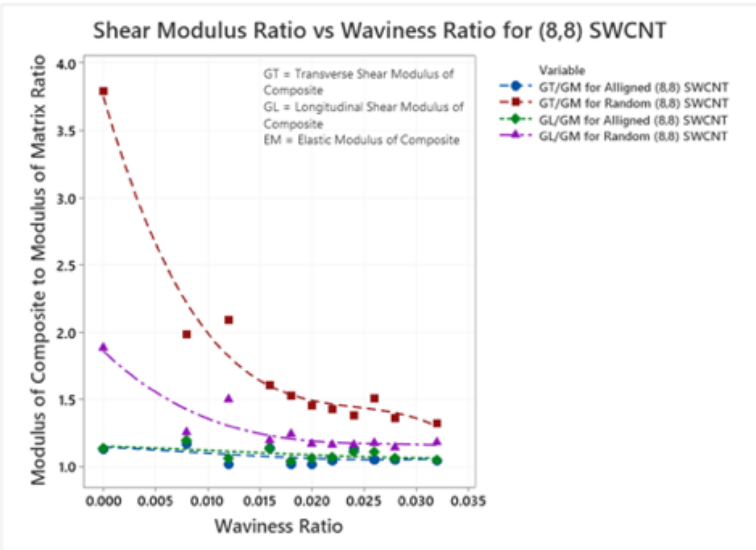

Figure 9. Shear Modulus Ratio vs Waviness Ratio for (8,8) SWCNT with 2.5% volume fraction and wavelength ratio = 22.73

Transverse shear modulus (Figure 9) decreases with increasing waviness ratio in an irregular way and decreases by maximum 10.1% as the waviness varies up to 3.2% for aligned orientation, whereas Longitudinal Shear Modulus decreases with increasing waviness ratio in an irregular way by 7.8%. For random orientation, Longitudinal shear modulus (Figure 9)

decreases with increasing waviness ratio in an irregular way and decreases by 40% as the waviness varies up to 3.2%, and the transverse shear modulus decreases with a few fluctuating values by 65.3%.
While the longitudinal elastic modulus has a smooth decreasing pattern, transverse elastic modulus and both types of shear modulus have fluctuating values with the variation of waviness. These effects are probably due to the non-uniformity caused by the waviness of the CNTs. The load is not distributed uniformly throughout the body in transverse direction. Hence, with increasing waviness, a wide scatter in data is observed.

Both longitudinal and transverse shear modulus increase significantly as the orientation is changed from aligned to random. Additionally, similar to the elastic modulus, the variation due to alignment decreases with increasing waviness, which implies that at higher waviness ratio, alignments of CNTs have less impact on the modulus of the composite.

3.6. Polymer composite reinforced with (14, 0) CNT

For (14, 0) aligned CNT reinforced composite, a wavelength ratio = 22.34 and volume fraction
= 2.5% were considered. From the simulation software, the values of the constants in stiffness matrix have been determined. Then Eqn. (13-18) were used to determine the values of elastic and shear modulus.

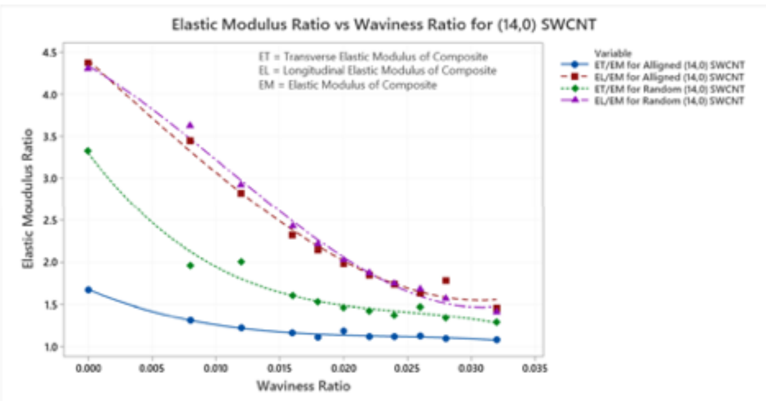

Figure 10. Elastic Modulus Ratio vs Waviness Ratio for (14,0) SWCNT with 2.5% volume fraction and wavelength ratio = 22.34

