**This paper is very confusing and requires major input from the two of you. It lack in rigor. Please address the 3 main objective of the work as described by my comments near end of paper. You seem to use bold whenever you feel like it. At the sametime, you using bold to define stress vectors and element stiffness matrices. You cannot use bold to define a diameter D or volume fraction Vf. The figures are very poor and unfit for a scientific paper. Redo!**

**Realistic Modeling of the Complex Morphology of CNT-Reinforced Nanocomposite using Immersed Finite Element**

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**Abstract**

In this article, we overcome the limitations of traditional finite element method (FEM) by providing a more appropriate and computationally efficient approach for treating CNT reinforced nanocomposites. It allows us to discretize each continuum in its most suitable reference frame. Specifically, the focus of our work is in modeling the behavior of nanocomposites containing high volume fractions and complex morphologies of CNTs without applying gross simplifying assumptions and/or costly re-meshing. Our newly devised approach relies on the use of unmatched meshing in an *immersed* FEM type algorithm in which the composite constituents are discritized independently, but simulated as a coupled system. The most important advantage of the newly developed approach is that the polymer can always be discretized as a regular grid, irrespective of the complex nature of the CNT network. In this approach, the fully bonded CNTs and the polymeric matrix strictly obey the equilibrium equations of the system.. The developed modeling approach allowed us to simulate realistic representative volume elements containing randomly dispersed CNTs of different morphologies, curvatures, orientations, aspect ratios and large volume fractions that are 10 times some of the existing efforts in the literature. The newly developed approach is used to determine the effect of CNT waviness and volume fraction on the mechanical properties of a polymeric nanocomposite. Our results are in excellent quantitative agreement with the corresponding reported data in the literature which are based on different simulation platform.

**Keywords:** Immersed finite element method, mechanical properties, CNT, polymer, nanocomposites, morphology.

1. Introduction

Carbon nanotubes (CNTs) have attracted considerable interest due to their remarkable mechanical [1–4], electrical [5–7], and thermal properties [5,8]. These superior properties make CNTs ideal choice as reinforcements and tailoring of properties for multifunctionality [9,10]. As consequence of their importance, intensive attention has been paid by the scientific community to understand their mechanical behavior experimentally [7,11,12], analytically [13–15] and numerically [16–19].

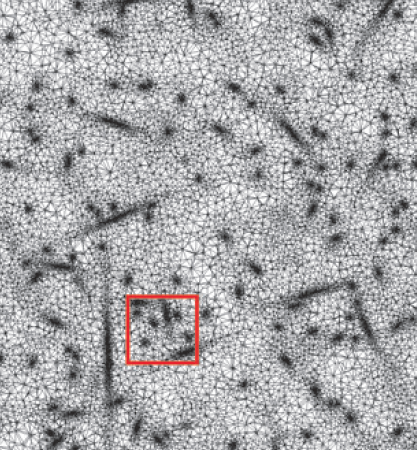
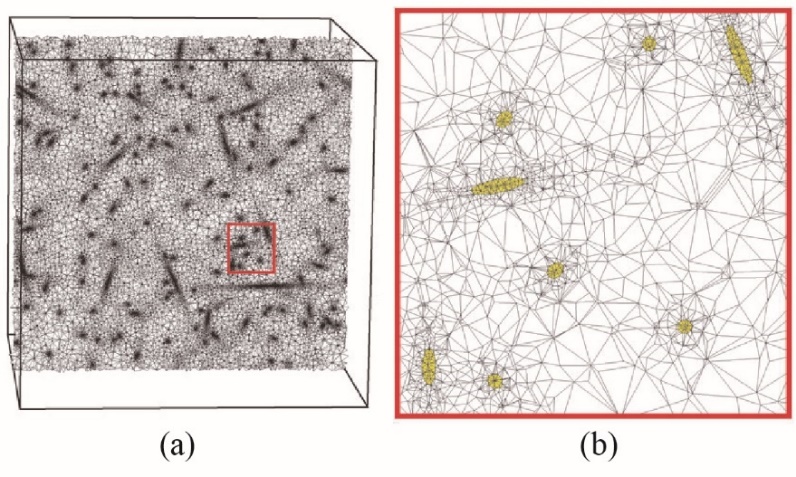
Numerical simulations are widely used in studying the mechanical properties of nanocomposites and a variety of modeling methods are developed for different scales of interest; see, e.g., Refs. [20–23]. Molecular dynamics (MD) is suited for investigating the nanoscale properties [24], where the constitutive relations are governed by interatomic potentials [25]. MD simulations can monitor the details of individual atoms, allowing us to study complex phenomena such as mechanical and interfacial properties of a single nanotube surrounded by a polymeric matrix [25–27], effect of chemical functionalization on the structural stability and strength of CNTs [28,29], and influence of defects on CNT properties [18,30]. Several studies attempted to utilize the increasing computational resources to conduct large atomistic simulations of composite systems [16,31,32]. The main objective was to simulate representative volume elements (RVEs) large enough to capture the atomistic behavior of nanocomposites[16]. However, even with the usage of the most advanced supercomputers, only ~ atoms, i.e. 1000 atoms in each direction, can be simulated; making it unsuitable approach to investigate microscopic composite systems reinforced with nanotubes of larger diameters and aspect ratios [33].

To enlarge the simulation scale, traditional continuum techniques were introduced which neglect the details of its atomic structure. Although the traditional continuum models cannot accurately describe the phenomena at the nanoscale, they are able to provide valuable information concerning the influence of the microscale parameters on the properties of CNT-reinforced composites, such as curvature [34–36], aspect ratio and volume fraction of the dispersed CNTs [37].

Both micromechanics and finite element methods are widely used in modeling the effective bulk properties of nanocomposites at the microscale level [38,39]. For example, Mori-Tanka micromechanical technique [40] has been used extensively in the literature to scale up the nanoscale properties of nanocomposites and evaluate the effect of morphological, dispersion state, and alignment on their overall performance [13,39,41]. However, such analytical techniques suffer from several drawback that result in unrealistic predictions of the properties of the material due to their inherent over-simplifications and limitations concerning problem size (DOF) [16]. For instance, to enable the treatment, very low concentrations (xx%) of CNTs were assumed in these analytical models [42]. Besides, the interactions between the reinforcements were neglected and all nanotubes were assumed to be of the same type, length, size, morphology, agglomerate size, and fully coupled to the matrix [39]. As a consequence, micromechanics models overestimate the properties of the composites and could not model RVEs representing the actual microstructure as imaged by electron microscopy techniques [16].

