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Continuum Modeling Techniques to Determine Mechanical Properties of Nanocomposites

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ABSTRACT: *Nanotechnology offers fundamentally new capabilities to architect a broad array of novel materials, composites and structures on a molecular scale. A review of modeling techniques for predicting the mechanical behavior of 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 analytical models discussed include Voigt and Reuss bounds, Hashin and Shtrikman bounds, Halpin–Tsai model, Cox model, and various Mori and Tanaka models. These micromechanics models predict stiffness of nanocomposites with both aligned and randomly oriented fibers. Three different approaches are discussed in finite element modeling, i.e. multiscale representative volume element (RVE) modeling, unit cell modeling, and object-oriented modeling.*

Keywords: *Finite element analysis (FEA), Nanocomposite, Mechanical properties, Multiscale modeling, Nanocomposite, Object-oriented modeling.*

I. INTRODUCTION

Nanoscience and nanotechnology refer to the understanding and control of matter at the atomic, molecular or macromolecular levels, at the length scale of approximately 1 to 100 nanometers, where unique phenomena enable novel applications 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. Computational modeling of 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.

II. 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

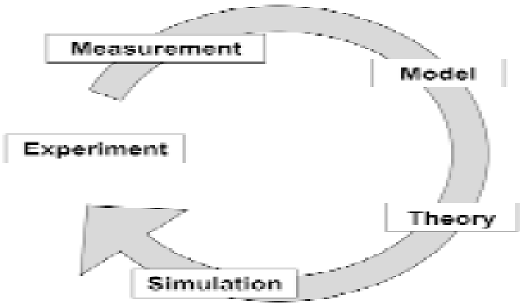


Fig. 1: Schematic of the process of developing theory and the validation of experimental data

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.

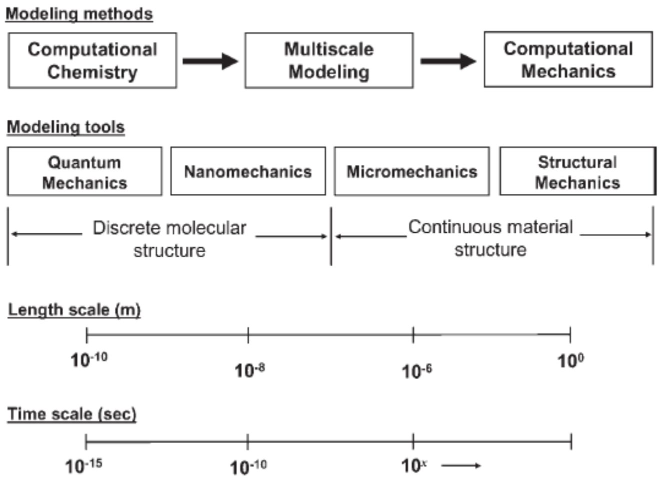


Fig. 2. Various length and time scales used in determining mechanical properties of polymer nanocomposites.

As indicated in Fig. 3, each modeling method has broad classes of relevant modeling tools. 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.