In Figure 10, variation of elastic modulus of nanocomposite reinforced with (14,0) CNTs with the increasing waviness ratio has been illustrated. For aligned orientation, the longitudinal elastic modulus decreases almost linearly and the value is reduced by maximum 66.8% for an increase in waviness up to 3.2%. Transverse elastic modulus decreases with some fluctuating values by maximum 35.4%. On the other hand, for random orientation, the longitudinal elastic modulus decreases almost linearly by around 68% as the waviness ratio is increased to 3.2%, whereas transverse elastic modulus decreases in a more irregular way by 49%.
Moreover, the longitudinal elastic modulus changes in a very small amount in comparison to transverse elastic modulus, but for this case (zigzag CNTs reinforced composite), the longitudinal elastic modulus for random-oriented is larger unlike that of armchair CNTs reinforced composite.

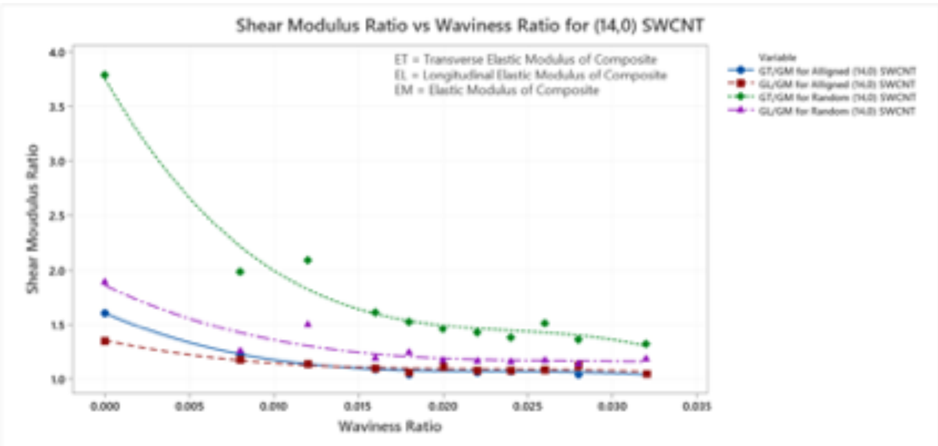

Figure 11. Shear Modulus Ratio vs Waviness Ratio for (14,0) SWCNT with 2.5% volume fraction and wavelength ratio = 22.34

Transverse shear modulus (Figure 11) and Longitudinal shear modulus decreases with increasing waviness ratio by maximum 35.3% and 22.4% as the waviness varies up to 3.2% for aligned orientation of CNTs.
On the other hand. Transverse shear modulus decreases with increasing waviness ratio with a few fluctuating values and decreases by 23.8% as the waviness varies up to 3.2%, whereas Longitudinal shear modulus decreases by 51.3%

3.7. Variation of Mechanical Properties in Nanocomposite with the change in volume fraction:

Polymer composite reinforced with aligned (8, 8) CNT
For (8,8) aligned CNT, at waviness ratio = 0.012, wavelength ratio = 22.73, elastic modulus of CNT = 0.68TPa: Volume fraction was varied from 0.5% to 10%. From the simulation software, the values of the constants in stiffness matrix have been determined.

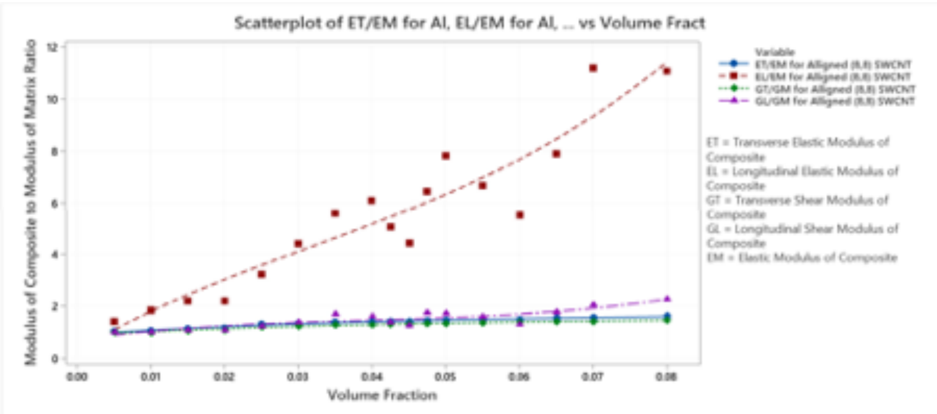

Figure 12. Modulus Ratio vs Waviness Ratio for (8,8) SWCNT with Waviness ratio = 0.012 and wavelength ratio = 22.73

