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Characterizing and Modeling Mechanical Properties of Nanocomposites

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Abstract.

This paper presents , theory of micro-nanomechanics, and numerical analysis on characterizing mechanical properties of nanocomposites. First, the classifications of nanomaterials are presented. Then nano indentation testing and the corresponding finite element modeling are discussed, followed by analytical modeling stiffness of nanocomposites. The analytical models discussed include Voigt and Reuss bounds, Hashin and Shtrikman bounds, Halpin–Tsai model, and various Mori and Tanaka models. These micromechanics models predict stiffness of nanocomposites with both aligned and randomly oriented fibers. The emphasis is on numerical modeling includes molecular dynamics modeling and finite element modeling. Three different approaches are discussed in finite element modeling, i.e. multiscale representative volume element (RVE) modeling, unit cell modeling, and object-oriented modeling. Finally, the mechanism of nanocomposite mechanical property enhancement and the ways to improve stiffness and fracture toughness for nanocomposites are discussed.

***Key words**: Nanocomposites; Mechanical properties; Multiscale modeling; Finite element analysis (FEA); Object-oriented modeling.*

1. 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. Nanotechnologies are the design, characterization, production and application of structures, devices and systems by controlling shape and size at nanometer scale. According to Braun et al. [1], from 1980s, the growth of research papers dealing with the prefix called ‘nano’ is exponential. Among all the work, characterizing and modeling mechanical properties of nanocomposites is one of the most important subjects.Nanomaterials are generally considered as the materials that have a characteristic dimension (e.g. grain size, diameter of cylindrical cross-section, layer thickness) smaller than 100 nm.Nanomaterials can be metallic, polymeric, ceramic, electronic, or composite. Nanomaterials are classified into three categories depending on their geometry, as shown in Fig. 1 [2,3]:

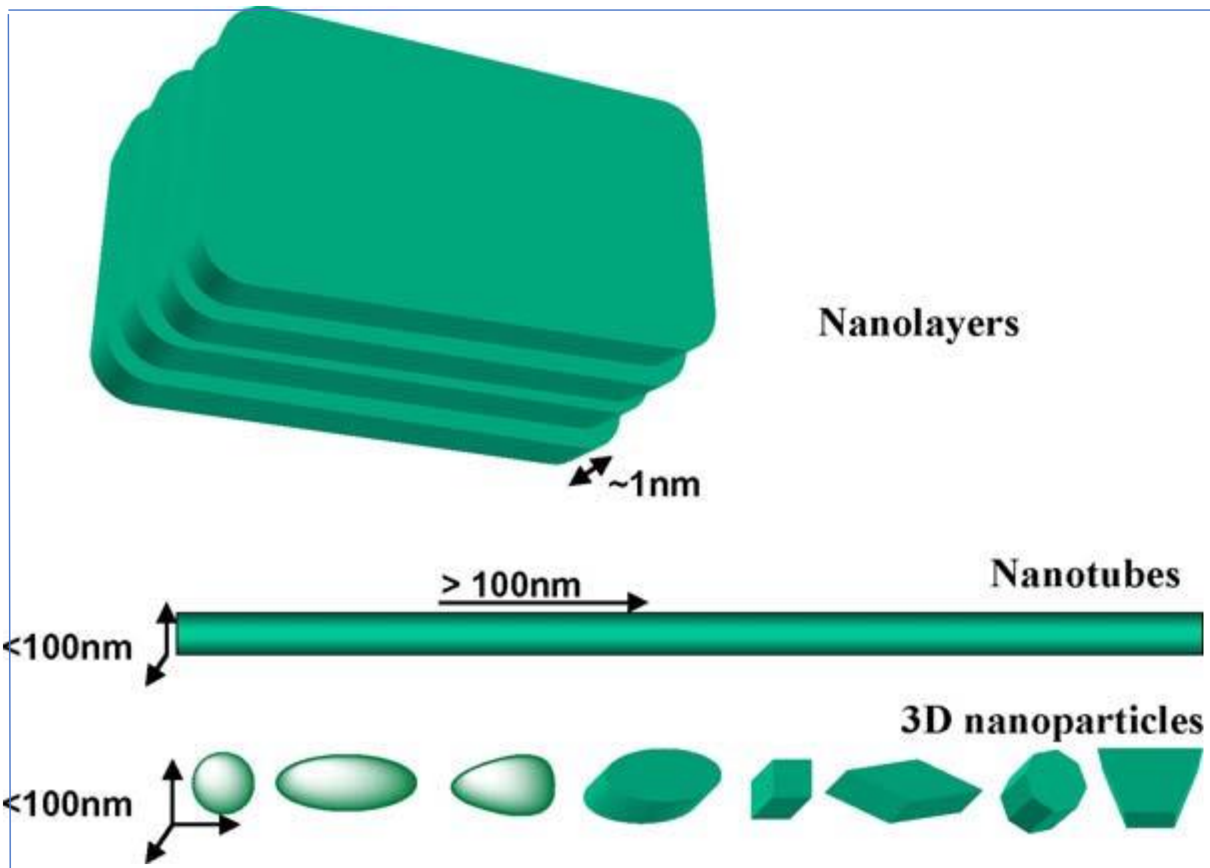

Figure 1. Various types of nanoscale materials [4].

