



Continuum Modelling of Carbon Nanotube Composites: A Review

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Abstract. Carbon nanotubes (CNTs) have been proven to show exceptional mechanical properties such as longitudinal elastic modulus of up to 1TPa and elastic strain of around 5%. Possessing these excellent properties, while having a fibre-like structure, CNTs have considerable potential to act as fillers in highly strong and light CNT composite (CNTC) materials. However, from experiments conducted, the biggest challenge before these nanocomposites can become a reality is that they do not show the expected excellent properties. This has led to extensive research into determining the effective properties of the CNTC using the preferred method of fully or semi-continuum modelling through the application of the finite element method (FEM). In this paper a review on aspects of the continuum representation of CNTCs is conducted. It covers the development, analysis and results of partial or full continuum modelling conducted in the last decades. A close-to-reality model must consider at least 5 CNT characteristics: length, interphase, waviness, orientation and agglomeration that cover 4 scales from nanoscale through micro- and meso- to macro-scale. The earlier nanocomposite continuum representatives mostly consisted of a CNT fibre surrounded by a matrix that could only catch the CNT characteristics at nano- and micro-scales and thus provided nanocomposite properties that were close to the rule of mixture (ROM) values but very far from experimental values. However, the recent representations manage to reach macro-scale level while representing important CNT characteristics such that the results were found to be close to the experimental results.

Keywords: Carbon nanotube · Nanocomposites · Multiscale modelling

1 Introduction

Carbon Nanotubes are known to possess many tremendously good mechanical, electrical and thermal properties [1, 2]. This is a result of their near-perfect seamless cylindrical microstructure, shaped naturally from a graphene sheet. With these advantages, CNTs have been proposed for use as nanofillers for polymer composites [3, 4] to form the so called CNT nanocomposites (CNTC).

In characterization studies of CNTC, its properties have been predicted using experimental [5], analytical [6] and modelling approaches [7]. While the experimental approach is expensive and time consuming, the molecular mechanics/molecular dynamics (MM/MD) approach [8, 9], requires huge computational time. Furthermore, the hard analytical method is limited to simpler geometry [10].

As such, the FEM based modelling approach that represents the CNT-matrix system as continuums has been the popular method as it is simpler, cheaper while giving greater insights to the CNT-matrix interactions.

In this paper, a review is conducted on the modelling of CNT nanocomposites using full and semi-continuum approaches that covers the representative volume elements (RVEs) both with and without the CNT-matrix interphase. In short, the review covers the journey of the continuum modelling in providing a close-to-reality model that gives results that agree closely with experimental results. The continuum modelling is explained starting by representing a lone CNT fibre encompassed by a matrix and then moving to models that exhibit the nanocomposites at the meso- and macro-scales. The processes of developing each representation are detailed out and the effectiveness of each model is discussed and compared. Finally, the conclusions are given along with recommendations for prospective future works.

2 The Continuum Modelling Approach

The challenge in conducting continuum modelling of a CNTC comes from the huge scale difference between the nano material and the matrix as all the characteristics of the CNT need to be considered. Failing to do so will cause the model to give solutions close to results due to the rule of mixture (ROM) but very far from the experimental findings.

Figure 1 shows how CNTs are typically positioned in a matrix, moving from nano-scale to micro-, meso- and macro-scales. While the length, waviness and defects of the CNTs can be considered at the nano- and micro-scales, the random orientation and agglomeration of the CNT can only be seen at the larger meso- and macro-scales [11]. As such, a full-scale model covering from nano- until the macro-scale is required to offer a close-to-real representation of the nanocomposite.

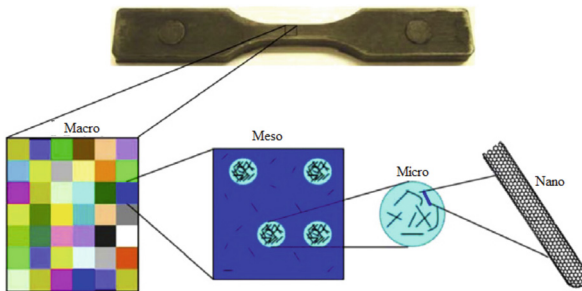


Fig. 1. From macro- to nano-scale in representing a CNT composite [11]

In the FEM continuum modelling approach, all or part of the constituents of the CNT composites are represented as equivalent continua. As an example, a CNT has been represented in FEM as a space-frame structure with each of its bonds is treated as an equivalent hollow cylinder, a solid cylinder, or simply an equivalent fibre (EF) [12]. The issue here is to get the right properties of the equivalent continuum to represent the real CNT structure.

2.1 The Representative Volume Element

The CNT composite in the FEM continuum modelling approach is represented as a unit cell or better known as the RVE, which basically consists of a matrix and a CNT.

With reference to Fig. 2, the characteristics of a CNT composite with repeated similar cells that give the global periodicity can be represented as a RVE with careful application of boundary and interface conditions.

The simplest RVE model assumes a perfect bonding or perfect load transfer between CNT and matrix where each phase is assumed to form a continuum. In this complete continuum representation, a long or short CNT fibre surrounded by a matrix is represented as a solid RVE at the nano-scale. The RVE is given appropriate boundary conditions and loaded such that the deformation obtained through the FEM can be applied in derived formulae to determine the CNTC's effective properties. While this representation does not consider the CNT-matrix interphase, it can still consider CNT characteristics such as CNT length, waviness and defects.