In Figure 12, variation of elastic modulus of nanocomposite reinforced with aligned (8, 8) CNTs with the increasing volume fraction has been illustrated. Change of the longitudinal elastic modulus with increasing volume fraction found in the study have lower rate of increment than the values determined from modified rule of mixture [31]. There are fluctuations in the values determined in this study as with the increasing volume fraction, the load distribution inside the RVE changes due to changing packing factor, which is not considered in the modified rule of mixture for short fiber, where fibers are assumed straight. Longitudinal elastic modulus becomes around 12.5 times of that of pure polymer matrix at the volume fraction of 10%. Transverse elastic modulus becomes around 1.7 times of that of pure polymer matrix at the volume fraction of 10%.
The RVE is composed of polymer matrix of very low Young modulus reinforced by CNTs with very high Young modulus. With the increment of volume fraction, the CNTs contributes more to the strength of the composite, as a result overall strength of the composite increases with the

increment of volume fraction.

Transverse shear modulus of nanocomposite reinforced with aligned (8, 8) CNTs increases with the increasing volume fraction. After a volume fraction of 2.5%, it increases linearly. At a volume fraction of 10%, transverse shear modulus becomes around 1.55 times of that of pure polymer matrix.

Longitudinal shear modulus of nanocomposite reinforced with aligned (8, 8) CNTs increase with the increasing volume fraction with some fluctuating values.

Longitudinal shear modulus increases with a few fluctuating values. At 10% volume fraction, it becomes around 2.2 times of that of the pure polymer matrix.

3.8. Polymer composite reinforced with aligned (14, 0) CNT

For (14,0) aligned CNT, at waviness ratio = 0.012, wavelength ratio = 22.34, elastic modulus of CNT = 0.60 TPa: Volume fraction was varied from 0.5% to 10%. From the simulation software, the values of the constants in stiffness matrix have been determined.

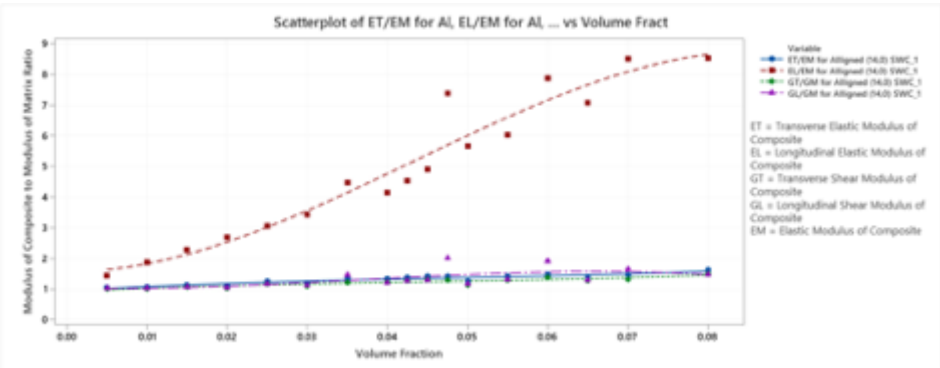

Figure 13. Modulus Ratio vs Waviness Ratio for (14,0) SWCNT with Waviness ratio = 0.012 and wavelength ratio = 22.34

In Figure 13, variation of elastic modulus of nanocomposite reinforced with aligned (14, 0) CNTs with the increasing volume fraction has been illustrated. Both Longitudinal and Transverse Elastic modulus increases with increasing volume fraction.