On the other hand, several research groups used finite element technique to overcome the some of the aforementioned limitations in micromechanics by modeling RVEs reinforced with CNTs [36,38,43,44]. However, due to the enormous computational cost associated with modeling systems containing large number of CNTs, these models were limited to RVEs reinforced with tens of CNTs that have relatively small aspect ratios [38]. Such small number of CNTs accounted for very small volume fractions and narrowed the scope of the investigations. Additionally, the preprocessing part of the analysis relating to the meshing stage is very challenging for larger systems, because the traditional FE method requires both CNTs and the surrounding matrix grids to at least be displacement compatible. For example, Lusti and Gusev [37] created a FE model of straight CNT-reinforced composites by using a complicated three dimensional mesh generator. Considerable efforts are typically applied to create these models but there were still many highly distorted cells which may decrease the accuracy of the results (see Fig. 1(a)). Moreover, the number of degrees of freedom (DOF) is also very large. For example, the volume fraction of CNTs in Fig. 1(a) is only 0.5%, but the composite is meshed with tetrahedral elements. Alian and Meguid [43] also used the traditional FE model to study the electro-mechanical behavior of composites reinforced by straight CNTs, but due to the difficulties in the meshing process, the CNT volume fraction was only limited to 0.3% in their research.

More recently, the “embedded element technique” [36,45] is used to simplify the meshing process (see Fig. 1(b)). The CNTs are meshed as beam elements and their DOF are embedded into the polymer by modifying the stiffness matrix of each polymer element. However, only the kinematic relations between CNT and polymer is considered in this method, while the more important issue; namely, the interacting forces in between are not accounted for. Therefore, the composite system is not in a rigorous equilibrium state and it decreases the accuracy of the results. In summary, unnecessary simplifying assumptions are introduced to overcome the difficulties in the discretization process, leading to a reduction in the accuracy of the simulations.

(a) (b)

**Fig. 1.** FE models of CNT-reinforced composites: (a) the traditional FE technique (from Ref. [37]) and (b) embedded is used for singularities element technique (from Ref. [45]).

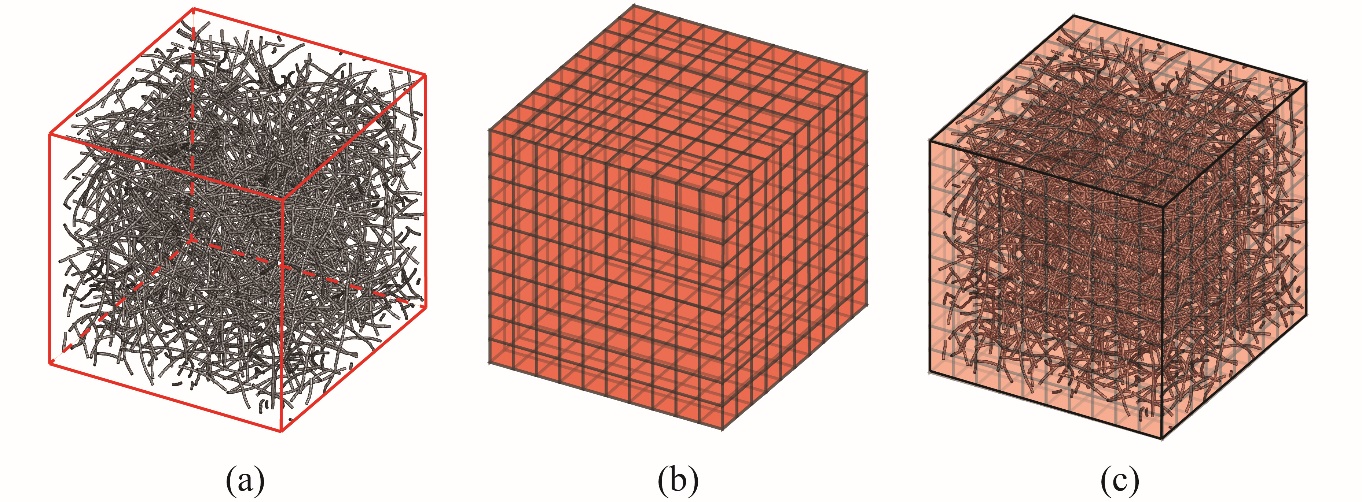
Since Ref. 45 addressed the problem already, why publish this work?

Answer: The previous embedded FE technique over simplified the interaction between CNT and polymers and our new approach addresses this problem.

In this study, we adopt the immersed FE approach that allows the dispersed CNTs and the polymer matrix to be meshed independently but simulated simultaneously as a coupled system. It means that the polymer can be discretized as a regular grid, irrespective of the complex nature of the CNT network. Using the developed technique, we managed to simulate realistic composite systems containing high concentrations of CNTs (3%) of varied complex morphologies. Immersed finite element algorithms assume a fully bonded interface between the randomly distributed nanotubes and the surrounding matrix. Unlike the previous embedded finite element approach, which represents the CNTs by beam elements and only embeds the DOF of the CNTs, our immersed finite element model uses 3D elements to represent the CNTs of a fully equiliberated system. Therefore, both kinematic and kinetic relations between the composite constituents are considered in the newly proposed immersed FE algorithm. The developed method is validated by comparing its results for different cases with those obtained with the traditional finite element simulations and then used to investigate the effect of volume fraction and waviness of CNTs on the mechanical properties of epoxy-based nanocomposites.

1. Immersed finite element modeling procedure

An immersed FE modeling scheme was developed in three consecutive steps, as shown in Fig. 2. A Monte Carlo based algorithm was developed to create RVEs reinforced with randomly dispersed CNTs (see Fig. 2(a)). The polymer cubic cell was then discretized with a regular grid, as shown in Fig. 2(b). The elements representing the CNTs network were then immersed into the polymer grid, as illustrated in Fig. 2(c). This procedure avoids the meshing step in traditional FE modeling that require matching nodes along the constituents’ interfaces. This allows us to create complex two-phased composite models, irrespective of their complexity. The basic concept, assumptions, governing equations and the solution scheme of the immersed Finite Element are presented in the subsequent subsections.



**Fig. 2.** Modeling steps of the immersed FE method: (a) Create the CNT network by the Monte Carlo based algorithm. (b) Create the regular polymer grid and (c) immerse the CNT network into the polymer grid

* 1. Basic assumptions and governing equations

The polymer and the CNTs considered in the study are meshed independently using 8-node hexahedral elements that are not matching at the CNT-polymer interface. The basic assumption is that the polymer and CNTs are fully bonded, thus ensuring a compatible system. This assumption is widely used in continuum models [34,37,43,46], although the matrix and the CNT are actually bonded at the atomic scale with a relatively weak van der Waal's (vdW) forces [39]. This approximation of the interface leads to an overestimate of the material properties [47], especially at higher strain levels. However, it is also reasonable to consider a fully bonded coupling for small deformation where the stress in matrix can be fully transferred to the embedded nanotubes [48].

In the immersed FE model, the CNTs' grid is not matched with the polymer grid. To specifically consider the interaction between CNTs and polymer, the “displacement gathering” and “force scattering” process are introduced. Fig.3(a) shows the “displacement gathering” process. Since the CNT and polymer are fully bonded, the displacement of the nodes on the CNTs’ surface, namely node *A* and *B* in Fig.3(a), is gathered from the surrounding polymer nodes. Fig.3(b) is the “force scattering” process. The brown arrows are forces that the polymer applies on the CNT surface nodes *A* and *B*. According to Newton’s third law, the forces that node *A* and *B* applies on polymer are the opposite, namely the green arrows in Fig.3(b). However, because nodes *A* and *B* are not coincident with any polymer node, should be scattered to the surrounding polymer nodes when creating the equilibrium equation of polymer, namely the yellow arrows in Fig.3(b).

