Mechanical Properties of Nano and Nano Based Composites - A Review

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Abstract
This paper addresses the mechanical behavior of nano reinforcement like carbon nanotubes, graphene sheets, nano particles which are used as a constituent in composite materials. Several authors explored the mechanical properties of nanobased composites. A review of the past research is presented, and several key findings and behavioral characteristics are discussed. An overview covers the prediction of mechanical properties of carbon nanotubes, graphene sheets, nano size particulates and different modeling techniques to represent the nanobased composites, behavior of the nanocomposites under different loading and boundary conditions. Some overall important findings of the studies are that a composite material reinforced with nano substances definitely improves the structural performance of the composite material.

Keywords: nano Reinforcement, Nano based composites

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Introduction

The research topic attracting the many researchers and having great applications are the nanocomposites. Conventional materials are replaced by composite material and now a day’s composite materials are replaced by nanocomposites. The uses of nanocomposites are found in aerospace structures because of their high stiffness to weight and strength to weight properties. These properties could ultimately yield significant weight savings for aircraft structures.

The need for mechanical characterization of nanobased composites is typically required to increase the applications of such material. For example composite material reinforced with carbon nanotubes, graphene, buckminster fullerene are using in aero space and marine structures, super conductors, lubricants, catalysts due to their high reactivity, drug delivery systems, and pharmaceuticals. Thus, understanding the mechanical behavior and properties of nanobased composites and different analyzing techniques are needed for their effective design.

Nanosized reinforcements are available in different forms such as nanotubes, nanosheets, nano particulates.

The present study focuses on prediction of mechanical properties of nano based composites. Knowledge of the basic response of the nanocomposites and nano reinforcement provides useful information for preliminary design of complex structures. In addition, this basic knowledge provides valuable insight into modeling complex structures with general purpose finite element method.

One objective of the present study is to describe the results of research that has been conducted on the nanobased composites and nano sized reinforcement. Another objective is to describe several of the key behavioral characteristics and trends in a coherent manner. For convenience, the primary studies conducted on nano reinforcement and nanobased composites behavior are also summarized in tables 1 and 2, respectively. Next, several key findings on the Nano sized reinforcement and nanocomposites behavior that have been identified since the early 1998’s are described and discussed. The table shown above addresses the type of reinforcement, modeling technique adopted by the author to reach their objective and the method incorporated to validate their work is presented.

Overview of Past Work
The structural application of carbon nanotubes (cnts) depends on its mechanical and thermal properties. Rodney S.et al [1] predicted some of the mechanical and thermal properties of single wall carbon nanotube and multiwall carbon nanotubes from graphine sheet properties. The stiffness, bending constant, bulk modulus and thermal properties of cnts are calculated by using properties of graphine sheet because the CNTs obtained by rolling the plane graphine sheet. The carbon nanotube reinforced composites important features also included in their study.

The particle reinforced composites have many applications in engineering field. In 2000 Hyoung Seop Kim evaluated et al [2] the hardness of the particulate composites by varying the volume fraction of the reinforcement using several models for rule of mixtures and the results are validated by finite element method. Comparison between the results from ROMs and FEA shows the stress states are nearly iso-strain at high volume fraction of the hard particle and iso-stress at low volume fraction of the particle.

The enhancement of stress developed inside the inclusion of particulate reinforced composite made of silicon carbide aluminum composites are studied computationally using micromechanics with finite element method by Wilkins et al [3]. The study is carried out by treating the constituent with elastic and plastic nature by taking simplified and refined finite models. The authors concluded that the simplistic two phase model of Al/Sic is adequate to predict the stress inside the inclusion with elastic behavior. The refined three phase model is needed for the plastic behavioral analysis. The study illustrated that, in analyzing composite materials related problems, if the objective is to obtain the overall response, then a simplified approach will be adequate. When the micromechanical details are of concern, the composite should be viewed as a structure not a simple material, so a well refined approach should be undertaken.

The tensile behavior of composites reinforced with ceramic particles aligned in strips are predicted by 3D finite element calculations and compared to axisymmetric calculations by D. Saraev [4]. The analyses conducted by selecting a unit cell model of periodic arrangement of reinforcements. The authors presented the results are in such a manner that can be directly compared for all possible aspect ratios and inclusion volume fractions. The results obtained in this work indicated that varying the distance between the stripes when particle volume fraction is kept constant significantly influences the overall mechanical behaviour of composites. During elastic state of deformation, 3D and axisymmetric formulations predicted similar results. The mechanical behaviour perpendicular to the stripe direction predicted by 3D and axisymmetric models may fluctuate depending on the inclusion volume fraction. The volume fraction and size and type of the reinforcement in composite material affect the resultant properties of composite significantly. F.V. Antunes et al [5] evaluated the fatigue life of three different particulate composite considering the effect of above mentioned parameters. To achieve the objective of their work the authors selected a specimen with central hole. Fe method is adopted to find the stress intensity factor. Numerical predictions are performed with the presence of crack of different shapes and different aspect ratios. Fatigue lives, crack shape evolution and final crack length were predicted assuming an initial crack size and considering that the crack maintains a quarter-elliptical shape. The results are compared with existing literature and experimental data.

A review of modeling techniques for predicting the mechanical behavior of polymer nanocomposite is presented. A detailed discussion of Computational chemistry and Computational mechanics modeling techniques is given by P.K. Valavala and G.M. Odegard [6]. The specific molecular-based and continuum based modeling approaches are described in terms of assumptions and theory. The approaches discussed are Ab initio simulations, Molecular Dynamics, Monte Carlo, Analytical Micromechanics, Computational Micromechanics, Finite Element Method, and Boundary Element Method.