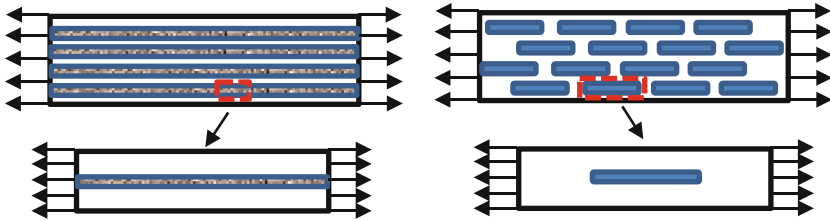


Fig. 2. Representing a unit cell as the whole CNT composite [11]

A strong CNT-matrix interface has been shown by CNTC along with an effective load transfer between the two constituents as indicated by experiments [13]. As such, more realistic models that consider the CNT-matrix scale difference i.e., an interphase is added to the RVE in order to cater for the CNT-matrix non-bonded relations. This so-called multiscale RVE model is a three-phase representation being made of matrix, CNT and their interphase. While considering the interphase improves the model, it can remain limited to considering CNT characteristics at the nano- and micro-scales as it considers only a single CNT fibre. Here, the macroscopic behaviours of the CNT composites are predicted assuming the well-dispersed and uniform distributions of the CNTs that result in the global periodicity of the nanostructures [14].

Referring to Table 1(b)–(d), depending on the phases whether they are in atomic (A) or continuum (C) forms, here the multiscale representative can be categorized into

3 types according to the order of arrangement of the CNT, interphase and matrix: the A-A-C [15], A-C-C [16] and C-C-C models [17]. As an example, in the A-A-C model, the CNTs are represented at the atomic level such that carbon atoms and the inter-atomic covalent bonds are modelled as FEM nodes and beam elements respectively. The CNT-matrix van der Waals (vdW) interactions between the matrix and CNT which is weak and non-bonded may be represented as a truss element while the matrix is taken as a solid continuum.

3 Modelling the Two-Phase CNT Composite

Referring to Table 1(a), For simplicity, modelling CNT composites began by representing a single CNT fibre that was surrounded by a matrix with the CNT-matrix bonding assumed to be perfect. This approach is expected to give results that is comparable to those from ROM because of their similar assumptions.

3.1 Predicting the Effective Properties

Using this approach, Liu and Chen [18] applied a quarter-scale continuum model to represent the CNT and the matrix. Here, a square RVE consisting of a matrix and a short SWCNT, both represented as continuum elements with assumed dimensions of the CNT continuum and stiffness ratio of $E_{cnt}/E_m = 10$, was analyzed using FEM to determine the RVE's load transfer capability.

The results from both FEM and boundary element (BEM) methods corresponded well. Furthering this study, investigations were conducted to predict the four transversely isotropic effective properties (longitudinal modulus, E_z , transverse modulus $E_x = E_y$, ν_{xy} and Poisson's ratio, $\nu_{zx} = \nu_{yz}$ of long and short CNT composites using a cylindrical RVE [19], square RVE [20] and hexagonal RVE [21] while applying three loading cases of axial stretch, lateral uniform load and torsional load. In all cases, derivations were made to determine formulae for the effective properties.

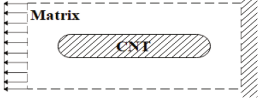
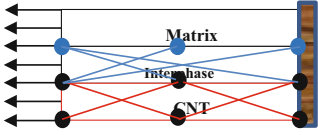
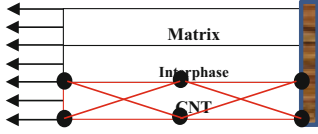
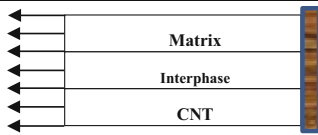
Comparing the results of the three RVEs, the hexagonal RVE was found to give results close to those of the cylindrical. The use of cylindrical RVE has been preferred by researchers [22] since CNTs with various radius can be easily modelled especially in a form of concentric cylinder [23]. The results of the effective properties showed the substantial contribution provided by the CNT to the nanocomposites.

3.2 The Effect of CNT Characteristics

Several researchers studied the influences of factors on the CNTC properties: CNT waviness [24], pinhole defects [25] and CNT orientation [26]. With the global periodicity assumption, the fibre-matrix bonding was assumed to be perfect and formulae for the effective property were derived.

The Effect of CNT Waviness. In reality, due to the vdW interactions along with electrostatic forces, CNTs are typically curled, agglomerated and aggregated [27]. Through a micromechanical modelling [24] and continuum modelling of the two-phase CNTC

Table 1. The categories of nanocomposite continuum models.

Types	Model	Descriptions
(a) No interphase		Both CNT and matrix are continuum elements
(b) A-A-C model		CNT and interphase are represented at the atomic scale while matrix is taken as solid continuum.
(c) A-C-C model		CNT in atomic scale but the interphase and matrix are in solid continua.
(d) C-C-C model		All constituents are modelled as continua

[28], the increase in the CNT waviness ratio ($w = a/L$) has significantly decreased the E_z and the ultimate strength of the CNT composite. The influence of CNT waviness was even more significant when completely randomly oriented CNTs with different waviness were applied [28]. In the analytical work of Stein and Wardle [29], a simulation framework that was capable of analysing 105 CNTs with realistic morphologies and waviness ratio, w , it was shown that the waviness was responsible for the huge over-prediction of the CNT composite elastic modulus and as such results from experiment [30] can be reproduced.