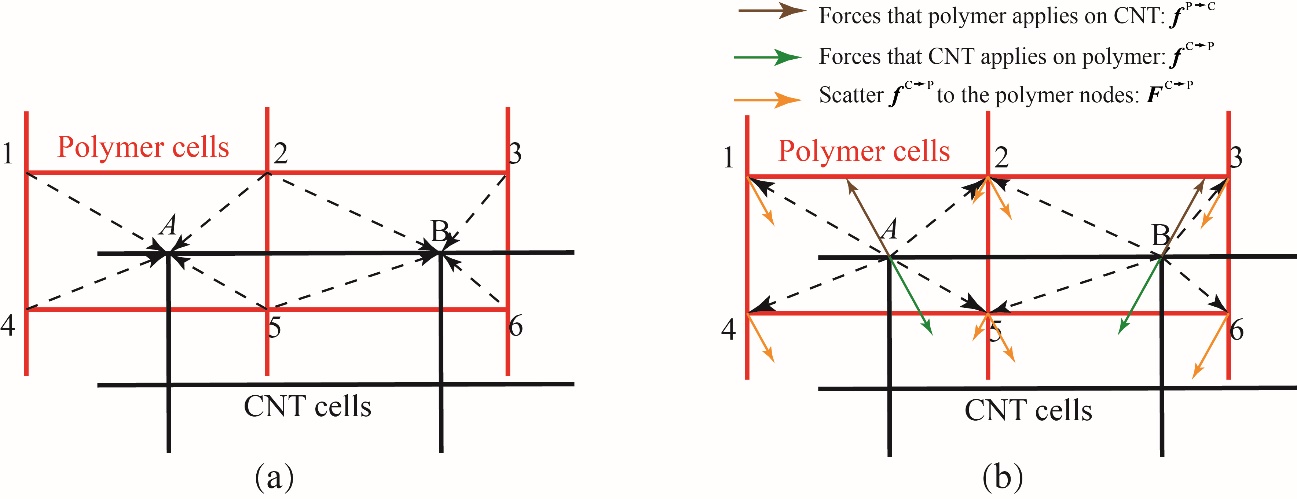


Fig.3. The “displacement gathering” process (a) and the “force scattering” process (b) to couple the non-matched CNT and polymer grid.

The equilibrium equations of CNTs and polymer can be derived from the “displacement gathering” and “force scattering” process, respectively. Denote the DOFs of polymer as and the DOFs of *i*th CNT as . can be divided into and , where is the DOFs of the surface nodes and is the DOFs of the other nodes inside *i*th CNT. The size of is and the size of is . In the “displacement gathering” process, is calculated from as:

(1)

where is the contribution of the *k*th polymer DOF to the *j*th component in . The superscript “d” means is used in the “displacement gathering” process. Equation (1) can be rewritten in the following matrix form:

(2)

where is the displacement gathering matrix of the *i*th CNT with dimension .

When considering the equilibrium equation of *i*th CNT, is regarded as constrained DOFs because it is calculated from . Accordingly, once is obtained, the equilibrium of *i*th CNT is also determined as:

(3)

is the stiffness matrix of *i*th CNT and it can be rearranged into sub-matrices associated with the active DOFs and constrained DOFs. The superscripts “II”, “IB”, “BI” and “BB” in the middle term represent the components related to active and constrained DOFs. is the reacting force on the CNT surface which equals to the force that polymer applies on *i*th CNT, namely the xxx in Fig.xxx(b). can be explicitly calculated from Equation (3) as

(4)

where must be a positive definite matrix due the conservation of energy. Equilibrium necessitates that the force that the *i*th CNT applies on the polymer is:

(5)

which corresponds to the xxx in Fig.xxx(b).

The equilibrium equation of polymer can be derived from the “force scattering” process. As shown in Fig.xxx(b), should be scattered to the polymer nodes and the scattered can be calculated as:

(6)

where is the total force from *i*th CNT that applies on the *k*th DOF of polymer and is the contribution of the *j*th component of to . Equation (6) can also be rewritten to a matrix form as:

(7)

where is the force scattering matrix of *i*th CNT with dimension . Accordingly, the equilibrium equation of the polymer can be expressed as:

(8)

By substituting Equation (2) and (5) into Equation (7), can be expressed as:

(9)

In this study, shape functions of the 8-node hexahedral element are used in the “displacement gathering” and “force scattering” processes, namely

(10)

where is the shape function of the node related to *j*th DOF of polymer and is the coordinate of the CNT node related to *k*th DOF in . Accordingly, , and equation (9) can be rewritten as:

(11)

where is a positive semidefinite matrix. Finally, substituting equation (11) into equation (8) gives,

(12)

where is the total stiffness matrix of the nanocomposite which contains the original stiffness from the polymer, , and the reinforced stiffness from the CNTs, .

It should be mentioned that matrix implicitly contains the equilibrium equation of CNTs and the interaction force between CNTs and polymer, so the solution of Equation (12) guarantees that both CNTs and polymer are in equilibrium state and the interaction forces in between are compatible.

Dividing into the active DOFs and the constrained DOFs, equation (12) changes to,

(13)

and can be obtained from the following equation:

(14)

It should be mentioned that is a positive definite matrix, but is a positive semidefinite matrix, so the coefficient matrix of equation (14) is also a positive definite matrix.

* 1. Solution scheme

Although equation (14) is a linear equation, it is almost impossible to calculate the coefficient matrix directly because the expressions and are very complicated. Note that and can be easily obtained from Equation (4), (5) and (7), so the conjugate gradient (CG) iteration is an appropriate approach to solve equation (14).

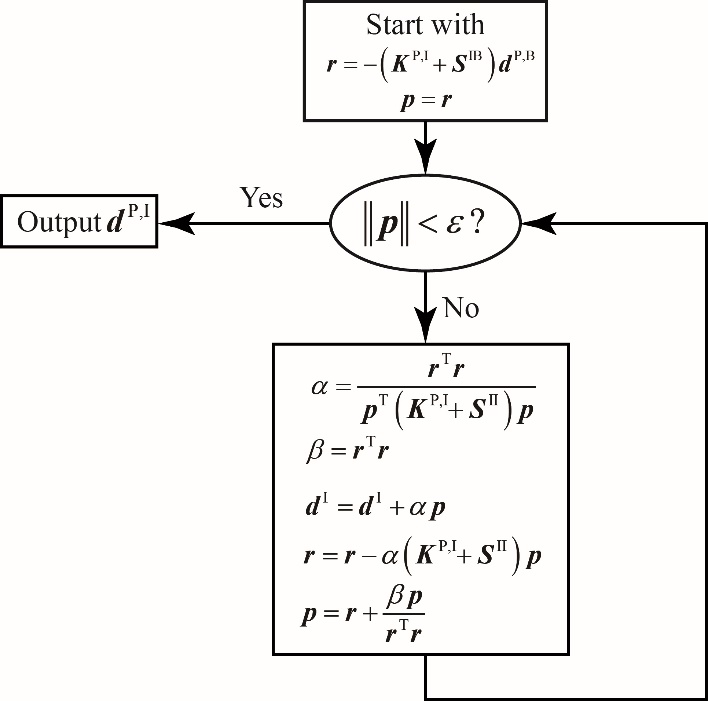
The flowchart of the CG iteration is shown in Fig. 3, where the values of and are known while and are unknown variables. Note that

(14)

so equals to the components of related to the active DOFs of polymer. Similarly,

(15)

so equals to the components of related to the active DOFs of polymer and subtracting .