G.M Odegard [7] has done great contribution on characterization of nanotubes and Nano composites. In their work the method they proposed provided a linkage between nano structured material to bulk material. The study is performed by reinforcing a swnts in two different polymers (LaRSSI & LaRCCP2) individually considering length, volume fraction and orientation and distribution of the reinforcement. The Young’s modulus and shear modulus are presented with varying the above parameters.

An analytical study is carried out to evaluate the effective stiffness of Multi walled nanotubes (Mwnts) by Tan Xiao [8]. The Mwnts are assumed as a concentric thin cylindrical shell. The interaction between layers of Mwnts is expressed by the Lennard Jones potential which is successfully employed to study nano structures. These Mwnts reinforced in matrix only the outer most layers is supposed to endure the axial load due to weak vander wall effect in axial direction. The work also includes the distribution of interfacial shear stress along the cnt length by conducting pullout test for different

coefficient of friction by considering linear and nonlinear effects.
The behavior of the material is different at nanolevel and macro level. One of the reasons to fabricate the material at nano scale is to get superior properties at macro scale, but the predictions of mechanical properties of these material is difficult due to the associated scale. M. Odegard et al. [9] made a brief relation between those scales. Authors evaluated bending rigidity of the graphene sheet using molecular, equivalent continuum and continuum modeling techniques. Correlation between the above modeling methods is obtained by equating the potential energy associated with the concerned modeling method. The interface of the particulate composite is as important as the type of reinforcement. As the load transferring medium it cannot be strong at every situation due to mismatch in the properties. R. Guo et al [10] determined the debonding effect of interface in particulate composites using Voronoi cell finite element method. The distribution of stress around the inclusion is determined considering uniform and random distribution particles in composite material. The toughness of nano composite ceramics may be influenced by many factors, e.g., the size, volume fraction, and distribution pattern of the nano-particles, etc. The influence of nano-particle clustering, crack pinning, and transgranular fracture on its toughness are evaluated identified from both the experimental and analytical studies by Ai Kah Soh et al [11]. From the work authors found that crack pinning toughens the nano-composite ceramics because a higher stress intensity factor is needed to cause crack propagation around or pull-out of the nano-particle. The grain boundary of nano particle guides the crack into the matrix due to strong cohesion between the nano-particle and the matrix. Transgranular fracture increases with the increase of the volume fraction of nano-particles. The nano-particle clustering can reduce toughening induced by crack pinning. Theoretical prediction, based on the combination of the three effects of nano-particles, is in agreement with the experimental data.

R. Byron Pipes [12] considered large arrays of carbon nanotubes, assembled in helical array geometries of circular cross-section for the prediction of the effective thermal expansion coefficients (CTE) of the array. The effective axial, transverse and shearing coefficients of thermal expansion of the array are determined in terms of the degree of twist, number of layers, properties of the carbon nanotube and surrounding polymer matrix. Results described that the axial coefficient of thermal expansion of the SWCN dominates the effective axial coefficient of thermal expansion of the array for small angles of twist, while the thermal coefficient of the polymer matrix strongly influences the axial coefficient at large angles of twist. The effective circumferential coefficient of thermal expansion of the helical array shows little influence of the angle of twist over large twist angle.

The experimental and theoretical studies on carbon nanotubes demonstrated that cts have great potential in mechanical and electrical applications. B. Liu et al [13] determined the load carrying capacity of the cnt is used to evaluate the electrical performance. The authors expressed that the conducting CNTs may easily become semi-conducting ones subject to mechanical deformation, but the semi-conducting CNTs never become conducting ones upon deformation.

Mechanical properties of cnt reinforced composites are evaluated by X.L. Chen, et al [14] in the year 2004 using continuum mechanics with the finite element method. The continuum mechanics method accuracy depends on the selection of representative volume element (RVE). The authors performed the analysis by taking square RVE. The material property constants are obtained from selected RVE under two different loading conditions with the concepts of elasticity theory. The results obtained from the analysis show that the load carrying capacity of the cts in the matrix are significant. For example, with the addition of CNTs in a matrix at a volume fraction of 3.6%, the stiffness of the composite can increase as much 33% in the axial direction with long CNTs. These simulation results are consistent with both the experimental ones reported in the literature. The rules of mixtures, for both long and short CNT cases, are found to be quite accurate in estimating the effective Young’s moduli in the CNT axial direction.

The tensile behavior of spherical shaped particle reinforced composites is studied by J. L. Lorca et al [15] considering elastic and plastic matrix material using three-dimensional finite element method. Damages are formed in the material due to void nucleation and their growth. Damages are located in the regions between the spherical reinforcement in close packing in the direction of deformation axis. The high strain concentration in those regions initiates voids, which grew by the tensile hydrostatic stresses. The authors considered all the above mentioned factors to characterize the particulate reinforced composites. The multi particle cell results were compared with those obtained from single-particle axisymmetric simulations, and the effect of reinforcement volume fraction was analyzed as well as
that of the matrix damage parameters on the composite behavior.

A three three-dimensional quadratic interfaces finite element is developed by Javier Segurado et al [16] to study the fracture behavior in composite materials. The particle fracture in the composite material is simulated by developed element. The study conducted by selection of represented volume element which reproduces the microstructure of the material which is very important foe micromechanics study. Overall properties of particle reinforced composites are determined using micromechanics approach. The formulated element is validated by two dimensional axisymmetric approaches.