The Effect of CNT Defects. Several defects in the CNT atomic network may be developed during the growth and purification of CNT, the irradiation process with energetic particles [31] and the functionalization process [32]. A process of adding a small organic group to the nanotube sidewall [33] may be conducted to upgrade the vdW interactions into the matrix–CNT covalent bonds [34]. In this process however, the strong chemical bonding and the formation of SP3 hybridised sites may cause defects such as the pinhole defect. A research was conducted on the influence of pinhole defects on the effective properties of the CNTC by applying a continuum representation for both the CNT and the matrix [25]. A single long and short CNT were modelled as a hollow cylindrical continuum with added pinholes and waviness. Two types of pinholes with diameter 0.4 nm and 0.8 nm were placed on the CNT in z -direction at equal gaps. It was discovered that even a waviness or a pinhole defect has immensely modified the overall properties of the CNT composites. A square RVE representing a perfectly bonded CNT-matrix interphase was used [35] to study the effect of CNT fibre breakages on the redistribution of stress at

the broken CNT location. The RVE was given a strain and a nonlinear behaviour of the CNT was incorporated into the analysis. It was determined that the ineffective length of the defective CNT was 28% for the CNT/Epoxy composite and only 3% CNT/Titanium composite.

The Effect of CNT Direction. The fully continuum two-phase model was used to determine the influence of the orientation of a single CNT on the axial and lateral modulus [26]. It was found that the higher the angle of inclination of the CNT angle the lower the effective axial and lateral modulus. The orientation effect was, however, reduced if the waviness factor was included. In a work by Moghaddam et al. [36], the consequence of the high CNT inclination angle that decreased the properties was insignificant as the angle reaches 60° , 30° and 15° for the axial modulus, Poisson's ratio and the transverse elastic modulus, respectively. The role of limiting certain effects of a CNT at a certain CNT angle of orientation was also discovered by Huang and Rodrigue [37] where at a 30° angle of orientation and volume fractions (VF s) greater than 0.74%, the stresses (tensile and shear) can no longer be influenced.

4 The Continuum Approach in Multiscale Modelling with interphase

In multiscale continuum modelling, CNT composites are represented in a form of RVE comprising the CNT, the matrix and the CNT-matrix interphase. Here, the models are given names based on the phases of the RVE's constituents, as given in Table 1. The major contribution of this modelling is the use of the vdW forces within the interaction between the CNT and matrix. However, only composites with one CNT fibre contained by the interphase and matrix are considered, thus exposing the weakness of this modelling that may consider the nanoscale level only.

4.1 The A-A-C model

The benefit of the A-A-C model is the CNT lattice structure is kept even though the model of the matrix is simplified to a continuum [38]. Several researchers have investigated the A-A-C model of the CNTC that vary mainly in terms of their modelling of the interphase between CNT and matrix. The effects of several CNT characteristics and the non-linearity assumption of the model were also considered.

Modelling Truss Rods as the Interphase. Li and Chou [39] used the multiscale modelling approach to determine the CNT-matrix load transfer within a nanocomposite loaded with a compressive load before the buckling behaviour of this nanocomposite was studied. Using a cylindrical RVE, both continuous and short CNT fibres were considered. Applying FEM, the CNTs were represented as nodes (carbon atoms) connected by beam elements (covalent bonds) whereas the epoxy matrix was represented as a continuum. The CNT-matrix interphase that was characterized by vdW interactions was represented as truss rods that connected the carbon atoms and the inner surface nodes of the matrix continuum, as shown in Fig. 3. The properties of the rods, representing the

vdW low level CNT-matrix interactions were determined based on the “6–12” potential of Lennard-Jones. The longitudinal modulus was determined to match well with the ROM’s result.

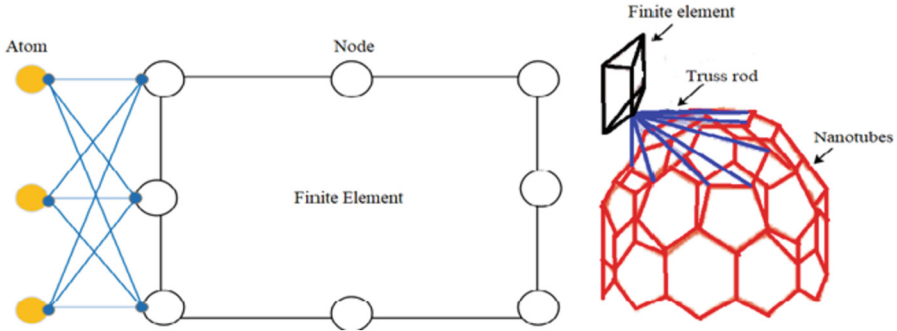


Fig. 3. The A-C-C model: (a) the lateral surface and (b) the end cap region of the nanotube [39]

Modelling Beams as the Interphase. Joshi et al. [40] used the A-A-C multiscale model to examine the effect of CNT chirality on the stiffness of the CNTs. In contrast to [39], the interfacial region was characterized discretely by beam elements that connected the atoms of the nanotubes radially with the corresponding nodes at the inner cylindrical surface of the matrix. Various parametric studies were conducted including the effect stiffness, tensile strength and chirality of the CNT on the mechanical behaviour of the CNTs. The results for the elastic and shear moduli were found to agree closely with those of the ROM. The same A-A-C model was applied to investigate the influences of chiral angle, vacancy defect locations and number of vacancy defects on the elastic properties and strength of the nanocomposites subjected to axial loading [41]. As the CNT was modelled in atomic form, the modification of the CNT atomic structure was done by omitting 1 atom and 3 bonds for a single vacancy representation. It was found that the nanocomposite strength increased as the chiral angle increased while the maximum stress of the nanocomposites decreased as the location of the vacancy defect was moved away from the fixed point of the RVE. Furthermore, it was found that even a single vacancy can highly influence the Young’s modulus of the CNT composites.

