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MODELING TECHNIQUES FOR DETERMINATION OF MECHANICAL PROPERTIES OF POLYMER NANOCOMPOSITES

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Abstract. A review of modeling techniques for predicting the mechanical behavior of polymer nanocomposites is presented. A detailed discussion of Computational Chemistry and Computational Mechanics modeling techniques is given. 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. In addition to the discussion of the methods, specific results from recent studies are presented and compared. From these results, the general focus of current polymer nanocomposite modeling studies is summarized.

1. INTRODUCTION

In 1985, Smalley and co-workers at Rice University discovered cage-like carbon structures known as fullerenes; named after R. Buckminster Fuller [1]. These fullerenes are C_{60} molecules with 'buckyball' or 'truncated icosahedron' structure consisting of 20 hexagons and 12 pentagons with a nearly spherical shape. In 1991, Iijma discovered carbon nanotubes [2]. Carbon nanotubes are closed graphene sheets with a cylindrical shape with end caps. They can be described as long and slender fullerenes. Research has shown that carbon nanotubes exhibit exceptional mechanical properties [3]. Although there has been some variation in the reported values for the carbon nanotube mechanical properties, the elastic modulus has been shown to be greater than 1 TPa and the tensile strength exceeds that of steel by over an order of magnitude. In view of the exceptional mechanical properties of carbon nanotubes, they have been considered as ideal reinforcements in composite structures. For nanotube composite materials, it has been shown that a carbon nanotube weight fraction of 1% results in the same increase in composite elastic modulus as a composite with a 10% weight fraction of carbon fibers, based on results from short-fiber composite theory [4]. This difference in elastic modulus is predicted even though the size scale of the two reinforcements differs by three orders of magnitude [5].

Nanopartcles with high aspect ratios have proven to be good reinforcing agents in polymeric materials [6]. Among all nanoparticle reinforced composites, the most widely investigated systems are based on silicates and clay particles. Ahn *et al.* reported that the tensile modulus of composites reinforced with unmodified silica nanoparticles improved upon increasing the silica content, however, the elongation to failure decreased [7]. A research group at Toyota developed an economic industrial process for the

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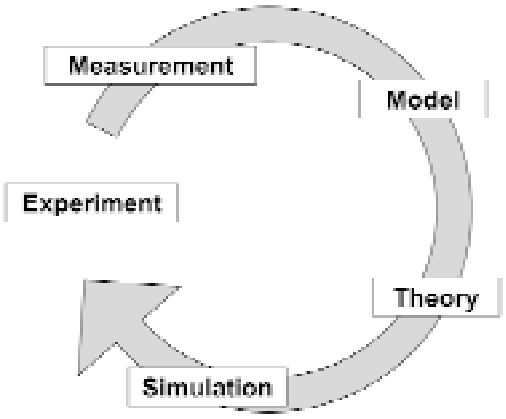

Fig. 1. Schematic of the process of developing theory and the validation of experimental data (adapted from [24]).

manufacture of polymer/clay nanocomposites. This work led to the development of composites with twice the Young's modulus as that of the pure polymer. The increase in Young's modulus was also observed at elevated temperatures [8,9].

The tremendous mechanical properties of carbon nanotubes and other nano-reinforcements can be realized only if efficient load transfer exists between the matrix and reinforcement [10-13]. It has been shown that in some cases the load transfer between nanotubes and the surrounding matrix can be increased by introducing non-bonded interfacial compounds or chemical crosslinks between nanotubes and the matrix [14-17]. Despite these early efforts, more research is required to fully understand the effects of molecular structure of the nanotube/polymer interface on overall composite mechanical properties. Although experimental-based research can ideally be used to determine structure-property relationships of nanostructured composites, experimental synthesis and characterization of nanostructured composites demands the use of sophisticated processing methods and testing equipment; which could result in exorbitant costs. To this end, computational modeling techniques for the determination of mechanical properties of nanocomposites have proven to be very effective [18-25]. Computational modeling of polymer nanocomposite mechanical properties renders the flexibility of efficient parametric study of nanocomposites to facilitate the design and development of nanocomposite structures for engineering applications.