Continuum modeling and self similar methods are two important approaches used by many authors for predicting elastic properties of single wall carbon nanotube reinforced composites. The above methods are compared and validated by G.M. Odegarda [17]. Both models include information about molecular interactions at the nanometer length scale into a continuum-mechanics based model. It is shown that the two approaches having the ability to predict elastic properties of SWCN/polymer composites in a combined range spanning dilute to hyper-concentrated SWCN volume fractions. In addition, the predicted Young’s moduli for a SWCN/polymer composite determined using both approaches are shown to be consistent and there is a reduction in predicted Young’s modulus compared to the classical rule-of-mixtures of about 15%.

The greatness of cnts as a reinforcement in composite material is studied by several authors. G. M. Odegard et al [18] predicted the effects of the chemical functionalization of a single-wall carbon nanotube on the resulting composites are evaluated using multiscale modeling techniques. Functionalization is nothing but making the strong covalent bond between cnts and matrix by some chemical agents. The effects of functionalization on the mechanical properties of cnt reinforced composites are determined that longitudinal elastic constants and longitudinal plane strain bulk moduli were reduced because of functionalization but transverse elastic , buckling and shear modulus are greatly enhanced. Similar study is extended to composite with aligned and random distribution of cnts in polymer matrix.

The sustainability of nanocomposites to different loading conditions is obtained by knowing the stress transfer between the nano reinforcement and the matrix material. The study of stress transfer in single walled carbon nanotube reinforced composites is evaluated analytically by A. Haque [19]. The proposed model of 2D representative volume element is able to determine axial stress and interfacial shear stress along the carbon nanotubes (CNT) embedded in matrix materials. The load transfer efficiency in cnt based composites is established in terms of an effective length of the cnt. H.L. Duan et al., [20] used micromechanical composites to deal the problem of surface/ interface stress effect at the nano-scale. The effective moduli of solids containing nano in-homogeneities in conjunction with the composite spheres assemble is analyzed by formulated micromechanical procedure. Closed form expressions are obtained for the bulk and shear moduli, which are function of the size of the in-homogeneities and interface properties.

The importance of surface/interface in the analyzing the deformations of the structures at nano scale is highlighted.

Composite material properties are improved by reinforcing highly potential carbon nanotubes in composite materials. The reinforcing carbon nanotubes are single walled carbon nanotubes, double walled carbon nanotubes, multi walled carbon nanotubes. Florian H. Gojney et al [21], focused on the assessment of the different type of nano-fillers and their influence on the mechanical properties of epoxy based composites. The significance of functionalization of nano reinforcements on the mechanical performance of the composites also included in the analysis. The influence of filler content, the varying dispensability, the aspect ratio, the specific surface area and an amino-functionalization on the composite properties are discussed and correlated to the identified micro-mechanical mechanisms. Authors suggested that CNTs are a valuable chemical additive for the modification of epoxies and other polymers. Especially, the combination with conventional fibre reinforcements can be a promising approach for future Perspectives in composite applications.

The interface of the carbon tube and matrix in the nano composites plays an important role in deciding the mechanical behavior of the resulting material. A.V. Desai et al [22] demonstrated the influence of nanotube polymer interface on mechanical performance of the composite materials. Extensive research has been performed on CNT–polymer composites using chemistry, mechanics and physics aspects. Various issues like processing of composites and experimental challenges are addressed which are required to get knowledge on understanding the structural applications.

Young’s moduli, Poisson’s ratio and stress- strain relationship of carbon nanotubes under tension and torsion loading are evaluated by J.R. Xiao [23] by adopting the principles of molecular structural mechanics. The cnt diameter and helicity has considerable effect on the Young’s modulus of the cnt. Young’s moduli of both armchair and zigzag carbon nanotubes reaches Young’s modulus of graphite when

the tube diameter is increased. Armchair nanotubes exhibit higher tensile strength than zigzag nanotubes but their torsion strengths are identical based on their study. G.M. Odegard et al [24] further extended the molecular modelling and continuum methodologies to silica nanoparticles/polyimide composites considering the interface. The micromechanics are one of the important analyses in the composite material using continuum approach. The authors included an effective interface between the polyimide and nano particle with properties and dimensions that are determined using the results of molecular dynamics simulations. The model proposed used to predict the elastic properties of silica nano particle/polyimide composites for a large range of nano particle radii, 10–10,000 Å. For silica nano particle radii above 1000 Å, the predicted properties are equal to those predicted using the standard Mori–Tanaka micromechanical approach, which does not incorporate the molecular structure. It is also shown that the specific silica nano particle/polyimide interface conditions have a significant effect on the composite mechanical properties for nano particle radii below 1000Å.

Dong-Li Shiet al [25] presented a multiscale mechanics method to study the deformation and fracture of CNTs embedded in a composite. The unit cell selected for the analysis is incorporated three regions, simulated by using atomic-potential method, the atomistic-based continuum method, and the continuum mechanics, respectively. Some represented CNTs embedded in a composite are used to calculate the critical strain. The influences chiral angle and diameter of CNTs as well as the elastic constant of matrix on the Stone–Wales defect formation and fracture behavior are investigated.

A three dimensional finite element method is applied to determine the mechanical properties of single wall carbon nanotubes with different configurations are studied by K.I. Tserpes [26]. The model is created by using the concepts of atomistic description of atoms and bond between the atoms. The influence of nanotube wall thickness, diameter and chiral vectors on the elastic properties of single wall nanotubes of armchair and zigzag configurations is considered in the analysis. The Young’s modulus of Swnts increases with diameter. The chiral nano tubes showed greater Young’s modulus than armchair and zigzag nano tubes.