Modelling Spring Elements as the Interphase. Applying the A-A-C multiscale modelling Method, Shokrieh and Rafiee [42] used ANSYS software to simulate a cylindrical RVE that predicted the effective elastic properties of a CNT. Referring to Fig. 4, a SWCNT was represented at the atomic level where carbon atoms were treated as nodes and the strong bonds between them were represented by Timoshenko beam elements. The interphase region was modelled using the Combin39 non-linear spring elements of ANSYS software to represent vdW interactions. The non-linear characteristic behaviour of the spring elements was according to the Lennard-Jones “6–12” [43]. Three load cases were given to the RVE in a process to determine the longitudinal, shear and transverse moduli. It was found that the RVE exhibited highly non-linear behaviour under tensile load. The longitudinal elastic modulus was shown to recover if the length of the CNT

was between 100nm and 10 μ m. The results show that the CNT and the interphase can be considered as having comparable properties to a long fibre as the results followed the trend in Odegard et al. [44].

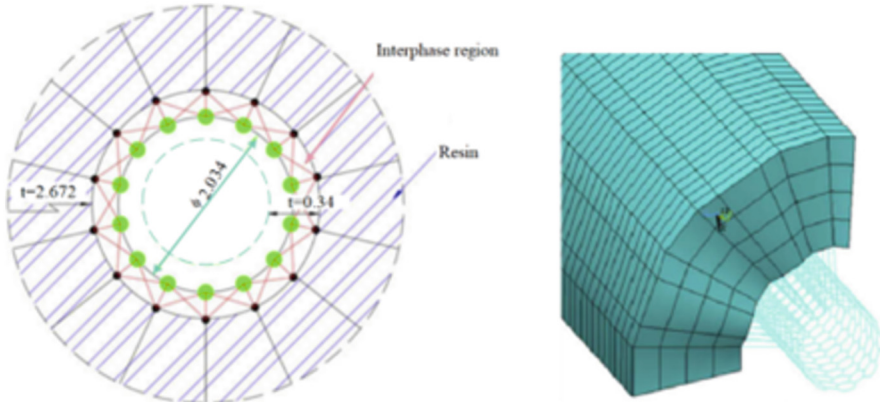


Fig. 4. (a) The schematic view of the CNT composite, (b) the cut section of the real FEM model [42]

Modelling Joint Elements or Links as the Interphase. A new method of representing the interfacial region was to treat it as a heterogeneous region that was constructed in a discrete manner by bringing together joint elements of varying stiffness [45]. While the CNT was represented at the atomic level using spring-based elements to represent the covalent bonds, the matrix was treated as an isotropic continuum. With this multiscale model, studies were conducted on the various stress-transfer characteristics of the CNTC in the RVE. When the interfacial region was tested with different values of stiffness, the normalized stiffness of the CNTC provided the meaningful influence of the interfacial stiffness on the elastic characteristics of the CNTC. The study also found that the transfer of stress was influenced by the atomic microstructure, VF of CNT and the E of the interphase region.

4.2 The A-C-C Model

An RVE such as shown in Fig. 5 was used to examine the influence of interphase thickness (t_{if}) and stiffness on the transfer of stress and the E_{eff} of CNT composites [16]. The SWCNT was represented based on an atomic molecular structural mechanical approach in which the covalent bond was treated as a Timoshenko beam. Being a continuum, the interface and matrix were modelled using brick elements while it was assumed that CNT-matrix stress transfer occurred fully. The 3-phase RVE was validated using past experimental results and the results from a CNT composite model without the interphase. It was found that both results using the fully continuum approach were in close agreement. However, the results for the 3-phase model with interphase were found

to give higher values than the experimental values for the SWCNT-polymer composite due to the presence of stress concentration regions as a consequence to the weak boundary layer in the interphase region.

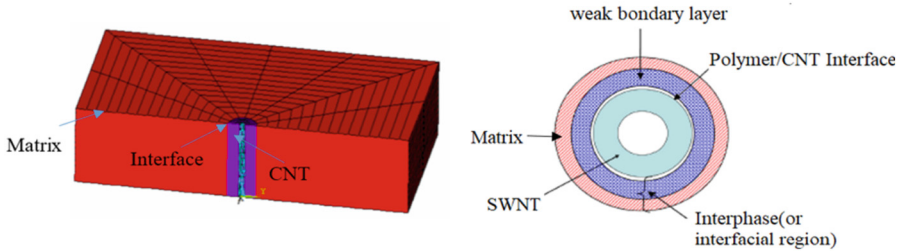


Fig. 5. (a) The RVE of the A-C-C model (b) The cross-section of the RVE [72]

4.3 The C-C-C Model

Several researchers have considered continuum modelling for all three phases of the CNT composites. The difference between these models was on how the properties and thickness for the interphase continuum were assumed or determined. As stressed by Zuberi and Esat [22], both mechanical properties and thickness of the interphase have not been reported yet, experimentally. As such, the difference in the results on the significance of the interphase on the CNTC's effective properties is expected.

Interphase Property as a Ratio-to-Matrix Property. Wan et al. [17] applied a full three-phase continuum model to conduct a numerical study on the effect of CNT dimension and the CNT-matrix interphase on effective moduli of the CNT composite. The CNT and the matrix were treated as a continuum while the interphase was a homogeneous continuum of the same width as the CNT and assumed to have hard stiffness ($E_{int} = 10 E_{matrix}$) or soft stiffness ($E_{int} = 0.3 E_{matrix}$). It was found that the effect of CNT length was significant in ensuring the occurrence of full load transfer and that the critical length of the CNT for this study was 271nm. The effect of the interface was found to be only slightly so for the effective properties. Similar effect was found by Ayatollahi et al. [46] that used an equivalent cylindrical beam element to represent CNT such that the nonlinear properties of the SWCNT was described using the beam elements. Golestanian and Shojaie [47] assumed the E of the interphase as 3.2 GPa and 100 GPa where the Young's modulus of the matrix was given values between 3.2 GPa and 100 GPa. The study revealed that for the interphase models, the effect of the interphase on the E_{eff} was significant only for low-modulus polymers. Zuberi and Esat [22] researched the influences of CNT diameters and chirality on the E_z and Poisson's ratio of CNTCs by applying a RVE with the C-C-C model. The E of the interphase was assumed to be 20GPa while the interphase thickness was 3 times the CNT thickness. The armchair RVEs gave the highest values of the E_z and ν followed by the chiral and zig-zag RVEs.