**Fig.** **3.** A flowchart of the developed algorithm to perform CG iteration.

1. CNT network generator

In this section, we will introduce the Monte Carlo algorithm that we developed to disperse straight and curved CNT inside the RVEs. The generated nanocomposite systems are used to study the influence of CNT waviness on Young’s modulus of the nanocomposites.

Straight CNTs are characterized by a segment . The start point and the orientation of the line segment are randomly generated inside the RVE. The length of the segment is equal to the length of the CNT. Once is determined, the corresponding cylinder is created to represent the CNT and discretized into hexahedral elements.

Curved CNTs are characterized by a series of segments . The length of each segment = and the relative orientation angle between any two adjacent segments is . The curved CNT is then created segment by segment from . Fig. 4 shows an example of two adjacent segments and . Once is determined, the new point is created at a random position on the bottom edge of the cone.

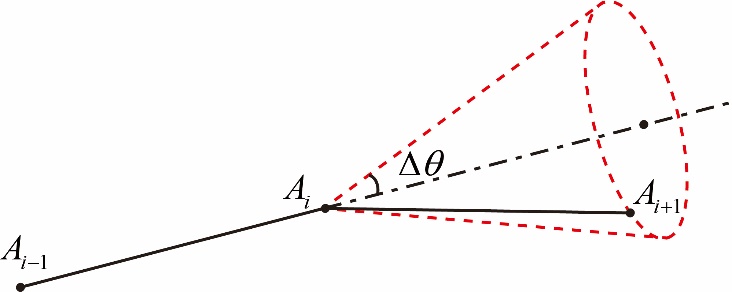


Fig. 4. Modeling of curved CNTS as adjacent segments of length △L and relative orientation angle .

Noting that is a constant value for a curved CNT with specific curvature, it can be varied to represent nanotube with different morphologies. The curvature of the CNT can thus be defined as:

(16)

A series of cylinders are created for each segment to represent the curved CNT and they are also discretized using hexahedral elements. Fig. 5 are examples of curved CNT with different curvatures. It should be mentioned that the morphology of each curved nanotube is different, indicative that our model is closer to reality than earlier studies which assume the morphology of all CNTs are same and were simplified as sinusoidal cylinders [34,35,41,49].

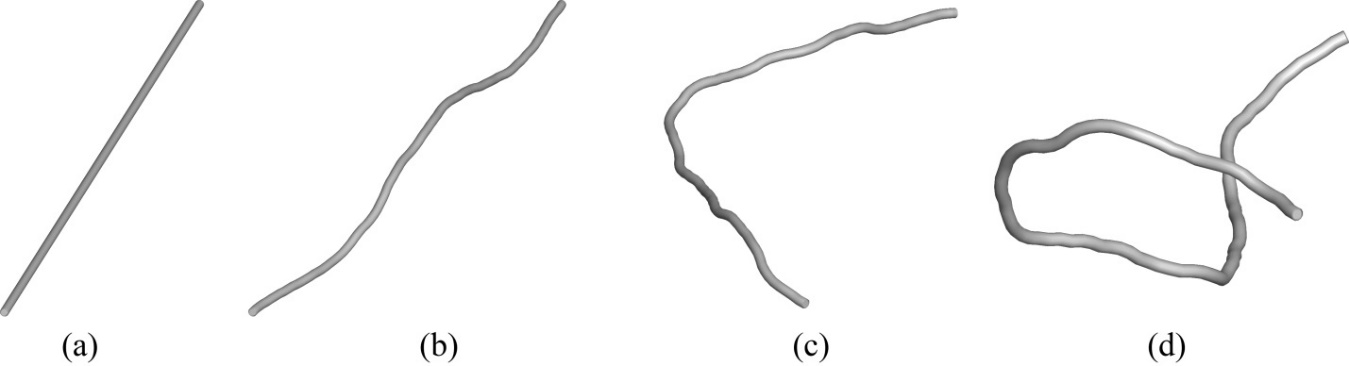


Fig. 5. Examples of CNTs of different curvature that were used as reinforcements in the RVE: (a) straight CNT , (b) curved CNT , (c) curved CNT . And (d) curved CNT .

The periodic boundary conditions are imposed on the dispersed CNTs in the RVE; namely, the CNT network should be repeated periodically in space. To this end, pseudo RVEs surrounding the actual RVE are also created when generating the CNT network, as shown in Fig. 6(a). The box with solid edges in Fig. 6(a) is the actual RVE and the surrounding boxes with dashed edges are pseudo RVEs. When adding a new CNT into the network, the copies of this CNT are also added into the pseudo surrounding RVEs. In Fig. 6 (a), the four thick segments are the distributed CNTs into the actual RVE, and other thin segments are their copies in the surrounding RVEs. Finally, as shown in Fig. 6(b), the CNT network in the actual RVE must strictly fulfill the periodic boundary conditions.

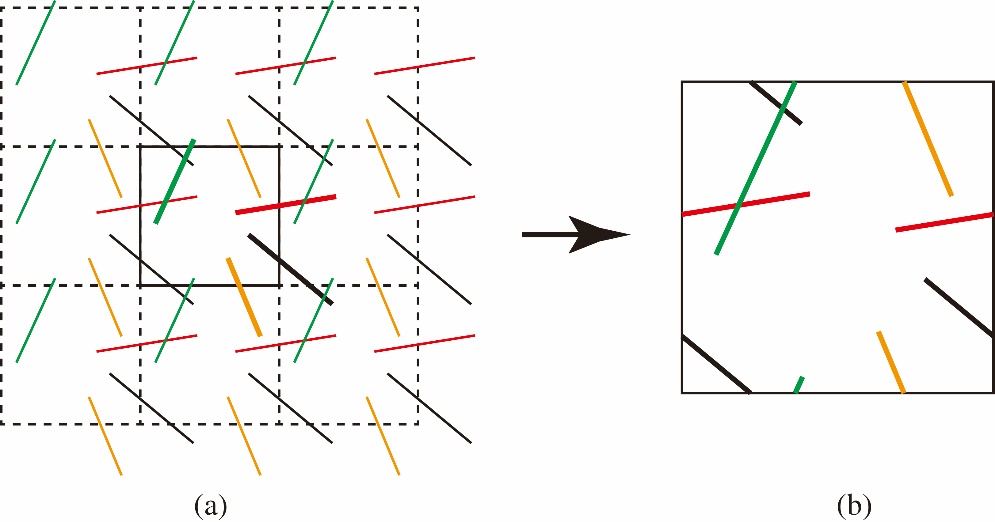


Fig. 6. The sequence used to impose periodic boundary conditions on the embedded CNTs: (a) the center box with solid edges is the actual RVE while the surrounding boxes with dashed edges are pseudo RVEs. The four thick segments are the CNTs dispersed into the actual RVE and the other thin segments in a same color are the copies of this CNT in pseudo RVEs, and (b) the RVE with CNTs fulfilling the periodic boundary conditions that is used in the analysis.