Behnam Ashrafi et al [27] predicted the elastic properties of single-walled carbon nanotube (SWNT) arrays and their composites. The twisted SWNT nano arrays with circular cross section properties are determined using the strain energy of the resulting structure applying finite element method. The study also includes the effect of aspect ratio of the nano array and volume fraction of the reinforcement of a composite material with aligned and random distribution of reinforcement using conventional micromechanics. Finally, elastic properties of the twisted SWNT nano-array/polymer composites are compared to the results from constitutive model of individual nanotube-reinforced polymer composites.

Stone–Wales (SW) defect is one of the most commonly present topological defects; which effects on the mechanical behavior of carbon nanotubes needs to be analyzed. In this work, the effect of SW defect on the tensile behavior and fracture of armchair, zigzag and chiral single-walled carbon nanotubes (SWCNTs) was studied by K.I. Tserpes [28] using an atomistic-based progressive fracture model with finite element method. Nanotube chirality is a controlling parameter of the defect (sw) on the tensile behavior of the SWCNTs. In armchair SWCNTs, a considerable reduction in failure stress and failure strain was predicted. In chiral SWCNTs, the effect of the defect is between those of the armchair and zigzag SWCNTs, depending on chiral angle.

The mechanical properties of single walled carbon nanotubes are predicted by Michele Meo [29] using finite element (FE) method with the association of molecular mechanics. Nonlinear and torsional springs are used to represent the bonds between the carbon atoms. The dependence of Young’s modulus on the Swnts diameter and chirality is also studied. In particular, armchair, zig-zag and chiral nanotubes, with different size, were tested under uniaxial load. The results show that good agreement was achieved with existing experimental results. The presented results demonstrate that the proposed FE model may also provide a valuable numerical tool for the prediction of the strength behaviour of single walled carbon nanotubes.

H. Ding et al [30] adopted atomic scale finite element (AFM) method to find out Young’s modulus of single wall carbon nanotube. The carbon nanotube is modelled by treating a carbon atom as a node and the bonding between the atoms are modelled as a beam element. The beam element selected for the analysis is able to show the covalent bond characteristics. The material properties of beam elements can be determined by using a linkage between molecular and continuum mechanics. The thickness of cnts has considerable impact on their Young’s modulus. The authors are also evaluated the thickness effect on the Young’s modulus of the cnt using same approach. For the values of wall thickness used in this study, the obtained values of Young’s modulus agree well with the corresponding theoretical results. Furthermore, the results also illustrate that Young’s modulus is inversely proportional to the wall thickness. The presented results demonstrate that the proposed AFE
The damage debonding on the particulate filled composite is evaluated by using two multiscale homogenization schemes: one is based on a closed form micromechanics solution and other on the finite element implementation of mathematical theory of homogenization by H.M. Inglis et al [31]. A detailed comparative assessment between the two homogenization schemes is presented, with emphasis on the effect of volume fraction, particle size and particle-to-particle interaction. The plane strain micromechanics model is effective at capturing key features of the macroscopic stress-strain response. The limitations of this model are that it cannot capture the instability inherent in the system or the heterogeneous stress and strain fields. Both models demonstrate that, for large differences in particle diameters, it is unnecessary to model the debonding of smaller particles, but it is sufficient to represent their contribution to damage nucleation and to the stiffness of the matrix.

A. Selmi et al [32] used micromechanics analogies to predict the elastic properties of polymer composites reinforced with single walled carbon nanotubes. The authors used several micromechanics approaches and compared their merits. Four homogenization schemes, a sequential one and three others based on various extensions of the Mori–Tanaka (M–T) mean-field homogenization model: two-level (M–T/M–T), two-step (M–T/M–T) and two-step (M–T/Voigt). Several composite systems are studied, with various properties of the matrix and the graphene, short or long nanotubes, fully aligned or randomly oriented in 3D or 2D. The results are validated by experimental and finite element methods. The comparative study showed that there are cases where all micromechanical models give adequate predictions, while for some composite materials and some properties, certain models fail in a rather spectacular fashion. It was found that the two-level (M–T/M–T) homogenization model gives the best predictions in most cases.

The finite element analysis is used to determine Young’s modulus, shear modulus and coefficient of thermal expansion for graphene sheet as well as SWCNTs. The analysis is performed by Sushen Kirtania et al. [33] by analyzing armchair and zigzag SWCNTs and graphenesheets based on the assumption that CNTs, when subjected to loading, behave like space-frame structures. From the analysis the important conclusions are revealed. The authors revealed that the increase in the size of the graphene sheet, the Young’s modulus increases, with the increase in tube diameter of SWCNT, the elastic moduli of both armchair and zigzag carbon nanotubes (CNTs) increase monotonically, and approach the Young’s modulus of graphene sheets for large diameters.

Reinforcing efficiency of two different nanoparticles with different cross section is determined by Hua Liu et al [34] using micromechanics approach. The inter-phase zone plays a crucial role to transfer the load from reinforcement to the matrix. The interphase created by host polymer on the nano reinforcement is highlighted. The authors showed that nano-tubes have superior mechanical reinforcement potential beyond that of nanoplatelets for aligned orientations, while the high in-plane isotropic modulus of nano-platelets allows better reinforcing in random orientations. The authors highlighted that at the same volume fraction of the reinforcement the interphase area is more in nanotubes than nano platelets this yields the higher stiffness for all configurations of nanotube reinforced composites.

Song Hai Yang et al [35] determined the Mechanical properties of nano-single crystal gold and carbon nanotube-embedded gold composites under axial tension using molecular dynamics (MD) simulation method. Lenard–Jones (L–J) potential is used to model the interactions between the constituents of nano composites. The yield strain and the yield stress of nano-single crystal gold are 0.092, 5.74 GPa respectively. The results of the present work show that the increase in Young’s modulus of the long CNT-embedded gold composite over pure gold is much large and yield stress and the yield strain of short CNT-embedded gold composite are evidently less than that of the nano-single crystal gold.