Gradient Functions of the Interphase Properties. In a study by Perez and Aviles [48], a cylindrical RVE consisting of CNT, matrix and an interphase was applied to determine

the influence of the interphase on the effective properties. All three phases were modelled as continuum with transversely isotropic material properties. Specifically, the interphase parameters considered were thickness and varying E across the interphase's thickness. The study showed that the CNT-to-matrix modulus ratio and thickness have significant effects on the properties of the CNTCs.

Molecular Dynamic Approach to Determine the Interphase Properties. A study by Guru et al. [49] combined the MD and FEM approaches to investigate the CNTC's constituent properties. The CNT was modelled as a space frame structure and the E of the covalent bond was calculated based on the modified Morse potential [50]. The MD method was used to predict the E of the matrix functionalized with a DETA curing agent. The modulus and thickness of the interphase were 18 GPa and 0.3 nm respectively, estimated through the MD method. Nonetheless, in the C-C-C modelling study using ANSYS software, the modulus and thickness of the interphase were simply varied. It was found that the effect of the E of the interphase on the E_z of the CNTC was substantial.

The Interphase Cohesive Law of Interphase Properties. Focusing on the effect of the CNT-matrix interfacial shear strength (ISS) on the ultimate strength of a CNT composite, Mohammadpour and Awang [51] conducted tensile tests using ANSYS on a multiscale cylindrical RVE with an interphase layer. The CNT-matrix non-bonded interaction that was based on the interphase cohesive law was characterized by the vdW force such that if the shear stress is above the ISS, the interface has failed at that specific element. The material nonlinearity of matrix was modelled using the multilinear isotropic hardening material model. The results in Fig. 6 shows that strong ISS gave good upgrading in the elastic behaviour of the CNTCs.

The Effect of Functionalization and Defects of CNTs. Rafiee and Pourazizi [38] conducted studies at micro level on the influence of functionalized CNT on the E of the CNT composites. Two types of interphase regions were used and compared. In the first type, the A-A-C model of CNT with C-C covalent bonds and the CNT-matrix vdW interactions were applied. The results was the functionalization reduced the E of the RVE. The contribution of the functionalization in improving the mechanical properties of the CNT composites will occur at the mesoscale. The combined improving and decreasing effects of the functionalization of CNT on the effective properties of nanocomposites were studied by Esbati and Irani [52] The studies considered six RVEs having parameters such as the non-linear behaviour of the CNT, nonlinear vdW interactions, nonlinear covalent bonds, structural defects and fractures in the matrix. The RVEs may also differ in length, chiral indices and interphase regions. In each case, a cylindrical RVE was used, applying the nonlinear FEM in ANSYS software. As in the study by Rafiee and Pourazizi [38], two types of interphases were considered. The study found that the RVEs containing functionalized CNTs provided a better representation of the mechanical properties compared to the RVEs with normal CNTs.

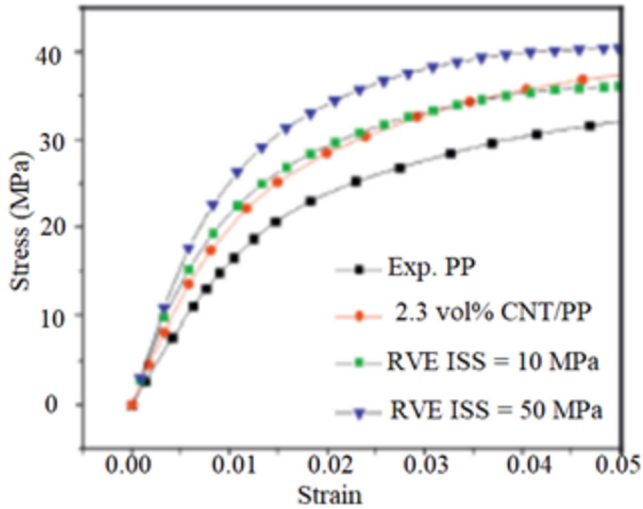


Fig. 6. The tensile test of CNT composites [51]

5 The Mesoscale Modelling of CNT Composites

The models previously discussed considered only one CNT fibre surrounded by a matrix. CNT characteristics such as length, chirality, orientation and defects were considered, all at nano- to micro-scales. To provide modelling closer to the real CNT composite at the macroscale, a representation of the nanocomposite should consider other characteristics of the CNT such as random orientation and agglomerations that can be seen at the mesoscale, as described in Fig. 2. It is known that CNT dispersion problems within the matrix have resulted in a random distribution of CNT and, due to high CNT length-to-diameter ratios and relatively strong intermolecular vdW interactions, there is a tendency for CNT to form bundles that later aggregate into agglomerates. To model a CNT composite with better accuracy, CNT-composite representations should consider CNT characteristics at all nano-, micro-, meso- and macro-scales. This is a big modelling problem as it involves a huge scale difference between nano- and macro-scales. Some of the meso- and macro-scale modelling described below can be referred in the diagrams in Table 2.

5.1 The Effect of CNT Randomness

In modelling the macroscopic properties of CNTCs, Afroos et al. [53] established the effect of short CNT fibre randomness on the elastic characteristics of the nanocomposites. CNT fibres were estimated as effective cylindrical fibres, represented by a 3D truss element applied in the MSC-Marc FEM software.