This review article will discuss the major modeling tools that are available for predicting the mechanical properties of nanostructured materials. Analytical and computational approaches to continuum-mechanics based modeling are discussed. Computational chemistry modeling approaches are also discussed in detail. Results found in the literature for the various modeling tools are tabulated and compared for six polymer nanocomposite systems. The comparison emphasizes the flexibility of the modeling approaches for different polymer nano-composite geometries.

2. MODELING METHOD OVERVIEW

The importance of modeling in understanding of the behavior of matter is illustrated in Fig. 1. The earliest attempt to understanding material behavior is through observation via experiments. Careful measurements of observed data are subsequently used for the development of models that predict the observed behavior under the corresponding conditions. The models are necessary to develop the theory. The theory is then used to compare predicted behavior to experiments via simulation. This comparison serves to either validate the theory, or to provide a feedback loop to improve the theory using modeling data. Therefore, the development of a realistic theory of describing the structure and behavior of materials is highly dependent on accurate modeling and simulation techniques.

Mechanical properties of nanostructured materials can be determined by a select set of computational methods. These modeling methods span a wide range of length and time scales, as shown in Fig. 2. For the smallest length and time scales, Computational Chemistry techniques are primarily used to predict atomic structure using first-principles theory. For the largest length and time scales, Computational Mechanics is used to predict the mechanical behavior of materials and engineering structures. Computational Chemistry and Computational Mechanics modeling methods are based on thoroughly-established principles that have been developed in science and engineering. However, the intermediate length and time scales do not have general modeling methods that are as well-developed as those on the smallest and largest time and length scales. Therefore, multiscale modeling techniques are employed, which take advantage of Computational Chemistry and Computational Mechanics methods simultaneously for the prediction of the structure and properties of materials.

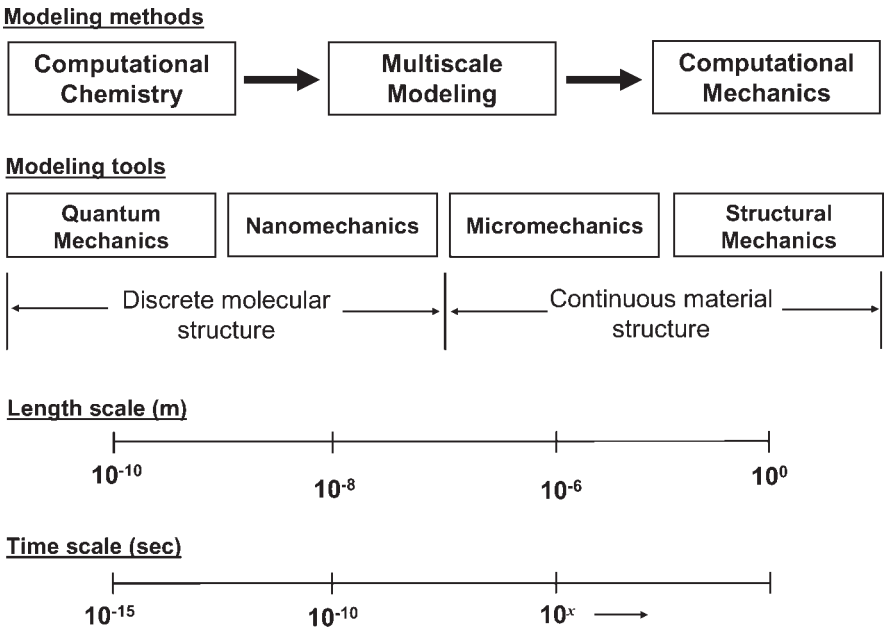

Fig. 2. Various length and time scales used in determining mechanical properties of polymer nanocomposites.