The differences between the response of the single walled and double wall carbon nano tubes are determined by R.C. Batra et al [36] using Molecular mechanics (MM). Vander Waals force expression is provided from the results of radial expansion/contraction of a SWNT. The multi wall nanotubes are modelled using continuum method. The mechanical deformation obtained using analytical expression is compared with results of MM simulations. The proposed continuum model is validated by studying bending and the onset of global buckling deformations of a DWNT and its proposed equivalent continuum structure. Carbon nanotubes can be replaced by their equivalent continuum structures when deriving mechanical properties of nanotube reinforced polymeric composites.

Elastic properties of single walled carbon nanotubes influenced by several parameters like temperature, environmental conditions. The influence of temperature on the elastic properties of swnts is determined by X.Chen et al [37] using molecular structural mechanics. Two node Euler–Bernoulli beams is used to model the
bonds between the carbon atoms. The effect of environmental temperature on force constants of the bond stretching, bending and twisting of the bonds are determined to reach the objective of the work. Nano-scale finite element simulations of the elastic properties of single-walled carbon nanotubes under different environmental temperatures reveal that the elastic modulus of single-walled carbon nanotubes decreases significantly with the increase of temperature. It is noted that the Young’s modulus of armchair nanotubes is more sensitive to environmental temperature due to the tube chirality.

The influence of swnt loading on the mechanical performance of the nano composites is investigated by Nyan-Hwa Tai et al., [38]. The Swnts used for analysis is synthesized by catalyst chemical vapor deposition method. Authors identified that a small of SWNTs can enhance significantly the mechanical properties of the composites. A small loading of swnts can improve the mechanical properties of composite material significantly like Young’s modulus increases 29.7% and the tensile strength increases 20.3% when 0.75 wt% and 2.0 wt% SWNTs were introduced to the phenolic matrix, respectively. The modified Halpin–Tsai equations were adopted to fit the experimental data of the tensile strength and Young’s modulus of the SWNTs/phenolic composites. The authors concluded that bundle bridging, SWNT loading, uniform dispersion of SWNTs, and the wetting at interface are the key parameters for strengthening the composites.

The mechanical performance of multi walled carbon nanotubes are depends on the environmental condition. Y.C. Zhang et al [39] studied the dependence of mechanical characteristics on the environmental factors using molecular mechanics. The covalent bonds are replaced by Euler–Bernoulli beam and the attraction or repulsion forces between the nanotubes i.e vander wall’s forces are simulated by nonlinear springs. The environmental temperature has significant influence on the Young’s modulus and Poisson’s ratios of multi-walled carbon nanotubes. The authors noticed that the Young’s modulus of multi-walled Zigzag CNTs is more sensitive to environmental temperatures due to the tube chirality. Last, the relationship between Young’s modulus of double-walled CNTs and environmental temperature is given by a simple formula.

In S.R Malik [40] work demonstrated that carbon nanotubes are obtained by rolling the plane graphite sheet. The carbon nanotubes have unique electrical and mechanical properties. The carbon nano tubes are used in two forms; one is single wall carbon nano tube (SWNT) and multi wall carbon nanotube (MWCNTs). SWCNTs tend to be stronger and more flexible than MWCNTs. Their interesting electronic structure makes CNTs ideal candidates for making novel molecular devices. Both metallic and semi-conducting SWNTs are found to possess electrical characteristics that are comparable favourably to the best electronic materials available. The interface of the constituents in the composite material plays very vital role in transferring load and resulting stresses. H.Wang et al [41] determined the interface effect on nano composites using molecular and continuum modeling techniques with finite element method. There study considers the Swnts of arm chire and zig-zag configurations and Dwnts as a reinforcement phase. The authors concluded that arm chair cnts reinforced composite shows good mechanical response than zig-zag cnts reinforced composites at same diameter. And Swnts reinforced composites having more beneficial than multi walled cnts reinforced composites. Heat transfer behavior of micro-nano fiber-reinforced composites developed analytically to predict the transverse thermal conductivity is proposed by Birgul Ascioglu et al [42]. The hexagonal unit cell is adopted to reach the objective of the problem. Thermal-electrical analogy method is used in the analytical model. The thickness of the interface (barrier) on the transverse thermal conductivity is studied by comparing the values with and without the barrier. The dependence of the transverse thermal conductivity on the filler volume fraction and interface thickness is studied. The model showed that increasing the volume fraction of the filler inside the matrix and barrier thickness increases the total effective thermal conductivity of the resulting composite. Material property characterization for tensile, fatigue life and inter-laminar fracture toughness were determined for hybrid composites and compared with the traditional fiber-matrix composite materials by Oladapo Akinyede et al [43]. Advanced composites are hybridized by the integration of alumina nanoparticles into the matrix and onto the fabric surface. Vacuum assisted resin transfer molding (VARTM) was used to fabricate the composite panels. Mode-I fracture toughness was significantly improved with the inclusion of alumina nanoparticles which is determined by experimental characterization. However, the influences on the tensile behavior and tension/tension un-notched fatigue behavior in [0/90] configuration were not significant. In applications that involve only tension/tension fatigue loading, hybrid composites with nano -particulate inclusions can provide improved delamination failure characteristics without impacting fatigue life and tensile behavior significantly. J. R. Xiao [44] determined the mechanical response of graphene sheet and single walled nanotubes under tension condition using the modified Morse potential function into a novel atomistic finite bond element.
molecular structural mechanics model. The model described by authors is used for predicting Young’s moduli, Poisson’s ratios, and stress-strain relationships of graphene sheets and nanotubes with or without a SW defect. A methodology to create multiple defects in a CNT at given locations has been implemented into our MATLAB code. The resulting simulations were able to predict the Young’s modulus, ultimate strength, and strain at failure. Results including the effects of defects more closely match experimental data reported in the literature.