The RVE is divided into several hexagonal elements and randomness was considered to increase as the number of nodes was increased. Up to 15 RVEs representing 0%, 2.5%, 5% and 10.48% of CNT were used. The study found that the increase in randomness

of the CNT fibres will decrease the axial modulus and the ultimate strength of the CNT nanocomposite.

Improving this study while continuing to use the parallel CNT fibres that experienced perfect bonding with matrix, Makvandi and Öchsner [54] considered CNT fibre positions that were overlapping one another and also CNT fibres that were joined at nodes to become long fibres. The results indicated that the E of the CNTC was significantly influenced by the CNT positions whether they are completely separated, overlapped, or sharing the same nodes.

Tserpes and Chanteli [55] estimated the linear characteristics of the CNT composite at micro/mesoscales utilizing their earlier work on homogenizing the elastic properties at the nanoscale. A composite of a polystyrene matrix with randomly-aligned CNTs was modelled with specimen dimensions reaching macroscale level. The dimensions of the CNTs and how they were distributed were obtained from experimental observations [56]. Assuming uniform dispersion, all elements of the CNT composites were treated as RVE and a pseudorandom function was used to match specific orientations and elements. The tensile modulus predicted for the polystyrene matrix reinforced with randomly aligned CNT was found to agree excellently with the experimental data. Furthermore, CNT orientation has a substantial effect on the elastic stiffness where the tensile modulus diminished for angles of orientation greater than 45° .

5.2 The Effect of CNT Agglomerations

A cylindrical RVE containing CNTs, matrix and their interphase was modelled to represent the CNT composite, giving the effective fibre (EF) characteristics of the CNT composite at nanoscale [57]. Using Cauchy–Born rule, the Lennard–Jones was associated with the Park–Paulino–Roesler potential to represent the CNT–epoxy interphase. In the so-called two-scale approach, the EFs were then dispersed into the matrix randomly to numerically create another micro-scale, EF–matrix RVE using the Python script in the ABACUS. Effective properties of this RVE at the micro-scale were determined with and without considering the effect of agglomerations. The agglomerations were created by clustering half of the CNT RVE into 1, 2 and 4 colonies. The numerical and experimental results were discovered to match the experimental results after considering the agglomeration effects at microscale.

In a study by Chanteli and Tserpes [58], a cubic RVE with CNT agglomerates surrounded by matrix was modelled using ANSYS software. Scanning electron microscopy (SEM) images were applied to provide the parameters for the agglomerates. The average diameter of the CNT was found to be 29 nm while the mean length was 210 nm. The study found the opposite effect of agglomeration and waviness where the increase of CNT agglomeration decreased the elastic properties while the increase of waviness increased the linear properties.

Bhuiyan et al. [59] integrated experimental and FEA to study the influence of four CNT characteristics: random dissemination, bundle formation, waviness and orientation with respect to the loading. In the FEA studies, 3D RVEs were applied consisting of multiple equivalent solid CNTs [60], polypropylene and the interphase. The C–C–C model was used. Random coordinates were given for the centre of mass of the CNT while the CNT orientations were modelled based on an angle θ with respect to the

direction of longitudinal loading (x) and an angle ϕ with respect to a defined ($x-z$) plane. The thickness and stiffness of the interphase were determined from the experiment conducted using atomic force microscopy (AFM) which gave the average values of the interphase thickness and modulus as 20 nm and 0.7 GPa respectively. Further, the AFM was applied to describe the tensile modulus, the size of the CNT agglomerates and the CNT distribution used in the FEA. The diameters of agglomerates comprising 3, 7 and 19 CNT were determined as 40, 65 and 100 nm respectively while Young's modulus values were 35, 30 and 12 GPa respectively. The FEA showed that the effective aspect ratio of the CNT was $L/D = 65$. Two leading factors working against the great potential of the CNT nanocomposites (see Fig. 7) were found to be CNT agglomeration and waviness. The FEA results from applying the experimentally-obtained data were found to agree excellently with experimental results.

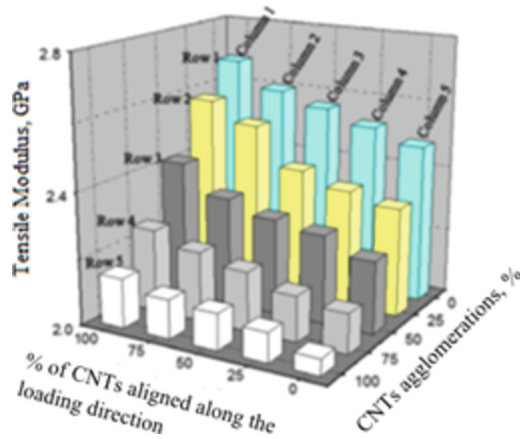


Fig. 7. The effect of CNT alignment and agglomeration on the tensile modulus of CNT composite [60]

5.3 The Stochastic Modelling of CNT Composites

In novel research by Shokrieh and Rafiee [11], a hierarchical, multi-scale, modelling technique called N3M was established to study the effective characteristics of CNTCs. Referring to Fig. 8, the approach used a stochastic modelling procedure with a different RVE applied each at the nano-, micro-, meso- and macro-scales where random parameters of length and interphase (nano), orientation, agglomeration, curvature (meso) and dispersion of CNT (macro) were considered.

