JCAMECH

Vol. 50, No. 2, December 2019, pp 413-419
DOI: 10.22059/jcamech.2019.293497.458

Computational Studies on Mechanical Properties of Carbon-based Nanostructures Reinforced Nanocomposites

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ARTICLE INFO

Article history:
Received: 04 December 2019
Accepted: 14 December 2019

Keywords:
Carbon Nanostructures
Nanocomposites
Representative Volume Element(RVE).

ABSTRACT

Computational methods can play a significant role in characterization of the carbon-based nanocomposites by providing simulation results. In this paper, we prepared a brief review of the mechanical properties of carbon nanotubes (CNTs), Graphene, and coiled carbon nanotube (CCNTs) reinforced nanocomposites. Varies simulation studies in mechanical properties of nanocomposites including representative volume element (RVE) approaches using the finite element, multiscale simulation and molecular dynamics studied is mentioned. All the simulation results show a significant role of interphase properties, interphase thickness, elastic properties of nanostructure, various loading conditions and orientation of the nanostructure on mechanical behavior of nanostructure reinforced nanocomposite. Some researchers employed various approaches for comparing simulation results of the effective elastic properties of nanostructures reinforced nanocomposite. Although it is a huge challenge for scientists to make a connection between MD simulations and continuum mechanics, in some researches scientists tried to couple MD and continuum mechanics for more precise results in nanocomposites.

1. Introduction

Nanotechnology can appropriately be defined as researchers at atomic and molecular scales in designing, modeling, fabrication, and manipulation. This topic is a multi-disciplinary field of different fundamental sciences and engineering. Nowadays, scientists are looking for new and advanced materials to draw out their utilization in order to improve world life quality[1-4]. Nanomaterials are one of the most recent and alluring fields in which several studies have been done in especially in design and fabrication[5-16]. The significance of nanomaterials becomes remarkable after an investigation of nanomaterials to use them in nanoelectronic circuits of new sensors. Although materials in nanoscale have excellent characteristics, carbon-based materials are more interesting for some of the scientists because of their unique mechanical, thermal and electrical properties [17]. Also, Nanoscale materials, with their high thermal, electrical and mechanical properties, have been widely used as reinforcements for improving mechanical properties of composites without increasing their weight significantly. For the same amount of mass, nanomaterials have a relatively high surface area to volume ratio as compared to larger forms of the material, which makes them more reactive[18]. Additionally, since the transference of load between matrix and fillers in composite materials occurs through their contacting surfaces, reinforcement with nanomaterials could be more effective than micro and macro reinforcement. Nanomaterials which are mostly used to enhance the properties of nanocomposites are as follows: graphene [19-30], graphite [31-37] carbon nanotubes (CNTs)[38-51], graphene spirals[52, 53], coiled carbon nanotubes (CCNTs) [54-67] and nanoclays [68-71]. In this review we have mentioned varies simulation studies in mechanical properties of nanocomposites including representative volume element (RVE) approaches using the finite element, multiscale simulation and molecular dynamics studies.

2. Carbon nanotube reinforced nanocomposites

CNTs are allotropes of carbon that have cylindrical structures, in which carbon atoms are bonded together in hexagonal arrangements. These nanostructures exhibit extraordinary properties that make them invaluable for many engineering applications. For instance, these lightweight structures are the strongest and stiffest materials that have been achieved by scientists to date and accordingly are widely used as reinforcements in nanocomposites. The development of new composite materials has long been of interest to researchers. Traditional CNTs are strong reinforcements for composite materials; incorporation of these fillers into the polymer matrix, however, can reduce fracture toughness of composite and increase its brittleness. Liu *et al* [72] employed representative volume element (RVE) approaches using the finite element method for simulation the effective elastic properties of CNT