The failure of CNT/polymer composites by combining micromechanics and finite element simulation are prescribed by Chunyu Li [45]. The waviness of cnts and random distribution of cnts in the matrix are investigated and compared with aligned distributed straight tubes. The results show that nanotubes waviness tends to reduce the elastic modulus but increase the ultimate strain of a composite. The randomness of nanotubes distribution tends to reduce both the composite elastic modulus and tensile strength. The damage initiation and evolution in composites with random wavy nanotubes have also been analyzed. But the evolution of damage is strongly influenced by the waviness as well as the distribution and aspect ratio of nanotubes. It should be noted that because of the randomness in nanotubes distribution, the mechanical behavior of such CNT/polymer composites is actually statistical in nature and variations in simulation results are expected.

The bending and buckling characteristics of SWNTs are carried out using finite element method by Ratnakar Pandu et al [46]. Natural frequencies and frequency response of Swnts are simulated by using shell element of Ansys software. The analysis is performed by modeling the cantilever beam and loaded at the free end to obtain model and harmonic analysis under axial compression and bending loading. The computed results for SWCNTs agree well with atomistic simulations in the literature and the FE approach is confirmed successfully. The crack closure techniques are applied for the Mode I interlaminar fracture of laminated composites reinforced with aligned carbon nanotubes by Joaquin Blanco et al [47]. The models considered for the analysis are independent of the scale of reinforcement and significant enhancement in the toughness is identified at the present scale. Analytical expressions are framed for crack growth resistance. The model is validated with experimental results of Z-pins and aligned cnts.

The mechanical properties of polymer composite material containing clay nanoparticles fillers are demonstrated by an analytical expression using micromechanical methods by Jin Y. Park et al., [48]. The effect of debonding is included in the analytical model between the reinforcement and the matrix of the composite material. The results obtained from the work are validated by experimental means. For the experimental program, clay/epoxy nanocomposite specimens were fabricated and tested. The developed model was also compared to the conventional and previously developed micromechanical models.

Damping characteristics of carbon nanotube-based composites are investigated with analytical method by R.M. Lin et al [49]. Interfacial slip is existed between the constituents of the nano composites. The proposed model is used to find the damping behavior of the nano composites considering the interfacial slip between the nanotubes and between nanotube and matrix material. The loss in the damping factor of the nano composites depends on its constituent’s properties, structural response, volume fraction of the phases and interfacial shear stress. The damping loss factor is high as 20% is obtained for small volume fraction of 1% of cnts in the composite material.

Interlaminar and intralaminar behavior of woven polymer matrix composites with aligned carbon nanotubes are determined by Sunny S. Wicks et al [50] using theoretical and experimental methods. Better performance is observed for Mode I interlaminar fracture toughness using CNT-pull-out toughening via bridging model compared to stitching and Z-pinning methods. The magnitude of predicted toughening is strongly dependent on CNT pull-out length, and is limited by the strength of the reinforcing CNTs. The toughness of the model is improved by 76% in steady state due to aligned cnts bridge at the ply interface. The developed analytical model is correlated to the experimental fracture data. In the plane of the laminate, aligned CNTs developed the tension bearing response of 19% in bearing stiffness, 9% in critical strength, and 5% in ultimate strength which changes the failure mode from shear-out failure (matrix dominated) without CNTs to tensile fracture (fiber dominated) with CNTs.

The first known model of damping behavior of cnt based composites was developed by Ailin Liu [51]. Damping behavior of nano polymer composites reinforced by nanotubes with aligned and random distribution is predicted. The shear strength at the interfaces are determined by using molecular dynamics simulation. The micromechanical damping model is generated by using shear strength at the interface determined from molecular dynamics. The resin is modeled as a viscoelastic material using a three-element standard solid model. The concept of stick-slip motion is used to describe the load transfer behavior between carbon nanotubes in a rope as well as between nanotubes and the surrounding sheath. Energy dissipated from the viscoelastic polymer matrix and from
the stick-slip motion contributes to the overall structural damping characteristics. The proposed model is used to study the damping behavior of CNT/polymer composites under tension tension and tension compression cyclic loads.

Giovanni Formica et al [52] determined the vibrational behavior of CNT reinforced composites by using equivalent continuum model based on the Eshelby-Mori–Tanaka approach. The global elastic model responses of nano structured composite plates are determined. Three different matrix materials (epoxy, rubber, and concrete) with embedded single-walled CNTs are considered for the analysis. The numerical simulations are performed with finite element method. The fracture response of graphene nano sheet with a center crack is analyzed by Jia-Lin Tsai [53] et al using atomistic and continuum mechanics. The change in the strain energy due to extension of pre existed crack is determined using atomistic approach. Mode I and Mode II were measured under tensile and shear loading are determined. Results indicated that the strain energy release rates obtained from the continuum model exhibit good agreement with those derived from discrete atomistic model. The interaction between CNT and matrix is modelled by nonlinear springs based on Lennar-Jonze potential. Horacio V et al [55] used the finite element method to perform the model analysis of laminated plate. The model analysis is used to obtain the tensile and shear modulus and Poisson’s co efficient of the composite plate. Similarly the study is carried out by preparing a laminate sample with S2 glass epoxy. Instead of using pure epoxy nanotube reinforced epoxy is used to prepare a laminate sample. The effective of nano mixed matrix is obtained. Antonio F. Avila et al [56] evaluated the vibration behavior of graphite nanostructures using molecular mechanics simulation. Under cantilevered condition nanotubes show the fundamental frequencies range is 10 to 250GHz and for bridged condition CNT can exhibit 100 to 1000 GHz frequency. The authors observed that for single wall nanotube, the stiffness was affected by two important factors, one is the curvature and another one is the diameter of the SWNT. The curvature effect is more evident on small diameter nanotubes. The Poisson’s ratio values are calculated for armchair, chiral, zigzag nanotubes. Moreover, in all three cases, i.e., armchair, zigzag and chiral the Poisson ratio seems to reach an asymptotic value after 1.0 nm diameter. Further the work is extended to study the multilayered graphene nano sheets by incorporating vander Waals forces between the layers.