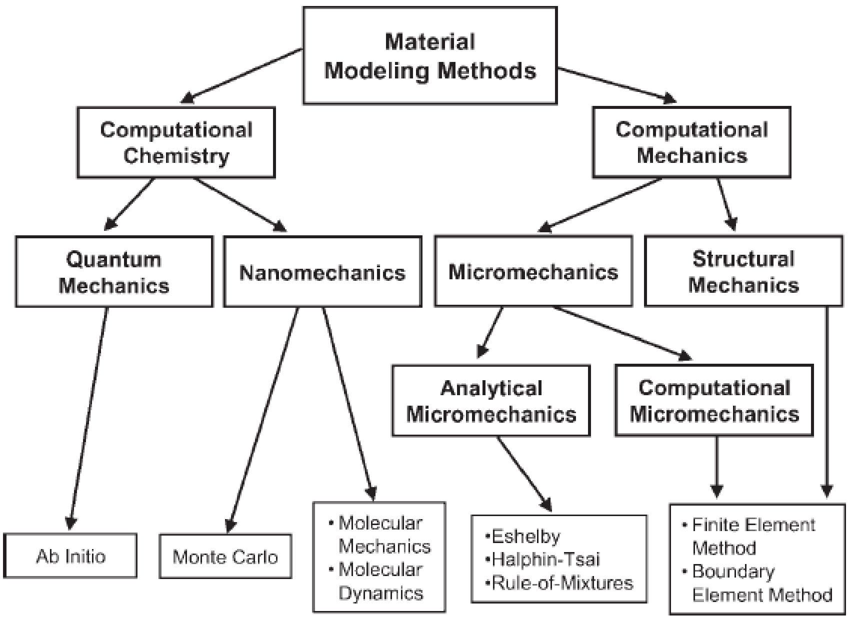


Fig. 3. Diagram of material modeling techniques.

III. CONTINUUM MTHODS

3.1. Analytical continuum modeling

The popular micromechanical models for prediction of modulus of elasticity are summarized and discussed in the following:

3.1.1 Voigt upper bound and Reuss lower bound (V-R model)

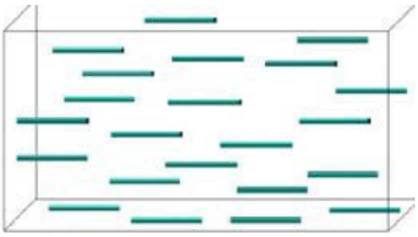
Assumed aligned fibers, and fibers and matrix are subjected to the same uniform strain in the fiber direction, Voigt got the effective modulus in the fiber direction as:

$$El = \varphi Ef + (1-\varphi)Em \quad (3.1)$$

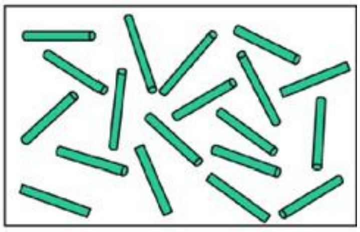
Reuss applied the same uniform stress on the fiber and matrix in the transverse direction (normal to the fiber direction), and got the effective modulus in the transverse direction as:

$$\frac{1}{Et} = \frac{\varphi}{Ef} + \frac{1-\varphi}{Em} \quad (3.2)$$

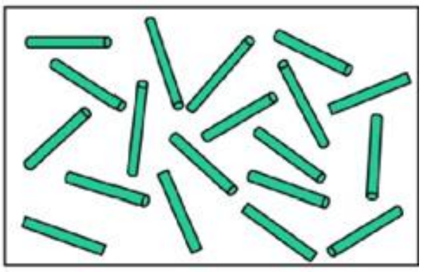
Where φ is the volume fraction of fiber in the two-phase composite system, and subscripts “f” and “m” respectively refer to the fiber and matrix, whereas the subscripts “L” and “T” refer to the longitudinal and transverse directions, respectively. Equation (3.1) is the parallel coupling , and it is also called the “rule of mixtures”, whereas (3.2) is the series coupling formula, and it is also called the “inverse rule of mixtures”.



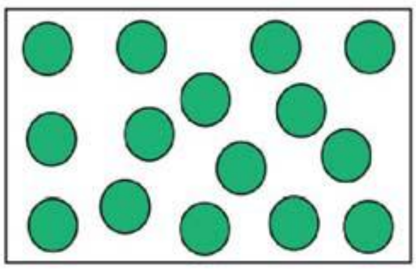
a. Aligned fibers



b. Randomly oriented fibers



c. Aligned platelets



d. Particulates

Fig 4. Schematics of nanocomposites: (a) with aligned fibers; (b) with randomly oriented fibers; (c) with aligned platelets; and (d) with randomly oriented particulates

Equations (3.1) and (3.2) can be extended to any two-phase composites regardless the shape of the filler, and E_L and E_T represent the upper and lower bounds of the modulus of the composite, respectively. Note that in these formulas, only three parameters are involved, i.e. modulus of the fiber and the matrix, and the fiber volume fraction.