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reinforced nanocomposite. Their results show that the reinforcing capabilities of the carbon nanotubes in a matrix are a significant influence on increasing stiffness of the nanocomposite. In another study [73] representative volume element (RVE) model is created to investigate the mechanical behavior of Single-walled carbon nanotubes (SWCNT) reinforced rubber nanocomposites using multiscale finite element method. Anifantis *et al* [74] investigated the effect of the interface on the effective elastic properties of CNT reinforced nanocomposite for various volume fractions using representative cylindrical volume element model. Ayatollahi *et al* [48] presented a multiscale simulation to investigate the nonlinear properties of SWCN reinforced nanocomposite under various loading conditions. Their results show that the ratio is the important factor in elastic properties of nanocomposite; also the strong interphase has more effects on the nanocomposite Stiffness in comparing weaker interphase. The effects of pinhole defects and waviness of carbon nanotube on the mechanical properties of nanocomposite are studied by Joshi *et al* [75]. In this study, the mechanical properties of representative volume element (RVE) model for nanocomposite are obtained for waviness index of carbon nanotube; also the effect of number and type of the defects on stiffness of nanocomposite is evaluated. According to the results with increasing number of pinhole defects, as well as with increasing the waviness number the stiffness of nanocomposite decreases. In another study [76] the effect of carbon nanotube (CNT) orientation on the mechanical properties, including Young's modulus and Poisson's ratio of nanocomposites under lateral and axial load was examined using representative volume element (RVE). Joshi and Upadhyay [77] investigated the effects of interphase properties on mechanical behavior of long and short multiwalled carbon nanotubes (MWCNTs) reinforced nanocomposite. Gupta and Harsha [78] studied the effects of vacancies on zigzag and armchair carbon nanotube on Young's modulus of CNT reinforced nanocomposite. Their results show that the presence of a vacancy on CNT significantly reduced the stiffness of nanocomposites.

Furthermore, some researchers studied the mechanical properties of CNT-based nanocomposites using molecular dynamics simulations. Odegard *et al* [79] studied the bulk elastic properties of a functionalized and nonfunctionalized single-walled carbon nanotube reinforced polyethylene nanocomposite in crystalline and amorphous polyethylene matrix using a hierarchical multiscale method. Their results reveal that the stiffness of nanocomposites for functionalized carbon nanotubes are less or equal to those of the nanocomposite without functionalizing nanotubes. Al-Ostaz *et al* [80] investigate the elastic properties, more precisely the engineering constants of carbon nanotubes and nanocomposites thereof with aligned and randomly oriented nanoparticles using molecular dynamics simulations.

Meguid et al [81] exhibited a different multiscale method to evaluate the elastic and interfacial properties of carbon nanotube (CNT)-reinforced nanocomposites. They used the two-step approach to estimate the bulk properties of nanocomposite, firs molecular dynamics simulation, and Second, the micromechanics models and combined Monte Carlo finite-element (FE) modeling. Wu et al. [82] worked on carbon nanotube and core-shell nanowire structures; they discussed electromechanical and resistance-change memory devices.

3. Graphene reinforced nanocomposites

Graphene sheets can be considered as an efficient substitution if their high electrical conductivity can be investigated to obtain a strong current-generated magnetic field [83]. Graphene nanostructures are scientifically and commercially crucial due to their special molecular structure, which is monoatomic in thickness, rigorously two-dimensional, and highly conjugated. Therefore, graphene presents extraordinary electrical, optical, thermal and mechanical properties. Liu et al. [84] discussed the surface modification of graphene which has a considerable advantage in sensors.

Moreover, they investigated the chemical sensors and biosensors and their application in different aspects. Zhang et al. [85] applied MD analysis to find the elastic modulus, fracture strain and fracture stress of graphene. They proved that the temperature gradient has more influence on graphene mechanical properties in comparison with the layer number in the multilayer graphene. Shiu and Tsai [86] used MD simulations to study the graphene reinforced nanocomposites different morphologies and revealed that composites with intercalated graphene possess greater elastic modulus than composites reinforced by graphene platelets. MD simulation provides detailed information on the deformation and damage of nanomechanism[26, 87-91].

On the other hand, to investigate the specimen's properties, continuum mechanics is more efficient. Although it is a huge challenge for scientists to make a connection between MD simulations and continuum mechanics, in some researches scientists tried to couple MD and continuum mechanics for graphene composites. By employing a combined approach of MD, molecular structural mechanics and FEM the elastic constants of nanocomposites were calculated [92]. Chandra et al. [93] applied multiscale modeling to estimate the effect of graphene sheets' orientation on the stiffness of the composites. Dai and Mishnaevsky [94] presented a 3D computational model of graphene-reinforced polymeric nanocomposites to evaluate damage and fracture of these materials. They applied inverse modeling to evaluate interface properties; it is found that the mechanical properties of the interface are almost 75% higher than pure matrix. Also, they found that by increasing the aspect ratio of the fillers, elastic modulus increases. K. Hbaieb *et al* [68] compared the results of two and three-dimensional finite element models for the stiffness of the nanocomposite. They show that the two-dimensional model is simpler and does not accurately predict the stiffness. Also, The MorieTanaka model results are compared with the MorieTanaka model. The results for randomly oriented particles show that the MorieTanaka model in compare three-dimensional model overestimates the stiffness of clay reinforced nanocomposites.