The influence of multi-walled carbon nanotubes (MWCNTs) on the mechanical properties of epoxy/MWCNT nano-composites were studied by M.R. Ayatollahi et al [57]. The fracture toughness of the nano composites depends on the type of loading. The presence of MWCNTs had a greater effect on fracture toughness of nano-composites under shear loading compared with normal loading. Fracture mechanisms are studied by using fracture surface images captured from scanning electron microscopy (SEM). An association was found between the characteristics of fracture surface and the mechanical behaviors observed in the fracture tests. J.S. Snipes et al [58] used Generalized Method of Cells (GMC) micromechanics model to predict the properties of nano composites. The nano composite material is prepared by reinforcing gold nano rods in polymer matrix. The interphase stiffness effect on the properties also included. Experimental studies exploded that an elastically stiff interface greatly increases the stiffness of the polymer in response to an ‘instantaneous’ step load, reduces the rapid creep response, and results in a rapid leveling off of the time-dependent strain curves. The response of the composite to increasing stiffness of the interface region eventually reaches a threshold value, where further increases in the stiffness of the interface produces negligible increases in stiffness, or further reduction in creep response.

Carbon nanotube reinforced composites mechanical properties are evaluated by U. A. Joshi [59] using continuum mechanics approach. Two different represented volume elements of Hexagonal and square shapes selected to carry out the work. Numerical equations are used to evaluate the mechanical properties from numerical solutions for the hexagonal RVEs under the lateral load case. An extended rule of mixtures is applied to evaluate the effective axial Young’s modulus, for validation of the proposed model. For long CNTs better stiffness is observed in CNT direction than transverse direction. Long carbon nanotubes reinforced composites are very effective than short CNTs reinforced composites and the resulting Young’s modulus are compared with the analytical expressions. Enhanced reinforcement is observed along the lateral direction compared to the axial, when short CNTs are considered under the effect of lateral load.


[52-71]
E. Jomehzadeh, and A.R. Saidi [60] presented large amplitude vibration analysis of multilayered graphene sheets. Nonlinear vibrations based on harmonic balance method are obtained for graphene sheet with three different boundary conditions. The numerical simulation is performed for single, double, triple layered graphene sheets of arm chire and zigzag type configuration are considered. The results obtained from the present work are compared with those available in the literature for linear vibration of multilayered graphene sheets and an excellent agreement is found. The nonlinear behavior of graphene sheet is extracted by varying the number of layers, geometric properties.

B. Ramgopal Reddy et al [61] investigated the free vibrational analysis of carbon nanotube reinforced laminated composite panels. Three types of composite panels are considered for the study such as flat, concave and convex. Numerical simulation is carried out using commercially available finite element analysis software ANSYS. Numerical homogenization is employed to calculate the effective elastic properties of randomly distributed carbon nanotube reinforced composites. To verify the accuracy of the finite element method, comparisons are made with existing results available in the literature for conventional laminated composite panels and good agreements are obtained. The results of the CNT reinforced composite materials are compared with conventional composite materials under different boundary conditions.

Size and shape effect of the inclusions in the composite properties are evaluated by V. K. Srivastava et al [62]. There study includes cylindrical fibers, spherical and elliptical particles and cylindrical fibers with hemispherical ends. The analysis is based on a numerical homogenization technique using finite element method in connection with three-dimensional representative volume element models. The effect of volume fraction, aspect ratio and particle distribution on mechanical performance of composites also studied.

Elastic properties of carbon nanotube reinforced composites are evaluated by analyzing the elastic deformation of a representative element (RVE) subjected to different loadings by N Hu et al [63]. The RVE of the analysis includes carbon nano tube, a transition layer between the nanotube and polymer matrix and an outer polymer matrix. The analysis is carried out by using force field theory of molecular mechanics and computational structural mechanics to construct carbon nanotube as equivalent beam model. From the analysis authors found that the shear modulus of transition layer strongly depends on the deformation in a form of nonlinearity. When the Young’s modulus of transition layer ranges from 3 to 100 GPa, a stronger transition layer can result in significantly higher Young’s modulus in longitudinal direction. However, when transverse Young’s modulus is higher than 100 GPa, the effect of stiffness of transition layer becomes weak. The interlaminar shear strength of carbon epoxy and carbon epoxy carbon nanotube composites is determined by P. Rama Lakshmi et al [64] using experimental and finite element methods. Double notched specimen mechanical properties are estimated from finite element based software Ansys. To determine the carbon epoxy carbon nanotube composite properties, finite element model of matrix and carbon nanotube is generated. From the obtained stretch and stress, the equivalent material property of combined matrix and carbon nanotube is achieved. The advantage of the carbon nanotubes in the composite materials is proved from experimental and finite element technique from the estimated fracture parameters.