In this study, the CNTs are uniformly distributed inside the polymer, namely the minimal distance of any two CNTs must be larger than , where is the Van Der Waals separation distance [43]. The distance requirement must be checked when adding a new CNT and Fig. 7 shows the flowchart of the steps to create a CNT network with periodic boundary conditions.

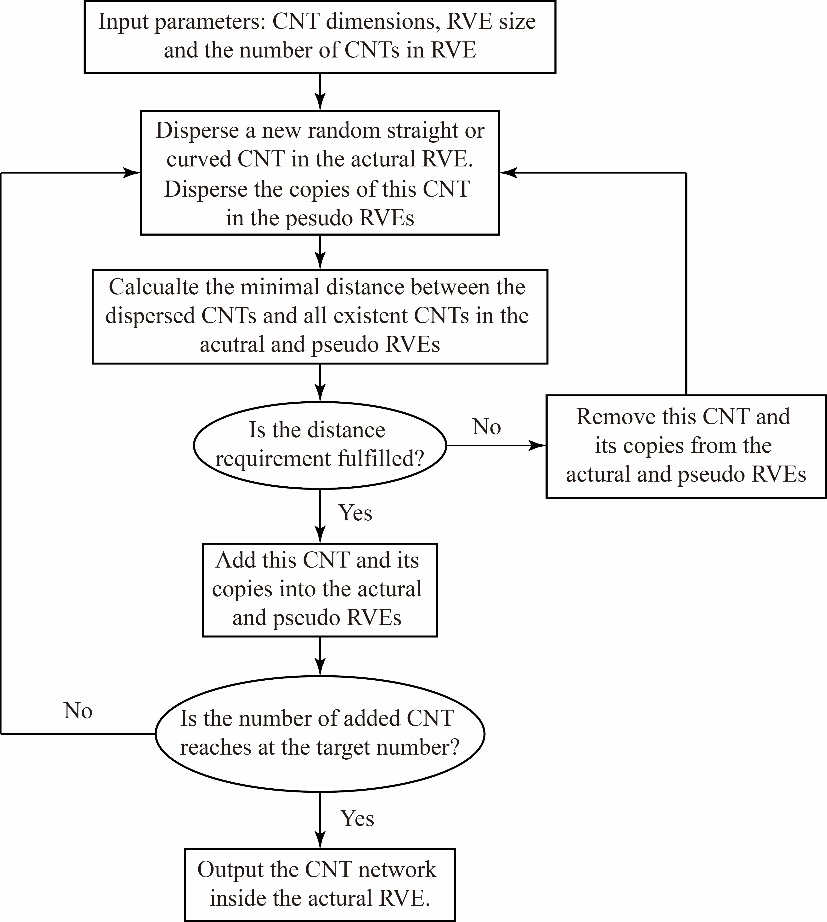


Fig. 7. The flowchart of the steps needed to create a fully dispersed CNT network with periodic boundary conditions.

1. Validation and numerical results

The validation of the proposed immersed FE approach was conducted by comparing its outputs with those obtained using traditional FE method. The immersed FE method is then used to study the influence of CNT waviness and volume fraction on the elastic properties of their epoxy-based composites.

* 1. Validation of an RVE reinforced with a single CNT

In this example, one SWCNT of (5,5) armchair chirality and of dimeter and length is placed at the center of the polymer matrix. The size of the polymer considered was selected to be and the CNT is placed at the center of the polymer as shown in Fig. 8. The material properties of the CNT and polymer were obtained from our previous MD studies [39,50], namely , and , . The following boundary conditions are applied on the FE model: at face , at face , at face z, and at face

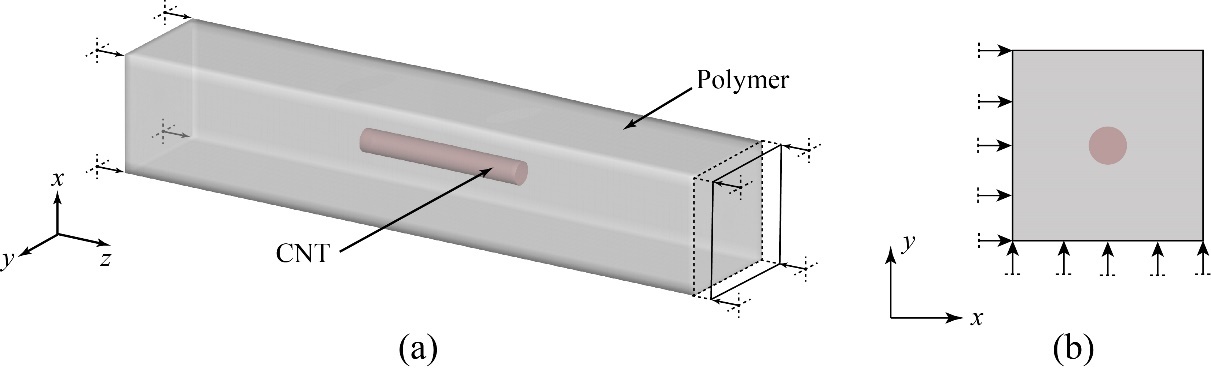


Fig. 8. The model used to verify the proposed immersed FE method: (a) a schematic drawing of a (5,5) CNT of length embedded in a polymer matrix of square cross-section of and length , and (b) the applied boundary conditions.

This simple problem is simulated both by traditional and immersed FE methods to determine the validity of the proposed immersed approach. Fig. 9 shows a cross sectional view of the grid in the traditional and immersed FE models. It shows clearly that the interface of the CNT and polymer are not matched in the immersed FE model. The number of elements in the traditional FE model is 168300 and the average element size is . In the immersed FE model, the CNT grid is the same one used in the traditional FE and the polymer matrix is meshed into elements. The average size of the polymer grid in immersed FE model is .