Change of the longitudinal elastic modulus with increasing volume fraction found in the study have lower rate of increment than the values from modified rule of mixture. Longitudinal elastic modulus becomes around 8.5 times of that of pure polymer matrix at the volume fraction of 10%. Transverse elastic modulus becomes around 1.6 times of that of pure polymer matrix at the volume fraction of 10%.

Both transverse shear modulus and longitudinal Shear Modulus of nanocomposite reinforced with aligned (14, 0) CNTs increase with the increasing volume fraction. At a volume fraction of 10%, transverse shear modulus becomes around 1.5 times of that of pure polymer matrix. Longitudinal shear modulus increases with a few fluctuating values. At 10% volume fraction, it becomes around 1.5 times of that of the pure polymer matrix.

3.9. Nanocomposite reinforced with aligned (8,8) CNT and an interface material

To study the effect of an interface material between the CNT and the matrix, Epoxy with elastic modulus of 15 GPa and Poisson's ratio of 0.35 was used in the model. The volume fraction of CNT fiber was 2.5% and the interface thickness was 10% of the tube diameter. A wavelength ratio of 22.73 was considered. From the simulation software, the values of the constants in stiffness matrix have been determined.

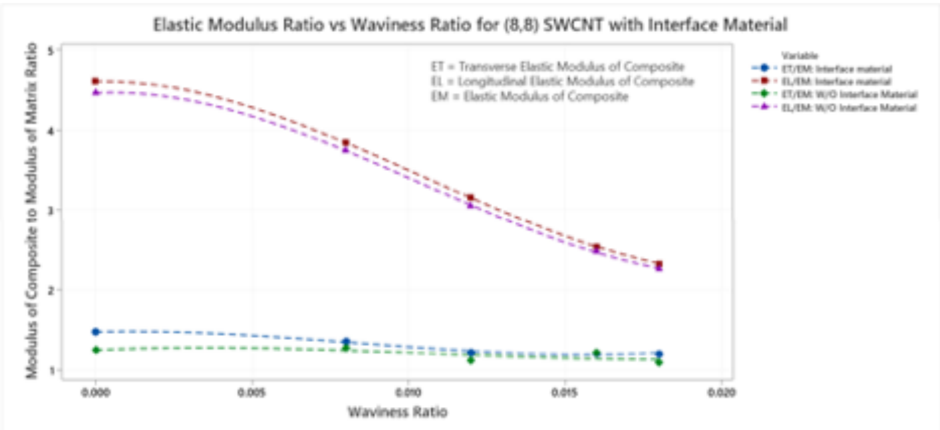

Figure 14. Elastic Modulus Ratio vs Waviness Ratio for (8,8) SWCNT reinforced nanocomposite with and without interface material of 10% thickness

In Figure 14, comparison of elastic modulus of nanocomposite reinforced with aligned (8, 8) CNTs with nanocomposites with an interface material have been illustrated. Longitudinal elastic modulus for a straight CNT with the interface material is around 3.6% higher than that of the straight CNT without interface material. For a waviness ratio up to 1.8%, longitudinal elastic modulus for nanocomposite with interface material decreases by 50%; where the value is 49% for the nanocomposite without interface material.

Transverse elastic modulus for a straight CNT with the interface material is around 18% higher than that of the straight CNT without interface material. For a waviness ratio up to 1.8%,

Transverse elastic modulus for CNT with interface material decreases by 18%; where the reduction is 12% for the CNT without interface material.