3.1.2 Hashin and Shtrikman upper and lower bounds (H-S model)

Hashin and Shtrikman assumed macroscopical isotropy and quasi-homogeneity of the composite where the shape of the filler is not a limiting factor, and estimated the upper and lower bounds of the composite based on variational principles of elasticity. Depending on whether the stiffness of the matrix is more or less than that of the filler, the upper and lower bounds of the bulk moduli, *Kupper* and *Klower* , and shear moduli, *Gupper* and *Glower*, of the composite are given as

$$K_{upper} = K_f + (1-\phi)\left[\frac{1}{K_m - K_f} + \frac{3\phi}{3K_f + 4G_f}\right]^{-1}$$

$$K_{lower} = K_m + \phi\left[\frac{1}{K_f - K_m} + \frac{3(1-\phi)}{3K_m + 4G_m}\right]^{-1}$$

$$G_{upper} = G_f + (1-\phi)\left[\frac{1}{G_m - G_f} + \frac{6\phi(K_f + 2G_f)}{5G_f(3K_f + 4G_f)}\right]^{-1}$$

$$G_{lower} = G_m + \phi\left[\frac{1}{G_f - G_m} + \frac{6(1-\phi)(K_m + 2G_m)}{5G_m(3K_m + 4G_m)}\right]^{-1}$$

(3.3)

Where the subscripts "f" and "m" refer to the filler (fiber) and matrix, respectively. The upper and lower bounds of the elastic modulus can then be calculated using the following relation:

$$E = \frac{9K}{1 + 3K/G}$$

(3.4)

Similar to Voigt and Reuss models, H-S model only involves three parameters.

3.1.3 Halpin-Tsai model (H-T model)

For aligned fiber-reinforced composite materials, Halpin and Tsai developed the equations for prediction of elastic constants based on the work of Hermans and Hill. The H-T model is a semi-empirical model, and the longitudinal and transverse moduli are given by:

$$E_L = \frac{1 + 2(l/d)\phi\eta_L}{1 - \phi\eta_L} E_m$$

(3.5)

$$E_T = \frac{1 + 2\phi\eta_T}{1 - \phi\eta_T} E_m$$

(3.6)

where l and d are the length and diameter of the fiber, and η_L and η_T take the following expressions:

$$\eta_L = \frac{E_f - E_m}{E_f + 2(l/d)E_m}$$

$$\eta_T = \frac{E_f - E_m}{E_f + 2E_m}$$

(3.7) For aligned nanoplatelets as shown in Fig.4 (c), equations (3.7) may still be used by replacing (l/d) with (D/t), where D and t are respectively the diameter and thickness of the platelet. H-T model takes the consideration of the fiber geometry, and has five independent parameters

3.1.4 Hui-Shia model (H-S model)

Mori and Tanaka developed analytical expressions for elastic constants based on the equivalent inclusion model of Eshelby . Taya and Mura and Taya and Chou used Mori-Tanaka approach to predict the longitudinal modulus of fiber-reinforced composites, Weng and Tandon and Weng further developed equations for the complete set of elastic constants of composite materials with aligned spheroidal isotropic inclusions. Based upon the results of Tandon and Weng, Hui and Shia and Shia et al. derived simplified formulas for predicting the overall moduli of composites with aligned reinforcements with emphases on fiber-like and flake-like reinforcements, and found that their theoretical predictions agree well with experimental results. The H-S model presents the Young's modulus as follows:

$$E_L = E_m \left[1 - \frac{\phi}{\xi}\right]^{-1}$$

$$E_T = E_m \left[1 - \frac{\phi}{4}(\frac{1}{\xi} + \frac{3}{\xi + \Lambda}\right]^{-1}$$

(3.8)

where

$$\xi = \phi + \frac{E_m}{E_f - E_m} + 3(1-\phi)\left[\frac{(1-g)\alpha^2 - g/2}{\alpha^2 - 1}\right]$$

$$\Lambda = (1-\phi)\left[\frac{3(\alpha^2 + 0.25)g - 2\alpha^2}{\alpha^2 - 1}\right]$$

$$g = \begin{cases} \frac{\alpha}{(\alpha^2 - 1)^{3/2}}[\alpha\sqrt{\alpha^2 - 1} - \cosh^{-1}\alpha] & \alpha \geq 1 \\ \frac{\alpha}{(1-\alpha^2)^{3/2}}[-\alpha\sqrt{1-\alpha^2} + \cos^{-1}\alpha] & \alpha \leq 1 \end{cases}$$

(3.9)

and α is the aspect ratio of the filler, defined as the ratio of the filler's longitudinal (with Young's modulus *EL*) length to its transverse (with Young's modulus *ET*) length.