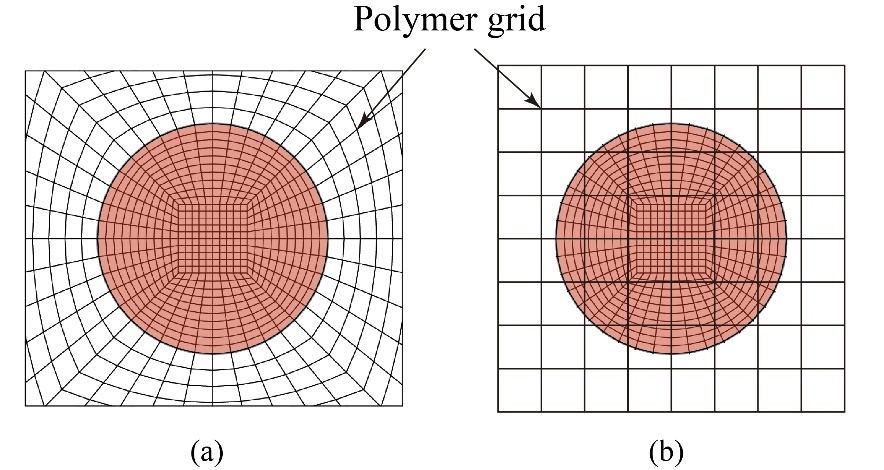
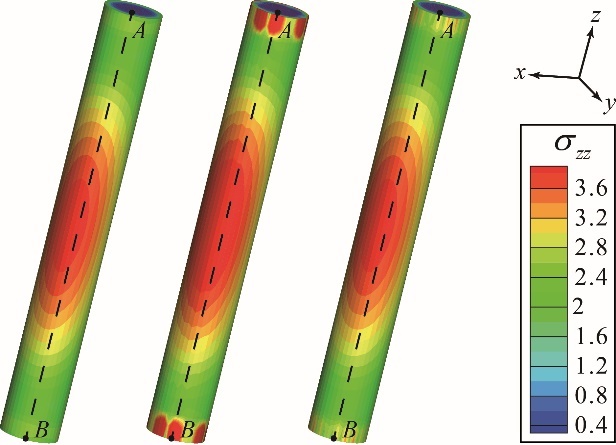


Fig. 9. The meshed CNT and polymer in (a) the traditional FE method model with matched nodes, and (b) the immersed FE method model with unmatched nodes.

The contour of the embedded CNT that were obtained by both methods are compared in Fig. 10. The distribution in Fig. 10(a) and (b) matches well everywhere except the area near the endpoints of the CNT. The simulations also reveal that the stress predictions were slightly overestimated in the immersed FE model (xx%). The overestimation typically occur if the difference between the polymer and the CNT is significant. Fig. 10(c) shows the contour if the polymer mesh was refined by using elements. It is very clear that stress overestimation is significantly reduced when we used a much finer mesh. A quantitative comparison of along a path on CNT surface is also presented in Fig. 10(d) to demonstrate the validity of our newly adopted immersed FE approach.



(a) (b) (c) (d)

Fig. 10. The contours of the CNT obtained by (a) traditional FE simulations, (b) immersed FE simulations using a coarse mesh for the polymer, (c) the immersed FE simulations using a finer meshing grid for the polymer. (d) is the quantitative comparison of at the CNT’s surface along the path .

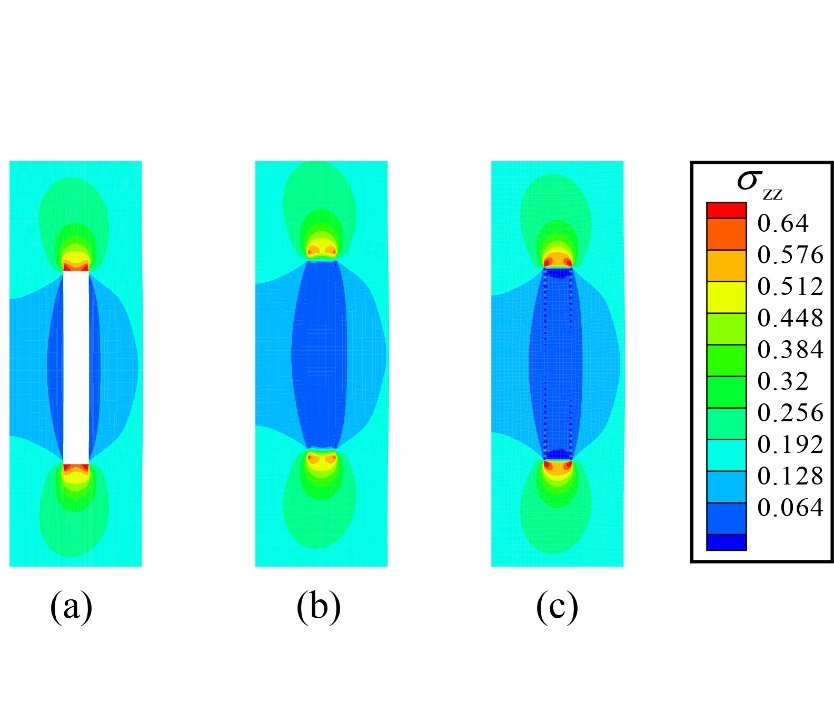
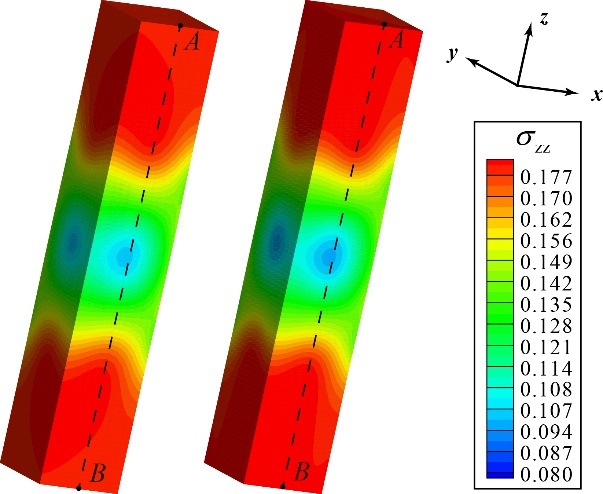


Fig. 11. The contours of the cross-sectional view in the polymer near the embedded CNT obtained by (a) the traditional FE simulations, (b) the immersed FE simulations using a coarse mesh, (c) the immersed FE simulations using a finer meshing grid.



(a) (b) (c)

Fig. 12. The contours on the boundaries of the polymer cell obtained by (a) the traditional FE simulations, (b) the immersed FE simulations. (c) is the quantitative comparison of at the polymer boundary along the path .

Fig. 11(a) and (b) presents the stress contours in polymer matrix near the embedded CNT that were obtained by the traditional and immersed FE techniques. The stress distribution is very similar in most locations in the polymer in both techniques. However, the degree of stress concentration near the CNT's endpoints is underestimated due to the non-matched polymer and CNT grid, and it can also be eliminated by using a refined polymer grid as shown in Fig. 11(c). It should be mentioned that the underestimation is localized due to the Saint Venant’s Principle, so it will not result in a sizable error when evaluating the effective material properties of the nanocomposite. Fig. 12(a) and (b) shows the contour at the polymer outer boundaries, and (c) is the quantitative comparison of along a path on polymer boundary. The numerical results clearly demonstrate the validity of the immersed FE method proposed in this paper.