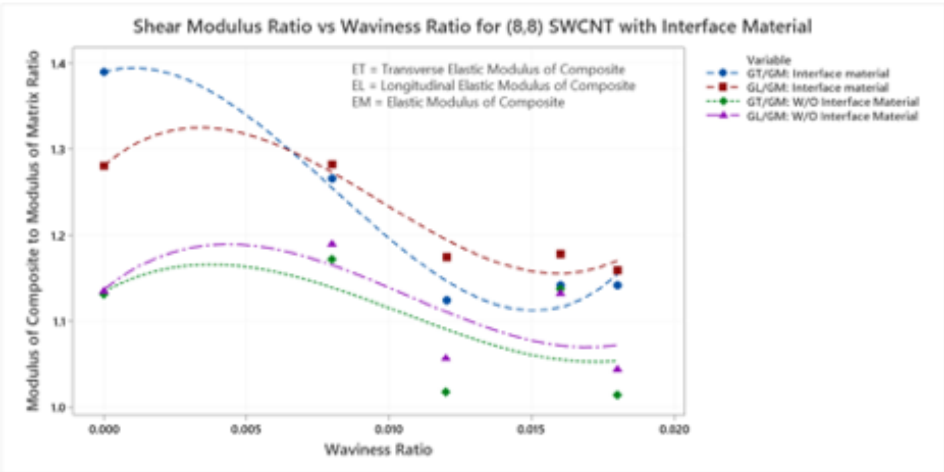

Figure 15. Shear Modulus Ratio vs Waviness Ratio for (8,8) SWCNT reinforced nanocomposite with and without interface material of 10% thickness

Transverse shear modulus and longitudinal shear modulus (Figure 15) of nanocomposite reinforced with aligned (8, 8) CNTs have been compared with composite with an interface material. With the increasing volume fraction both Transverse and Longitudinal, shear modulus decreases with less fluctuating values for composites with interface material.

Transverse shear modulus for a straight CNT with the interface material is around 22% higher than that of the straight CNT without interface material. For a waviness ratio up to 1.8%, transverse shear modulus for CNT with

interface material decreases by 18%; where the reduction is 10% for the CNT without interface material.
Longitudinal shear modulus for a straight CNT with the interface material is around 18% higher than that of the straight CNT without interface material. For a waviness ratio up to 1.8%, longitudinal shear modulus for CNT with interface material decreases by 10%; where the reduction is 8% for the CNT without interface material.
While studying the effect of interface material, the interactions like chemical reactions between the interface and matrix or interface and fiber were not considered. As the interface material added a layer of stronger material on the fiber inside the matrix, it is expected that it becomes stronger than the composite without interface material. Longitudinal shear modulus decreases with increasing waviness ratio in an irregular way and decreases by 22.4% as the waviness varies up to 3.2%.
In the case of (14, 0) CNT, the curves for transverse elastic modulus, longitudinal shear modulus and transverse shear modulus have less amount of fluctuation than that of the (8,8) CNT.
Interface material has a consistent effect on elastic modulus, whereas the change of shear modulus is inconsistent.

4. CONCLUSION

The strength and flexibility of carbon nanotubes makes them of potential use in controlling other Nano-scale structures, which suggests that they will have an important role in nanotechnology engineering. In a composite material the embedded CNTs are not straight rather wavy in nature. The literature review proves that there is interest in the effect of waviness on the bulk property of the composite. Nevertheless, in this study it was observed how the waviness affects the strength of CNT itself.
In this work, the change of mechanical properties in a single walled CNT with the increasing waviness has been studied. It is found that waviness significantly impacts the moduli of a CNT, resulting in almost 85% decrease for a waviness value of 3.2%. Using the derived values, polymer nanocomposite containing wavy Single-Walled Carbon Nanotubes (SWCNTs) has been characterized by utilizing a continuum approach. The CNTs used in the study was modeled as a curved solid beam in a representative volume element (RVE) of a polymer matrix. The study was carried out with randomly oriented CNTs that provided similar pattern of

curves for longitudinal and transverse directions. In addition, the effect of increasing volume fraction on strength of composite was compared with modified rule of mixture for short fiber, which validates the method of this study.
Effect of interface material between the polymer and the CNTs were studied to observe the reinforcement of strength of the nanocomposite.
It was observed that the Elastic modulus decreases with increasing waviness of CNT, but after a certain value of waviness ratio, the decreasing rate becomes insignificant. Additionally, the modulus of the CNT decreases with diameter, while having drastic change in the larger diameter region. The atomic bonds within the cusp zones could attribute to this phenomenon.

Though composite reinforced with CNTs follow similar trend with the atomic model, at higher waviness ratio, alignments of CNTs have less impact on the modulus of the composite.
Moreover, the overall strength of the composite increases non-linearly with the increment of volume fraction, and finally, interface material reinforces the mechanical properties of the composite. Interface material has a consistent effect on elastic modulus, whereas the change of shear modulus is inconsistent.

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