3.1.5 Wang-Pyrz model (W-P model)

For a composite material composed of an isotropic matrix and randomly oriented transversely isotropic spheroids, Qiu and Weng and Chen et al. gave the formulas for the overall bulk and shear moduli using the Mori-Tanaka method. These formulas are expressed in terms of the Eshelby tensor, thus are not final. Wang and Pyrz further gave the closed and concise formulas for the overall bulk modulus and shear modulus as follows:

$$K = K_m + K_m \frac{\phi\varphi}{1 - \phi(1-\alpha)}$$

$$\mu = \mu_m + \mu_m \frac{\phi\psi}{1 - \phi(1-\beta)}$$

(3.10)

The expressions for ϕ , ψ , α and β are given in the Appendix.

Note that W-P model is based on the Mori-Tanaka approach, and deals with the composite materials reinforced with randomly oriented and transversely isotropic spheroids. By varying the aspect ratio, the oblate spheroids can be approximate to platelets, and the prolate spheroids can be approximate to fibers.

3.1.6 Cox model (Shear lag model

Shear lag model was the first micro-mechanics model for fiber-reinforced composites. Cox analyzed a single fiber of length *l* and radius *f r* , which is encased in a concentric cylindrical shell of matrix having radius *R*. He derived the longitudinal modulus as

$$E_L = \eta_L \phi E_f + (1-\phi)E_m$$

(3.11)

where η*L* is a length-dependent efficiency factor,

$$\eta_L = 1 - \frac{\tanh(\beta l/2)}{\beta l/2}$$

(3.12)

With

$$\beta^2 = \frac{4\mu_m}{r_f^2 E_f \ln(K_R/\phi)}$$

(3.13)

K_R is a constant that depends on the fiber packing arrangements. For some typical fiber packing arrangements, the values of K_R are given in Table 1

Table 1. Values for K_R in Eq. (3.13)

FIBER PACKING	K_R
Cox	$2\pi/\sqrt{3}=3.628$
Composite cylinders	1.000
Hexagonal	$\pi/2\sqrt{3}=0.907$
Square	$\pi/4=0.785$

It is well known that the orientation of the dispersed phase has a dramatic effect on the composite modulus. It is apparent from their geometry that flake-like platelets can provide equal reinforcement in two directions, if appropriately oriented, while fibers provide primary reinforcement in one direction. If the longitudinal modulus *ET* and the transverse modulus *E T* are known, then the effective modulus of the composite with randomly oriented fibers and platelets in all three orthogonal directions are given by,

$$E_{3D}^{fiber} = 0.184E_L + 0.816E_T$$

$$E_{3D}^{platelet} = 0.49E_L + 0.51E_T$$

(3.14)

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.

3.2.1. Finite element method: FEM can be used for numerical computation of bulk properties based on the geometry, properties, and volume fraction of constituent phases In the following, three finite element modeling approaches will be discussed. They are multiscale representative volume element (RVE) modeling, unit cell modeling, and object-oriented modeling.

Multiscale RVE modeling: 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. However, high complexity of models, expensive software, and time-consuming simulations limit the utility of this method.

Unit cell modeling: The conventional unit cell concept is the same as the RVE . Here we define a unit cell as a special RVE that it has a relatively big size (usually in micrometers) and contains a significant number of fillers (usually in tens to hundreds or more). Such defined unit cell is still the building block of the composite, but as it gets more complicated, analytical models are difficult to establish or too complicated to solve, and numerical modeling and simulation become a necessity.

Object-oriented modeling*:* The object-oriented modeling which is able to capture the actual microstructure morphology of the nanocomposites becomes necessary in order to accurately predict the overall properties. It incorporates the microstructure images such as scanning electron microscopy (SEM) micrographs into finite element grids. Thus the mesh reproduces exactly the original microstructure, namely the inclusions size, morphology, spatial distribution, and the respective volume fraction of the different constituents. A objectoriented finite element code, developed by National Institute of Standards and Technology (NIST), has been extensively used in analyzing fracture mechanisms and material properties of heterogeneous materials and mechanical properties of nanocomposites.

3.2.2 Boundary element method

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

IV. CONCLUSION

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. 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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