4. Coiled Carbon nanotube reinforced nanocomposites

CCNTs are a form of CNTs where unique properties of straight CNTs are combined with morphological characteristics to promote the properties of CNTs [64, 95]. For example, load transfer and bonding strength between CCNTs and polymer matrix are greater than those between straight CNTs and polymer matrix in nanocomposites [65, 96]. Due to these potentials, more attention is paid to CCNTs, and CCNTs reinforced nanocomposites in recent years. Lau et al. [65] examined synthesis methods of CCNTs and their potential applications in advanced composites. They stated that the use of CCNTs as reinforcements not only can increase composites' strength but also can increase their toughness. Li et al. [54] investigated the mechanical behaviour of CCNTs reinforced epoxy-based composites using tensile and nano-indentation tests. They also studied dispersion and interlock action of CCNTs embedded in epoxy resin by in situ scanning electron microscopy (SEM). According to this research, the hardness, elastic modulus, and tensile strength of the composites increase by increasing the weight percentage of the fillers. Also, CCNTs dispersed well and interlocked tightly with the matrix. Experimental study of the behaviour of nanomaterials is a challenging task and says little about the physics of deformation process and the effect of various parameters [64]. Also, the results of the tests depend intensively on the fabrication of nanostructures with controlled such characteristics as shape and size [97]. As a consequence, experimental tests to characterize the mechanical response of the nanomaterials have serious limitations. However, computational methods—such as molecular dynamics and finite element—have been proved to be successful. Molecular dynamics simulations are so time-consuming for simulation of mechanical behaviour of complex systems like nanocomposites containing a great number of fillers with various shapes, sizes and orientations then Finite element method, nevertheless, is considered to be a more promising tool for prediction and assessment of the mechanical behavior of such complex systems as carbon-based nanocomposites. The quality and properties of fillers are key to the performance of composite materials. Parameters of fillers—namely geometry, concentration and properties—play an important role in the reinforcement of composite materials. As to nanocomposites, thickness and properties of the interphase layer are other influencing factors [97, 98]. This issue is not true in the case of micro composites as the thickness of the interphase layer is in the range of 1-2 nm [99]. Therefore, it could be neglected in micromechanical modelling. Mortazavi et al. [97] studied the effect of fillers geometry, volume fraction, and properties contrast and, in particular, the effect of interphase thickness and properties contrast on effective thermal conductivity and elastic stiffness of nanocomposites utilizing 3D finite element simulation. The considered geometries for fillers are a long cylinder, sphere, and thin disc. They have found that although the effect of interphase is considerable for spherical fillers, it is less effective when fillers' geometry deviates more from the spherical shape. CCNTs are helical structures that have several geometric parameters such as tube diameter, coil diameter, helix angle and number of coils. When these structures are used as reinforcements in nanocomposites, the parameters mentioned above affect the overall behavior of nanocomposites. Khani et al. [66] developed a 3D finite element model and employed it to study the effect of interphase, volume fraction, orientation and geometric parameters on the elastic behavior of nanocomposite with CCNT fillers. They also proposed an algorithm to answer the question of whether or not nanocomposites with spring fillers are appropriate alternatives to those with single-walled CNT (SWCNTs) fillers. The authors concluded that SWCNT fillers provide better reinforcement compared to CCNT inclusions with the same volume to surface area ratio.

Among carbon-based nanofillers, recently, a significant number of researches focused on Carbon Nano Coils (CNCs) because of their particular geometry and physical properties. The electric conductivity of CNC was calculated between 107 to 180 s/cm by Hayashida et al. [100]; thus, CNC is an appropriate material for nanoscale electronic applications. The spring constant of CNC was determined equal to 0.12 n/m which has an acceptable agreement with experimental results [101].

Molecular Dynamics (MD) and Molecular Mechanics (MM) are one of the practical methods to study and to model carbon-based nanomaterials. Wu et al. [64, 102] analyzed the CNC's energy absorption capacity. Buckling analysis of CNTs shows that length decrease and diameter increase lead to greater buckling loads. Also, by increasing the pitch number of CNCs, the natural frequencies decline [61]. Ghaderi and Hajiesmili [57] investigated the fracture strain and fracture load of CNCs using MD and Finite element method. They revealed that the fracture load per atom of the CNCs are lower than the corresponding armchair CNTs. Fakhrabadi et al. [103] presented an MM based FEM modeling of CNCs and their application as mass sensors. Besides, FEM has been used in several works to evaluate the influence of interphase zone between fillers and matrix on the nanocomposite's properties.

5. Conclusion

Development in simulation methods for nanocomposites based on carbon nanostructure rapidly evolving this research area. In this review varies simulation studies in mechanical properties of nanocomposites including representative volume element (RVE) approaches using the finite element, multiscale simulation and molecular dynamics studied is mentioned. All the studies show a significant role of interphase properties on mechanical behavior of nanostructure reinforced nanocomposite.

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