As indicated in Fig. 2, each modeling method has broad classes of relevant modeling tools. The Quantum mechanical and Nanomechanical modeling tools assume the presence of a discrete molecular structure of matter. Micromechanical and Structural Mechanics assume the presence of a continuous material structure. Fig. 3 is a schematic that details the relationship of specific modeling techniques in Computational Mechanics and Computational Chemistry. The continuum-based methods primarily include techniques such as the Finite Element Method (FEM), the Boundary Element Method (BEM), and the micromechanics approach developed for composite materials. Specific Micromechanical techniques include Eshelby approach, Mori-Tanaka method, Halpin-Tsai method [26-36]. The molecular modeling tools include molecular dynamics, Monte Carlo, and Ab-initio tech-

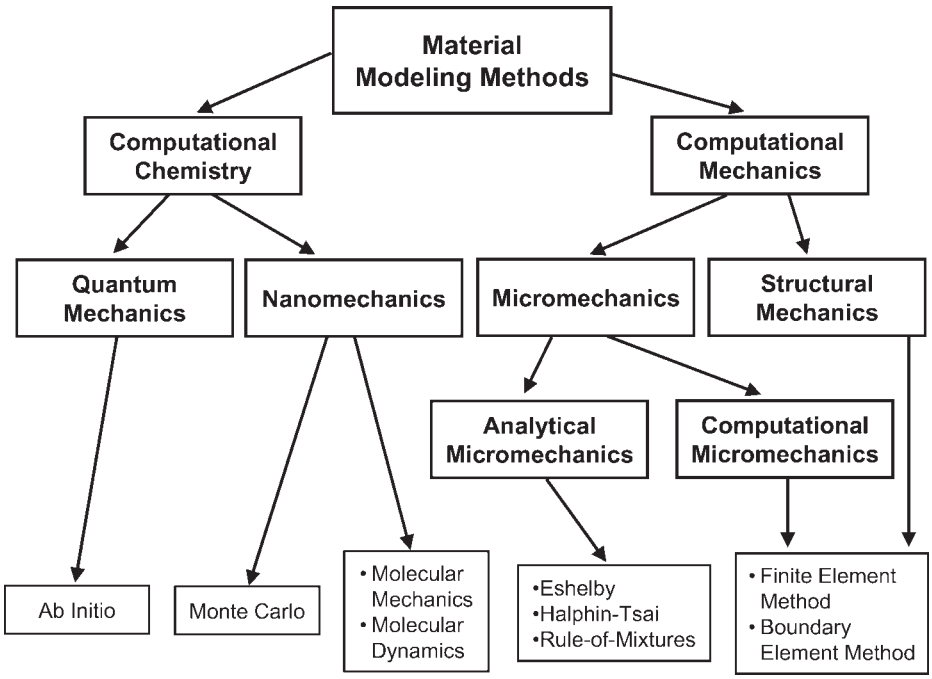

Fig. 3. Diagram of material modeling techniques.

niques. Each of these continuum and molecular-based modeling methods are described below.

3. CONTINUUM METHODS

These modeling methods assume the existence of continuum for all calculations and generally do not include the chemical interactions between the constituent phases of the composite. These methods can be classified as either analytical or computational.

3.1. Analytical continuum modeling

The overall properties of composites can be estimated by a volume average stress and strain fields of the individual constituents [37]. The overall stress and strain of a composite with *N* distinct phases can be represented as follows

$$\bar{\sigma} = \sum_{r=1}^{N} c_r \bar{\sigma}_r, \tag{1}$$

$$\bar{\varepsilon} = \sum_{r=1}^{N} c_r \bar{\varepsilon}_r, \tag{2}$$

where σ_r is the stress tensor and ε_r is the strain tensor of phase *r*, c_r is the volume fraction of phase *r*, and the overbar denotes a volume-averaged quantity. The constitutive equation for each phase is given by

$$\sigma_r = C_r \varepsilon_r, \tag{3}$$

where C_r is the stiffness tensor of phase *r*. The constitutive relationship between stress and strain for a composite material is given in terms of volume averaged stress and strain fields

$$\bar{\sigma} = C\bar{\varepsilon}. \tag{4}$$

The volume average strain of phase *r* is

$$\bar{\varepsilon}_r = A_r \bar{\varepsilon}, \tag{5}$$

where A_r is the concentration tensor of phase *r* and

$$\sum_{r=1}^{N} c_r A_r = I, \tag{6}$$

where *I* is the identity tensor. Combining above equations results in the stiffness tensor in terms of the constituent stiffness tensors,