At nanoscale, a composite consisting of a CNT fibre, the matrix and their interphase was modelled to give an EF. EFs with different lengths were distributed randomly within a matrix to become another RVE at microscale. At macroscale, the bulk CNT composite was divided into several blocks using a regular tessellation technique where each block was an RVE at mesoscale that consisted of several spherical agglomerated CNTs and fully-dispersed CNTs. The properties of each block at mesoscale were calculated using

an improved micromechanical model and the overall properties at macroscale were calculated using an averaging method. The results of the elastic stiffness and Poisson's ratio were determined and agreed excellently with past experimental results. Improvements were made to the N3M model [11] by Rafiee and Firouzbakht [61] who now used an irregular tessellation technique that considered the local position of each aggregate of CNT. The irregular tessellation was used to divide the RVE at mesoscale into heterogeneous polygons based on an irregular pattern provided by the Bayes classification algorithm combined with the Voronoi approach. The new method gave results that agree well with the findings of the N3M model and the experimental observations.

In a different approach without considering CNT-matrix interphase, the hierarchical multiscale modelling of CNT composites was used to study the influence of weight fraction of the CNTs and ISS based on sensitivity analysis on the damping characteristics of the CNTCs. Savvas et al. [62] used the space frame structure to model the CNTs that was later converted to EBE, the equivalent beam element (EBE) of the CNT. Applying the FEM, this EBE at nano-scale was used as the basic micro-scale building block for the construction of full length CNTs covering several EBEs embedded in the polymer. While the EBEs were assumed to behave linearly, the polymer, modelled as continuum was equipped with viscoelastic behavior applying the Maxwell–Wiechert material model. Without considering the interphase region, a nonlinear bond-slip friction-type model was used to represent the interfacial load transfer mechanism between the CNT and the matrix. While the straight CNTs can be considered easily, the average properties of wavy CNTs were determined using stochastic Monte Carlo simulation. The study showed the importance of a successful functionalization process that gives an increased ISS to achieve optimum damping characteristics. Furthermore, to improve damping properties of the CNTCs, it is crucial that CNTs are made to be straight. The results here were quite close to those of [63].

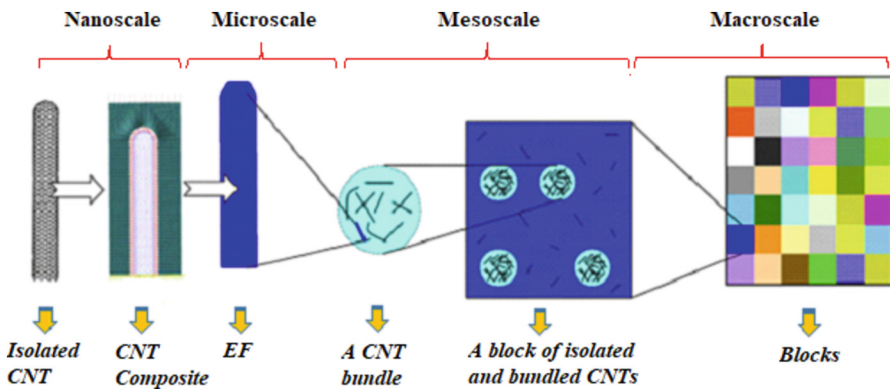


Fig. 8. Steps in hierarchical multi-scale modelling [11]

5.4 The Multiscale Modelling with Fuzzy CNT-Matrix

The difficulties to get the expected properties even after great deals of studies conducted on modelling of the CNT composites due to the agglomeration of CNTs, among others in the manufacturing process of the CNTs have led to attempt to grow CNTs directly on the fibre surface [64], a procedure that was found to be advantageous [65].

In the study by Kundalwal and Ray [64], the implementation of the radially grown CNT on carbon fibre surfaces or better known as fuzzy fibre [66] that can be assumed as transversely isotropic was proven to significantly improve the transverse effective properties of the fuzzy fiber-reinforced composite (FFRC). Applying the micromechanics model, two methods of cell approach and FEM were used to determine the effective properties of the nano composites.

A study [67] was conducted to toughen the interfacial fiber-matrix region with carbon nanostructures (CNS) while considering the effect of the orientation of the CNS. A multiscale micromechanical model consisted of the simplified unit cell (SUC) and Eshelby methods were used in finding the effective elastic modulus properties of FFRC [68]. For accurate property prediction with respect to experimental values, the study revealed that CNT should be characterised as wavy, randomly distributed, behaving in transversely isotropic manner and having interphase region with the matrix. The study found that the improvement of longitudinal modulus can be neglected while the transverse modulus was found to improve significantly.

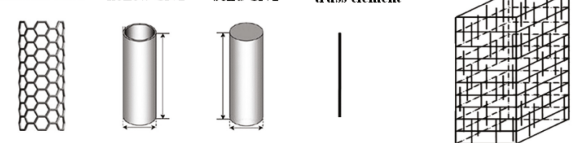
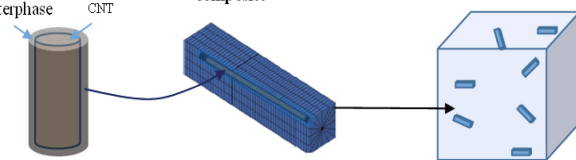

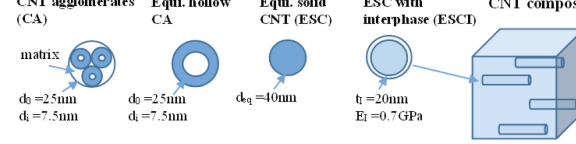
In a study by Rafiee and Ghorbanhosseini [69], Young's modulus of unidirectional FFRP having radially aligned CNTs on the surface of the core fiber was theoretically predicted following their previous work of bottom-up modelling CNT composites [11] that covers the four nano-, micro-, meso- and macro-scale. While the Young's modulus of the FFRP was determined using the deterministic modelling, the Monte-Carlo simulation technique for stochastic modelling was employed as the effects of CNT curvature and VF were considered as random variables. The results showed a very closed agreement with the experimental findings from Kulkarni et al. [70].