The variation of Young’s modulus of carbon nano tube with respect to the wall thickness is estimated by S. Prabhu et al [65] using molecular mechanics in association with finite element method. The developed model is based on the assumption that cnts behaves like space frame structures subjected to loading. In the finite element model generation nodes are used as carbon atoms and covalent bond between the atoms are represented by spring elements. The study includes different cnt configurations effect on the Young’s modulus.

Bi axially compressed graphene sheet buckling properties are obtained by S C Pradhan [66] using non-local elasticity theory. Levy’s approach is applied to solve the governing equations for various boundary conditions of the graphene sheet. Present results from Levy’s solution agree with the results for all edges simply supported available in the literature. The authors observed that non-local parameter and boundary conditions significantly influence the critical buckling loads of the small size graphene sheets.

The Young's modulus of carbon nanotubes are determined by Roham Rafiee [67] with non-linear finite element model. The molecular interactions in atomic structure of carbon nanotubes are represented by spring elements. Non linear finite element method is adopted to model a graphene sheet and several Armchair and Zigzag CNTs. The effect of chirality and diameter on cnt on the Young’s modulus of single walled carbon nanotubes is performed. Unlike the results of presented linear finite element models, the results of non-linear model imply on independency of Young’s modulus from chirality and...
diameter. The results obtained from their study are in a fine agreement with experimental observations and published data.

One of the important tools useful for predicting the behavior of composite material is Finite Element modeling. G.S. Venkatesh et al [68] predicted the finite element analysis results quantitative information on the effect of reinforcing polypropylene (PP) with various proportions of nanoclay is obtained through experiments. The Young’s modulus, tensile strength and failure strains are obtained from the experiments conducted on the above mentioned material. The validity of the modeling procedure is established by micromechanical finite element analysis in association with Monte Carlo simulation and accuracy of prediction is examined by comparing against experimentally determined stiffness moduli of nanocomposites.

Gouthamkumar Yarlagadda et al [69] modelled carbon nanotube using molecular and finite element method. The nodes of carbon atoms are connected with shell elements of finite element based software Ansys. The elastics properties of the shell elements which represents the bond between the carbon atoms are obtained by using the linkage between molecular and continuum mechanics. Influence of elastic moduli to diameter and length of the nanotubes is also obtained. M. Zakeri et al [70] determined different structures of short single-walled CNTs mechanical properties using finite element method. The geometry of CNTs is generated by using a simple algorithm. The effect of chiral angle from 0 to 30 degree at constant length to radius ratio, on its mechanical properties is evaluated. It is observed that the tensile modulus of CNTs changes between 0.93-1.02 TPa for different structures, and it can be higher for chiral structures than zigzag and armchair ones. Also, for different chiral angles, the bending modulus changes between 0.76-0.82 TPa, while the torsional modulus varies in the range of 0.283-0.301TPa.

P.K.Chidambaram [71] proposed a work on synthesis, mechanical testing and structural analysis of four ratios of Nylon6,6/MWNT new nanocomposite material to a tennis racket frame. The string of the racket frame is modelled by nylon fibers. The mechanical properties of the nanocomposite are obtained by using universal testing machine. To design the racket the author used PRO/ENGINEER software. The racket model can be export to ANSYS analysis software in order to analysis the mechanical properties of the new nanocomposite and structural analysis of the racket, especially the impact of tennis ball with string bed of the racket frame. Natural frequencies of single wall carbon nanotubes are determined by Mostafa Mohammadian Ref [72] using finite element method. Theoretical equation is used to find the natural frequency of a cantilever beam. The finite element model of molecular level cnt is prepared for zig zag and armchair configurations. Diameter of the cnt is considerable effect on the Young’s modulus for both zigzag and armchair. Also the values of Young’s modulus obtained by this method are in good agreement with the findings of other researchers.

The usage of the nano graphene sheets as a filler material in the composite material is demonstrated by Avinash Parashar et al [73]. The representative volume element using finite element method is developed to predict the buckling behaviour of graphene reinforced composites. Two modelling techniques are used to evaluate the buckling behaviour of the resulting nano composite material. The graphene sheet is modelled by using molecular mechanics method and the matrix is modelled with continuum approach. Representative volume elements are modelled for graphene sheet and for graphene reinforced composites. Considerable improvement in buckling strength is observed for graphene reinforced composites under compressive load over the pure polymer.

The virtual crack closure technique is used to know the fracture behaviour of the graphene reinforced composites using multi modelling techniques by Avinash Parashar et al [74]. The graphene is nano sheet and the matrix is a continuum material. The graphene sheet is modelled with atomistic modelling technique and the interaction between the nano graphene sheet and matrix material is modelled with truss elements which is able to define the vander wall forces. The graphene volume fractions, high aspect ratio, distribution of graphene in the polymer matrix are enhancing fracture toughness of resulting composites.

The high slenderness of cnts has significant curvature effect in the polymer when these are reinforced. Md. A. Masud et al [74] determined the curvature effect on the effective tensile elastic modulus of cnt based composites using three dimensional finite element methods. The analysis is performed for both long and short cnt reinforced composites. The effective tensile elastic modulus of nanocomposites decreases with the increase in wavelength of CNT for a fixed amplitude and CNT diameter for both the case of short and long CNT. The nano reinforcement can improve the properties of composite material in terms of wear resistance, damping properties and mechanical strength and stiffness. Generally used metal matrix materials are Al, Mg and Cu. Riccardo Casati et al [75] reviewed several important manufacturing techniques in synthesis of bulk metal matrix nanocomposites. The mechanical properties
improvements through some strengthening mechanisms are also highlighted.

Conclusion
The present paper addresses the key findings of nano reinforcement and nano composites using different approaches like molecular, continuum, analytical studies.

References