$$C = C_1 + \sum_{r=2}^{N} c_r (C_r - C_1) A_r. \tag{7}$$

Different methods exist for evaluation of the concentration tensor. When $A_r = I$; the above equation results in the rule-of-mixtures approach. Neglecting the interaction between the reinforcing particles results in the dilute concentration approximation. The dilute concentration tensor is given by

$$A_r^{dil} = \left[I + S_r C_1^{-1} (C_r - C_1) \right]^{-1}, \tag{8}$$

where S_r is the constituent eshelby tensor [31]. The eshelby tensor can be evaluated as a function of reinforcement dimensions, a_i^r, of the reinforcing phase *r* and properties of the matrix,

$$S_r = f(C_1, a_1^r, a_2^r, a_3^r). \tag{9}$$

Various expressions for the eshelby tensor can be found in literature [28-36]. For Mori-Tanaka approach, the concentration tensor is given by

$$A_s^{MT} = A_s^{dil} \left[c_1 I + \sum_{r=2}^{N} c_r A_r^{dil} \right]^{-1}, \tag{10}$$

where A_r^{dil} given by Eq. (8). Another form of concentration tensor used in the Self-consistent scheme is given by

$$A_r^{SC} = \left[I + S_r C^{-1} (C_r - C) \right]^{-1} \tag{11}$$

where *C* is the unknown composite modulus. The Self-consistent scheme utilizes an iterative technique to evaluate the modulus of the composite material.

Pipes *et al.* used an anisotropic elasticity approach to study the behavior of a layered cylinder with layers of discontinuous CNT following a helical path in each layer [38,39]. Odegard *et al.* used the Mori-Tanaka method to predict elastic properties of polyimide/CNT composites at various lengths, orientations, and volume fractions [25]. A similar micromechanics-based approach was used by Odegard *et al.* to predict the properties of CNT/polyethelene composites. This study also examined the effects of CNT functionalization in CNT/polyethylene composites and showed that functionalization deteriorated the composite mechanical properties. In another study, MWNT/polystyrene composite elastic properties were shown to be sensitive to nanotube diameter by an approach based on Halpin-Tsai micromechanical method [40]. Lagoudas *et al.* predicted elastic properties of CNT/epoxy composites using a variety of analytical micromechanics approaches [41].

3.2. Computational continuum modeling

Continuum-based computational modeling techniques include FEM and BEM. While these approaches do not always supply exact solutions, they can provide very accurate estimates for a wide range of assumptions. These approaches are described in detail below.

Finite element method. FEM can be used for numerical computation of bulk properties based on the geometry, properties, and volume fraction of constituent phases [42-44]. FEM involves discretization of a material representative volume element (RVE) into elements for which the elastic solutions lead to determination of stress and strain field. The coarseness of the discretization determines the accuracy of the solution. Nanoscale RVEs of different geometric shapes can be chosen for simulation of mechanical properties [18,19]. However, high complexity of models, expensive software, and time-consuming simulations limit the utility of this method.

FEM-based micromechanics has been used extensively for the prediction of mechanical properties of nanostructured composites. Li *et al.* used an FEM-based approach to investigate the stress concentration at the end of carbon nanotubes and the effects of nanotube aspect ratio on the load transfer between nanotubes and matrix [45]. Bradshaw *et al.* used FEM to evaluate the strain concentration tensor in a composite consisting of wavy carbon nanotubes. Fisher *et al.* used FEM to determine the effect of waviness on effective moduli of CNT composites. Chen *et al.* used different shapes of RVEs to understand the dependence of predicted properties on the element shape.

Boundary element method. BEM is a continuum mechanics approach which involves solving boundary integral equations for the evaluation of stress and strain fields [46]. This method uses elements only along the boundary, unlike FEM, which involves elements throughout the volume; thus making BEM less computationally exhaustive than FEM [47-49]. BEM can be applied from micro to macro scale modeling [20]. In BEM, it is assumed that a material continuum exists, and therefore, the details of molecular structure and atomic interactions are ignored.