* 1. Validation of an RVE reinforced with randomly dispersed straight CNTs

In this section, we tested out the immersed FE approach against a more complicated problem by modeling RVEs reinforced with randomly dispersed straight CNTs. In this example, the immersed and traditional FE models of nanocomposites reinforced with different CNT volume fractions are created. The Young’s modulus of the polymer is and other material properties are similar to those used in Section 4.1. Cubic RVEs of width are used in this analysis, where eight different composites are modeled with CNT volume fractions vf varying from 0.025 to 0.2 %. Fig. 13(a), (b), and (c) show the RVEs reinforced with CNT at , % and , respectively.

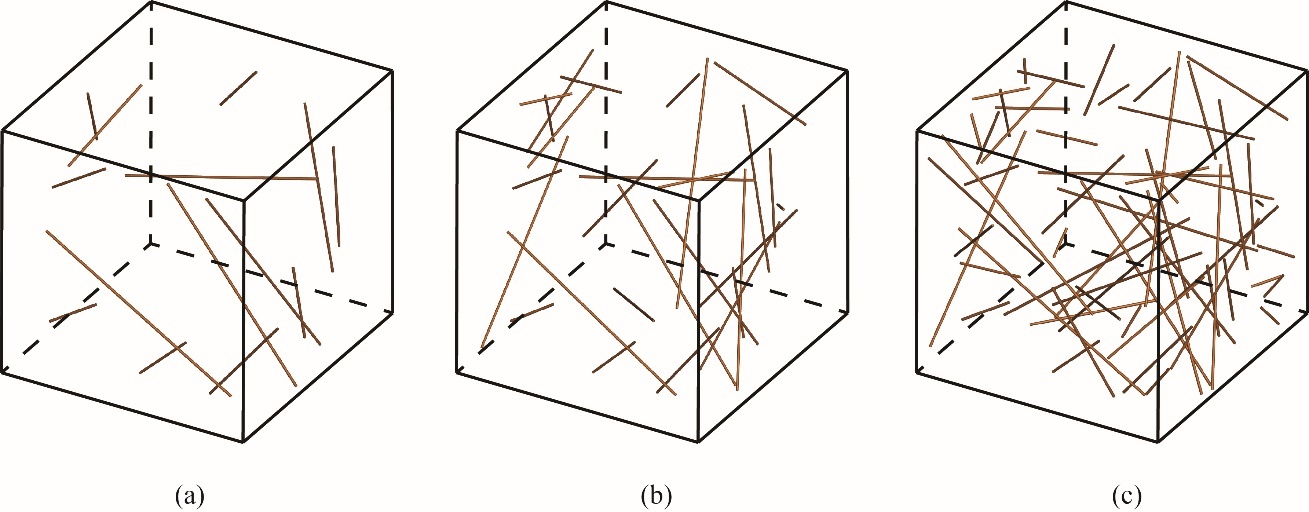


Fig. 13. RVEs represent nanocomposites reinforced with CNTs with different volume fractions: (a) , (b), and (c)

The elastic moduli , and of these RVEs are calculated by the immersed and the traditional FE techniques, and the average Youngs modulus from the two methods are compared. The traditional FE models are meshed with 4-node tetrahedron elements. In the immersed FE model, the number of elements along axis and circumference of CNT is the same with the traditional FE model while the polymer is discretized as regular grid with different resolutions. The polymer grid resolution is defined as

(17)

where is the diameter of the CNT and is the size of the polymer element.

Fig. 14 shows the variation of Young’s modulus of the nanocomposite with different vf predicted by the immersed and traditional FE techniques. The results of immersed FE method are dependent on the polymer grid resolution. The difference between the two methods almost diminishes when a higher grid resolution is used. At resolution , the average Young’s modulus from the immersed and traditional FE method are almost coincident. Fig. 15 shows the variation of the average relative error between the immersed and traditional FE methods with the grid resolution. We can conclude that the results of the immersed FE method are more accurate when using higher grid resolution for the polymer matrix.

Fig. 14. Comparison of Young’s modulus for CNT-reinforced composites containing randomly orientated CNTs obtained by the traditional FE method and the immersed FE method with different polymer grid resolution.

To demonstrate the advantages of the immersed FE method, Fig. 16 shows the variation of the total number of elements in the immersed and traditional FE models with increasing the CNT volume fraction. The number of elements reflects the difficulties of creating the composite models. The results indicate that the number of elements in the traditional FE method increase 24 times faster than the immersed FE method with increasing the number of dispersed CNTs. In fact, once the polymer grid resolution of the immersed FE model is fixed, the increment of the total element number equals to the number of elements of the added CNTs. However, in the traditional FE model, the polymer should be re-meshed when adding new CNTs and many new polymer elements are created around the CNT-polymer interface, which leads to a significant increase in the total number of elements and thus, the difficulty in the meshing process increases dramatically at high CNT volume fractions. The immersed FE method does not face these challenges and provides similar results to the traditional FE method, making it an effective approach to simulate CNT-reinforced nanocomposite with complex morphologies.

Fig. 15. Variation of relative error of Youngs modulus of CNT-epoxy composites with polymer grid resolution in the immersed FE method.

Fig. 16. Variation of the total number of elements in the immersed and traditional FE models with the limited increase of CNT volume fraction.

* 1. Influence of CNT waviness on material properties of nanocomposites

In this section we used the proposed immersed FE approach to solve complex nanocomposite structures by modeling RVEs reinforced with CNTs of different morphologies. The effect of CNT volume fraction and waviness on the elastic modulus of epoxy-based composites was investigated.

The (5,5) armchair SWCNT with and is selected as the reinforcement. The material properties of CNT and polymer are similar to those used in Section 4.1. The CNTs are uniformly dispersed in a cubic RVE whose size is selected to be equal to the CNT length. Our previous studies demonstrate that the material properties will converge around this RVE size [38,43]. The fully dispersed straight and curved CNT networks are created by the Monte Carlo method described in Section 3.

In this investigation, three volume fractions are investigated and four curvatures are considered for each volume fraction. To reduce the effect of the system size and increase the accuracy of the results, for each combination, three RVEs samples filled with randomly dispersed CNTs are modeled. Therefore, a total of 36 composite models with different volume fractions and curvatures are simulated in this study.

Fig. 17 shows three RVEs reinforced with CNTs of volume fraction and different curvatures. The morphology of every CNT in the RVE is different and the CNT networks are very similar to the actual microstructure of nanocomposites as imaged with scanning electron microscopy [35] (see Fig. 17 (d)). The polymer grid resolution in this study is selected to be for all cases and the details of the composites models are listed in Table.1. There are 12 composite models for each volume fraction and the element and node number in Table.1 is the average of them.