6 Concluding Remarks and Future Perspectives

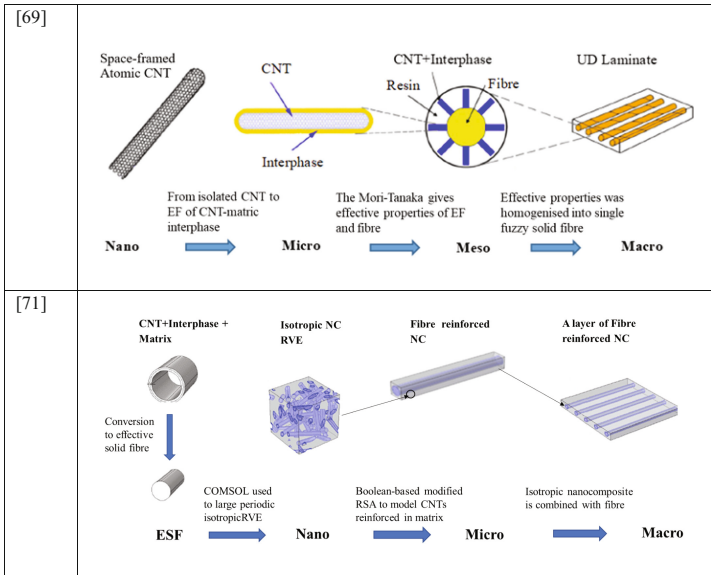
It had been expected that CNTs would improve mechanical properties of CNTCs but experimental researches have shown that CNT provided improvements that are much lower than those predicted by the ROM. This paper reviews the progress of FEM-applied continuum representation of CNTCs over the last two decades as the most suitable method of analysis in predicting close-to-reality values of effective properties of CNT nanocomposites. The journey of this continuum modelling has gone through several stages:

1. It started with the 2-phase continuum representation with an assumption of perfect bonding between the phases. Hence, the results are similar to the results of the ROM, as expected. Here, the linkage between the nanoscale and the upper scales in the form of an interphase was neglected.

Table 2. CNT composite modelling: from nana to macro

Ref	Modelling of Marco-scale CNT composites
[53]	<p>Space-framed Atomic CNT An equivalent hollow CNT An equivalent solid CNT A CNT FEM truss element CNT composite</p>  <p><i>Representing a space-framed CNT as a truss element</i></p> <p><i>Randomized CNTs into matrix for tensile test</i></p> <p>Nano → Nano → Macro</p>
[55]	<p>CNT with interphase RVE of a MWCNT composite CNT composite</p>  <p><i>Forming an RVE with a CNT with interphase</i></p> <p><i>Dispersing RVE randomly into matrix for tensile test</i></p> <p>Nano → Micro → Macro</p>
[57]	<p>Equivalent Fibre CNT composite</p>  <p><i>Homogenization of randomly oriented and agglomerated (clustered) CNTs for tensile test</i></p> <p>Nano → Macro</p>
[60]	<p>CNT agglomerates (CA) Equi. hollow CA Equi. solid CNT (ESC) ESC with interphase (ESCI) CNT composite</p>  <p>$d_b = 2.5\text{nm}$ $d_i = 7.5\text{nm}$</p> <p>$d_b = 2.5\text{nm}$ $d_i = 7.5\text{nm}$</p> <p>$d_s = 40\text{nm}$</p> <p>$t = 20\text{nm}$ $E_i = 0.7\text{GPa}$</p> <p><i>Representing agglomerated CNTs as ESCI applying data from AFM</i></p> <p><i>Dispersing randomly oriented ESCI into matrix for tensile test</i></p> <p>Nano → Nano → Macro</p>

(continued)

Table 2. (continued)

- The journey then progressed to considering the CNT-matrix interphase where CNT, matrix and their interphase have been treated in atomic or continuum forms. The nanocomposites have been classified in this paper as the A-A-C, A-C-C and C-C-C models, referring to the atomic (A) or continuum (C) representation of the phases. As in the first stage model, these models merely consisted of a CNT fibre surrounded by matrix and with the assumption of the CNT dispersion being globally symmetrical; the considered RVE can only capture the CNT characteristics as composite fillers at the nano- and micro-scales. As such, even with tackling the scale difference between CNT and matrix in considering the interphase, these representations considered CNT characteristics of length, waviness, orientation and defects only whilst ignoring the important characteristics of CNT randomness and agglomeration which give results close to those of the ROM.
- Several researchers have modelled mesoscale nanocomposites that can capture the randomness and agglomeration of the CNT. By applying the concept of EFs, one method is simply taking an RVE with a greater number of randomized EFs so that the size of the RVE now reached mesoscale. In hierarchical modelling, an RVE has been used at each of the nano-, micro-, meso- and macro-scales where the EF representation of the previous scale can be applied in a random fashion in the next higher scale. The hierarchical representation was proven to give results close to the experimental values.

With mesoscale modelling providing some success, the accurate continuum modelling for CNT nanotubes is closed to giving the full elastic constitutive relations of the CNT nanocomposite. Further, deeper understanding on the main culprit in the reduction

of properties may lead to simpler modelling at nano- or micro-scale that may also provide results that are close to experimental results. For example, the analytical work of Stein and Wardle [41] that used the better representation of waviness to give the elastic properties that were close to experimental values should be emulated in continuum modelling. With these modelling successes, the main task is to improve the CNT characteristics that lead to the failure of the CNTC. The manufacturing process of the CNT composite needs to be improved such that the scattering of CNT within the matrix will be straighter, more uniform and less agglomerated.

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