The rigid fiber model has been shown to be very effective in estimation of fiber composites [50]. Ingber *et al.* have shown agreement in predicted modulus using BEM and analytical results for fiber composites. Liu *et al.* used a fast multipole method to model CNT composites. They treated CNTs as rigid fibers and the properties were obtained in an analogous manner to a rigid inclusion problem. The estimated modulus was found to be very close to that predicted by MD simulations [20]. They concluded that BEM can be a very useful for first-order approximation of mechanical properties in large-scale modeling of CNT composites.

4. MOLECULAR MODELING

In recent years molecular modeling has emerged as an important tool in the prediction of physical material properties such as elastic response, atomic structure, vibrational frequencies, heat of reaction, electric permitivity, and binding energies. Molecular modeling assumes a noncontinuous composition of the material, which makes it a powerful tool for studying atomic interactions at the nanometer length scale. Due to the discrete nature of these techniques, they are often limited by the length and time scales that can be achieved in the simulations, and thus the techniques can be computationally exhaustive. Three widely used molecular modeling techniques for the prediction of mechanical properties of nanostructured materials are molecular dynamics (MD), Monte Carlo (MC), and ab initio simulation.

4.1. Molecular dynamics

MD is the most widely used modeling technique for the simulation of nanostructured materials. MD allows accurate predictions of interactions between constituent phases at the atomic scale. It involves the determination of the time evolution of a set of interacting atoms, followed by integration of the corresponding equations of motion. The equations of motion are given by Newton's second law:

$$F_i = m_i a_i \,, \tag{12}$$

where F_i is the force on atom i and m_i and a_i are the mass and acceleration, respectively, of atom i in a system of N atoms.

MD is a statistical mechanics method. A set of configurations is distributed according to a statistical ensemble or statistical distribution function. The trajectories of the motion of the atoms are calculated under the influence of interaction forces of the atoms. The trajectory is calculated in a phase space with $6N$ dimensions; three position and three momenta components for each atom. Calculation of physical quantities by MD simulation is obtained by arithmetic averages of instantaneous energy val-

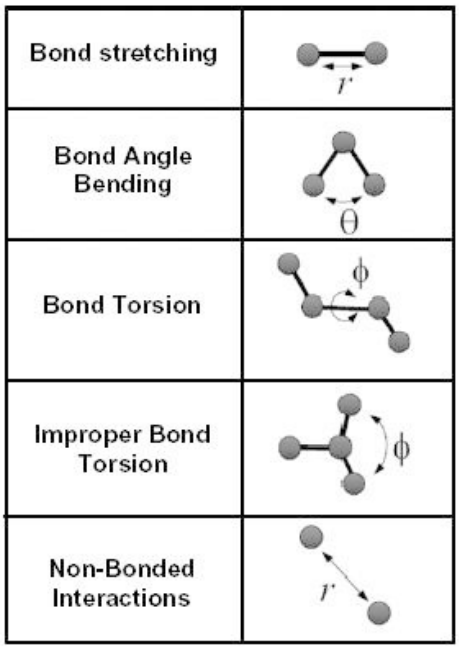

Fig. 4. Force field degrees of freedom.

ues from individual simulation steps. MD simulations, if run for a sufficiently long time, can completely sample the phase space, however, in practice, simulation times are limited. Physical quantities are sampled after the molecular system reaches a thermodynamic equilibrium.

Interactions of different atom types are described by an atomic potential. The total potential energy of the system can be evaluated as a function of the position of the atoms at a given time,

$$V = V(r_i, \ldots, r_N), \tag{13}$$

where r_i is the position of atom i in a system of N atoms for a particular simulation step. The positions of atoms are expressed relative to each other so that the atomic potential is invariant with respect to coordinate transformations. The force on an atom i is determined from the gradient of the potential V with respect to atomic displacements r_i,

$$F_i = -\nabla V(r_1 \ldots r_N). \tag{14}$$

The total energy of the system is

$$E = K + V, \tag{15}$$

where K is the kinetic energy and V is the potential energy of the system.