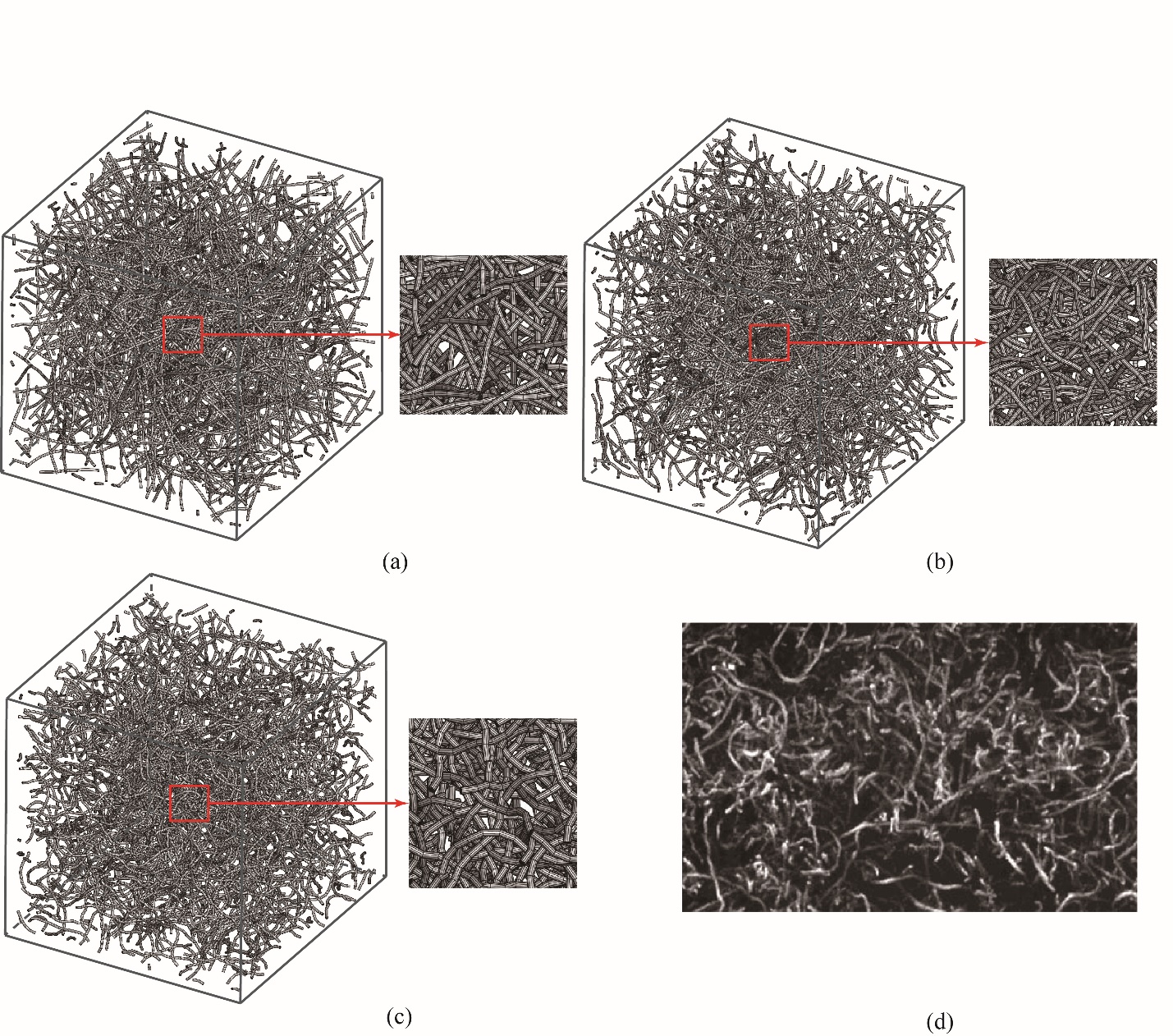


Fig. 17. The curved CNT networks with volume fraction and different curvatures: (a) , (b) and (c) . (d) is the scanning electron microscopy image of an actual nanocomposite (from Ref. [35])

Table.1. The details of the composite models with different CNT volume fractions.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Case # | CNT Vf (%) | # CNTs | # elements | # nodes |
| Case #1 | 0.5 | 64 | 1091971 | 1147861 |
| Case #2 | 1.5 | 191 | 1273933 | 1379901 |
| Case #3 | 2.5 | 318 | 1455433 | 1611941 |

Fig. 18 and Fig. 19 show the variation of Young’s modulus of the nanocomposites with increasing the CNT curvature and volume fraction, respectively. The effective Young’s modulus at each combination is the average of 3 different samples. Fig. 18 indicates that the RVE reinforced by the straight CNT networks produce the highest enhancement on effective Young’s modulus which is improved by 70% when the volume fraction of CNT increased to 2.5%. However, the elastic modulus decreases significantly if the CNT is curved. The decrement is more obvious with higher CNT curvatures and roughly 40% of the reinforcement lost when the CNT curvature increased to . This conclusion is in a good agreement with those obtained in the literature by atomistic and analytical techniques [34–36,50]. The numerical results are also compared with the experimental results of CNT-epoxy composites [51] and the obtained elastic moduli at curvature matches well with the experimental data. The good agreement between the reported experimental data and the numerical results also validates the capability of the proposed method in modeling actual nanocomposite materials.

Fig. 18. Variation of the effective Young’s modulus of CNT-epoxy composites with increasing the volume fraction of CNTs of different curvatures.

Additionally, Fig. 19 demonstrates that the decrement of effective Young’s modulus is almost linear from to and the slopes for , and are , and , respectively. These results demonstrate that the reduction of Young’s modulus becomes more tangible at higher CNT volume fractions and this conclusion is in agreement with the study by Roham [41].

Fig. 19. Variation of the effective Young’s modulus of CNT-epoxy composites with increasing the curvature ratio of the CNTs obtained for at different CNTs volume fractions.

1. Conclusion (did not review. Waiting your input to many of my revisions and changes)

In this study, we developed a modeling approach based on the immersed finite element method to determine the mechanical properties of CNT-reinforced polymer composites. In this model, the dispersed CNTs and the surrounding polymer matrix were created independently but simulated as a coupled system. The nanocomposite model can be easily created by eliminating the associated difficulties in creating a compatible mesh faced in the traditional finite element method. When coupling the independent CNT and polymer grids, both kinematic and mechanic relations in between are considered by embedding the equilibrium equation of each CNT into the equilibrium equation of the polymer. Since no additional unnecessary assumptions are introduced, the results of the immersed FE method are very close to the traditional FE method.

The polymer is discretized as a regular grid and the results depend on the polymer grid resolution. According to the numerical results, the size of the polymer element should be selected around or less than the dimeter of the CNT to obtain reliable results.

The proposed method is used to study the influence of CNT waviness on elastic properties of CNT-epoxy composites. The morphology of CNTs in our study is very similar to actual nanocomposites and the numerical results indicate that the CNT waviness deteriorates the performance of the material. Straight CNTs have the biggest reinforcement effect on the elastic modulus of the composite. Young’s modulus dropped by ~40% when the CNT curvature increased to . Moreover, the influence of the CNT waviness becomes more tangible at higher CNT volume fractions.

The numerical results show good agreements with previous experimental and numerical studies, thus validating the capability of the immersed FE technique in simulating realistic composites with complex microstructures. behaviour

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