The potential describing the interaction of atoms in an organic material is given in many forms. For a system involving only carbon and hydrogen, Brenner's potential is widely used for bonded interactions [51]. Brenner's potential is based on the principle that the strength of the bond between two atoms is not constant, but depends on local conditions. It can be expressed as

$$V = \sum_i \sum_{j(>i)} \left[V_R(r_{ij}) - B_{ij} V_A(r_{ij}) \right], \tag{16}$$

where the summation is performed over bonds of the system, r_{ij} is the distance between atoms i and j, $V_R(r_{ij})$ and $V_A(r_{ij})$ are repulsive and attractive interactions, respectively, and B_{ij} is the manybody coupling between atoms i and j and the local environment of atom i. Force fields provide a simple and effective approach for describing the atomic potential of interacting atoms consisting of many different atom types [52-56]. The force field can be described by the sum of the individual energy contributions from each degree of freedom of the system of N atoms, as shown in Fig. 4. The non-bonded interactions shown in Fig. 4 represent van der Waals, hydrogen, and electrostatic bonding. The force field equation developed by Cornell *et al.* for organic molecular systems is [52]

$$V = \sum_{bonds} K_r \left(r - r_{eq} \right)^2 + \sum_{angles} K_\theta \left(\theta - \theta_{eq} \right)^2 + \sum_{dihedrals} \frac{V_n}{2} \left[1 + \cos(n\phi - \gamma) \right] + \sum_{I<J} \left[\frac{A_{IJ}}{r_{IJ}^{12}} - \frac{B_{IJ}}{r_{IJ}^{6}} \right], \tag{17}$$

where K_r is the bond stretching force constant, r is the distance between atoms, r_{eq} is the equilibrium distance between atoms, K_θ is the bond-angle bending force constant, θ is the bond angle, θ_{eq} is the equilibrium bond angle, V_n is the torsion force constant, γ is the phase offset, n is the periodicity of the torsion, A_{IJ} and B_{IJ} are van der Waals force constants between non-bonded atoms I and J, and r_{IJ} is the non-bonded distance between atoms I and J. The van der Waals interaction term in Eq. (17) is in the form of the Lennard-Jones potential. Tables 1 and 2 list force constants for bond stretching and bond angles bending, respectively, for different atom types [52].

The Equivalent-Continuum Method (ECM) is used to determine the bulk-level mechanical properties of a material from the molecular model. ECM is a methodology for linking computational chemistry

Table 1. Bond stretching force constants for aromatic carbon (CA) and aliphatic carbon (CT) [52].

Interacting Atom Types	Equilibrium Spacing r (Å)	Force Constant K_r (kcal/mol/ Å^2)
CA-CA	1.4	469
CT-CT	1.526	310
CA-CT	1.510	317

Table 2. Bond-angle bending force constants for aromatic carbon (CA), aliphatic carbon (CT), and hydrogen (HC) [52].

Interacting Atom Types	Equilibrium Angle θ (deg)	Force Constant K_θ (kcal/mol/rad^2)
CA-CA-CA	120	63
CA-CT-CT	114	63
CT-CT-HC	109.5	50

and solid mechanics. An equivalent continuum, identical to the MD model in geometry, is developed and a constitutive law is used to describe the mechanical behavior of the continuum. Fig. 5 shows a molecular model of a nanotube reinforced polymer composite and its equivalent continuum model. The energies of deformation of the molecular and equivalent-continuum models are derived for identical loading conditions. The unknown mechanical properties of the equivalent continuum are determined by equating the energies of deformation of the two models under these loading conditions. The properties of a larger-scale material are then determined using the equivalent-continuum volume element properties.

Odegard *et al.* have used the ECM and MD to predict the properties of various CNT based composite systems. They predicted the elastic properties of PmPV CNT/polyimide composite for a wide range of nanotube lengths, orientations, and volume fractions. They also used a similar approach to predict behavior of functionalized and non-functionalized CNT/polyethylene composites [57]. Frankland *et al.* used MD to study the influence of chemical functionalization on the CNT/polyethylene composites [14]. They also studied the critical nanotube length required for effective load transfer. Frankland *et al.* predicted stress-strain curves from MD and

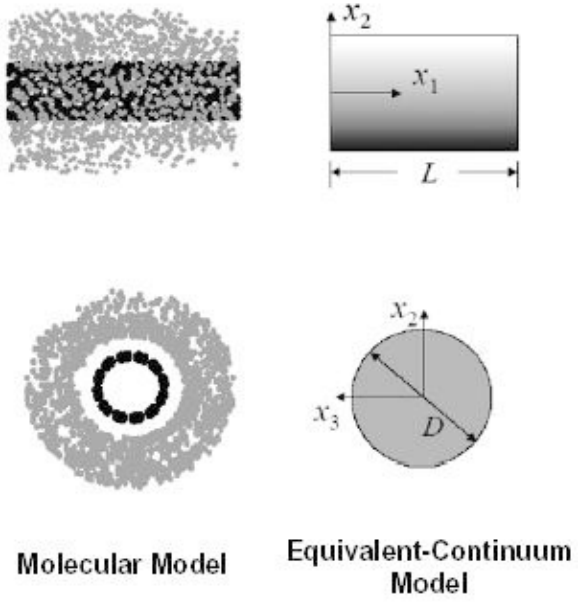

Fig. 5. The Equivalent-continuum model of a PmPV-nanotube composite [25].

compared them to those obtained from micromechanical models for CNT/polyethylene composites [58]. Hu *et al.* [15, 16] used MD to understand the effect of chemical functionalization on toughness of CNT/polystyrene composites.

MD has been used for simulation of other physical properties of nanocomposites. Wei *et al.* showed that addition of CNTs to polyethylene resulted in an increase of thermal expansion, glass transition temperature, and diffusion coefficients of the polymer [59]. Lordi and Yao calculated sliding frictional stresses between CNT and various polymer substrates based on molecular mechanics simulations [60]. Liang *et al.* showed the presence of an attractive interaction between SWNTs and epoxy polymer matrix [61]. Frankland et.al. characterized the interfacial friction model for the pull-out of SWNTs from a polyethylene matrix [62].

4.2. Monte Carlo

MC is a class of probabilistic mathematical models for the prediction of the behavior and outcome of a system. The outcomes of MC are statistical in nature and subject to laws of probability. In most cases it involves a multidimensional integration over the sample space. Different MC techniques can be used for determination of material properties; classical MC, quantum MC, volumetric MC and kinetic MC. Classical MC involves drawing samples from a probability distribution, often the classical Boltzmann distribution, to obtain thermodynamic properties or minimum-energy structures. Quantum MC utilizes random walks to compute quantum-mechanical energies and wave functions to solve electronic structure problems, generally using Schrödinger's equation as starting point. Volumetric MC generates random numbers to determine volumes per atom or to perform geometrical analysis. Kinetic MC simulates process by the use of scaling arguments to establish time scales. It also includes MD simulations which involves stochastic effects.

Based on the dependence of time, MC simulations can be classified as either metropolis MC or kinetic MC. Metropolis MC applies to systems under equilibrium, and thus is independent of time. This method generates configurations according to a statistical-mechanics distribution, whereas kinetic MC deals with systems under non-equilibrium. The kinetic MC technique uses transition rates that depend on the energy barrier between the states, with time increments formulated so that they relate to the microscopic kinetics of the system.

Ford *et al.* used MC techniques to study the mechanical and phase behavior of quartz, cristobalite, coesite, and zeolite structures. The bulk modulus predicted from their model was found to be in good agreement with experimental values. They concluded that the model can be used to determine properties of silica nanostructures with atomistic detail. Chui *et al.* used a MC-based modeling approach to study deformation, rate of deformation, and temperature dependence of large strain deformation in amorphous polymeric materials [63].

4.3. Ab initio

Unlike most materials simulation methods that are based on classical potentials, the main advantages of ab initio methods, which is based on first-principles density functional theory (without any adjustable parameters), are the generality, reliability, and accuracy of these methods. They involve the solution of Schrödinger's equation for each electron, in the selfconsistent potential created by the other electrons and the nuclei. Ab initio methods can be applied to a wide range of systems and properties. However, these techniques are computationally exhaustive, making them difficult for simulations involving large numbers of atoms.

There are three widely-used procedures in ab initio simulation. These procedures are single point calculations, geometry optimization, and frequency calculation. Single point calculations involve the determination of energy and wave functions for a given geometry. This is often used as a preliminary step in a more detailed simulation. Geometry calculations are used to determine energy and wave functions for an initial geometry, and subsequent geometries with lower energy levels. A number of procedures exist for establishing geometries at each calculation step. Frequency calculations are used to predict Infrared and Raman intensities of a molecular system. Ab initio simulations are restricted to small numbers of atoms because of the intense computational resources that are required.

Ab initio techniques have been used on a limited basis for the prediction of mechanical properties of polymer-based nanostructured composites. A study conducted by Mylvaganam *et al.* demonstrated that nanotubes of smaller diameters have higher binding energies in a polyethylene matrix [64]. Bauschlicher studied the bonding of fluorine and hydrogen atoms to nanotubes [65]. He showed that fluorine atoms favored to bond to existing fluorine atoms.

Table 3. Material systems characterized by different modeling techniques.

Material System	Simulation Method	Predicted Properties	Conclusions/Remarks
CNT/Polyethylene	MD, Mori-Tanaka	Elastic Modulus	The moduli of functionalized and non-functionalized systems were determined and compared [17]
	MD	Elastic Modulus	Effect of chemical crosslink density on load transfer was established [14]
	MD	Stress-Strain	Comparisons of composite modulus from MD and rule-of-mixtures techniques for three different cases of nanotubes was predicted [66, 67]
CNT/ Polyimide	MD, Mori-Tanaka	Elastic Modulus	Critical length for maximum load transfer was determined and the use of chemical interface between nanotube and matrix was explored [40]
Nanoclay/ Polyamide	MD,Halpin-Tsai	Elastic Modulus	The effects of interlayers, the structure of clay clusters, and platelet distributions on properties were determined and compared to Halpin-Tsai predictions [66]
	MD, Halpin-Tsai, Mori-Tanaka, FEM	Elastic Properties	Multiscale modeling of nanoclay reinforced polymer composites was presented [23]
CNT/ Epoxy	MD	Interfacial Bonding	Effect of nanotube loading on mechanical properties was established [67]
CNT/ Polystyrene	MD, Halpin-Tsai	Load Transfer	The effects of nanotube diameter and cross-links between nanotubes and polymer on mechanical properties were studied [16,41]
Nanoparticle/ Polyimide	MD, Eshelby	Elastic Modulus	Effect of the nanoparticle/ polyimide interface on elastic properties was determined [68]

5. SIMULATED RESULTS

As indicated in the review above, numerous attempts have been made to study the mechanical behavior of polymer nanocomposites using modeling techniques. A summary of some of these techniques as applied to six material systems is shown in Table 3. For each material system, one or more simulation methods have been applied to examine elastic modulus, constitutive behavior, interfacial bonding, or load transfer between the reinforcement and polymer matrix.

From the general results from these studies, several conclusions can be drawn. First, there is a strong effect of the interfacial conditions between the nano-reinforcement and matrix on the mechanical properties. The interfacial conditions can improve the load transfer via bonded (functionalization) or non-bonded means. Second, there is a measurable influence of nanotube length and diameter on the

overall composite properties. Third, use of traditional micromechanical theories to predict overall composite properties without the aid of molecular modeling do not always result in accurate predicted mechanical properties. Fourth, the study of CNT-based composites has been the focus these studies, with less attention given to nanoclays and nanoparticles. Fifth, the models have generally only examined elastic properties of composites. To date, little work has been performed on nonlinear mechanical behavior or failure of these materials.

6. SUMMARY

The modeling and simulation of polymer-based nanocomposites has become an important topic in recent times because of the need for the development of these materials for engineering applications. A review of the most widely used modeling techniques used for prediction of mechanical properties of polymer nanocomposites has been presented in this paper. In addition, results from recent modeling studies have been presented and discussed.

Because of the complex interactions between constituent phases at the atomic level, a combination of modeling techniques is often required to simulate the bulk-level behavior of these composites. The Computational Chemistry techniques assume the presence of a discrete molecular structure, and are primarily used to predict the atomic structure of a material. Computational Mechanics techniques assume that the matter is composed of one or more continuous constituents, and are used to predict the mechanical behavior of materials and structures. These two types of modeling techniques must be combined to an overall multiscale mode that is capable of predicting the structure and properties of polymer nanocomposites based on fundamental and scientific principles.

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