The nanomaterials can also be distinguished in three types as natural, incidental, and engineered nanomaterials depending on their pathway [4]. Natural nanomaterials, which are formed through natural processes, occur in the environment (e.g. volcanic dust, lunar dust, magneto-tactic bacteria, minerals, etc.). Incidental nanomaterials occur as the result of man made industrial processes (e.g. coal combustion, welding fumes, etc.). Engineered nanomaterials are produced either by lithographically etching of a large sample to obtained nanoparticles, or by assembling smaller subunits through crystal growth or chemical synthesis to grow nanomaterials of the desired size and configuration. Engineered nanomaterials most often have regular shapes, such as tubes, spheres, rings, etc. U.S. Environmental Protection Agency divides engineered nanomaterials into four types. They are carbon-based materials (nanotubes, fullerenes), metal based materials (including both metal oxides and quantum dots), dendrimers (nanosized polymers built from branched units of unspecified chemistry), and composites (including nanoclays).

2. CHARACTERIZING AND MODELING OF NANOCOMPOSITES

2.1. Nano Indentation Tests And Computing Simulations

There are different ways to experimentally characterize nanocomposites. For example, tensile and flexural tests (mostly conducted on Instron machines), impact tests (conducted on pendulum impact testing machine) [5-11], and micro-compression tests [12,13]. Nanoindentation test is one of the most effective and widely used methods to measure the mechanical properties of materials. This technique uses the same principle as microindentation, but with much smaller probe and loads, so as to produce indentations from less than a hundred nanometers to a few micrometers in size. During the past dozen years or so, it has been widely used in measuring the mechanical properties of various nanocomposites [14-25] and human enamel and dentin [26-38].Hardness (H) and elastic modulus (E) are

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calculated from the load-displacement curve obtained from a nanoindentation test. A typical load-displacement curve is shown in Fig. 2. As the indenter penetrates into the specimen, the loading curve climbs up. At some point, the maximum load *P*max is reached, and then followed by the unloading. If the material is perfectly elastic and has no hysteresis, the loading curve and the unloading curve will be identical. *h*max gives a measure of the total maximum deformation, while *h*f represents the maximum permanent(plastic) deformation (final penetration depth).

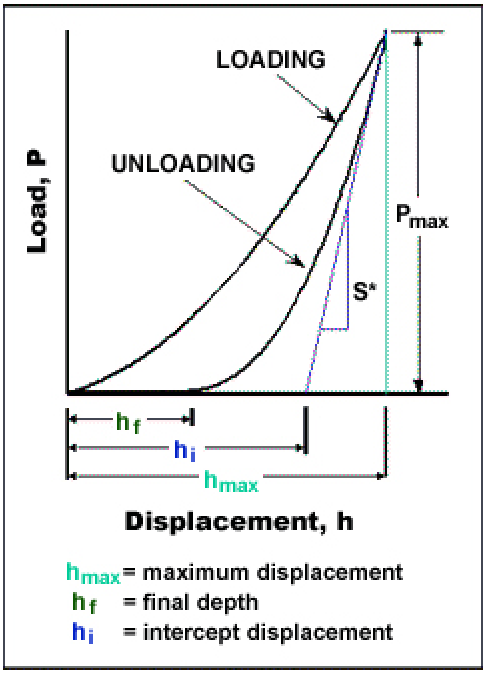


Figure 2. Typical load-displacement curve of the nanoindentation test.

Equations

The most commonly used method to obtain the hardness and the elastic modulus of a material by nanoindentation is the Oliver-Pharr method . According to this method, the nanoindentation hardness as a function of the final penetration depth of indent can be determined by:

$H = P_{max} / A$ (2.1)

where Pmax is the maximum applied load measured at the maximum depth of penetration (hmax), A is the projected contact area between the indenter and the specimen.

For a spherical indenter,

A = 2πRhf (where R is the radius of the indenter), whereas for a pyramidal (Berkovich or Vickers) indenter, A can be expressed as a function of hf as

$A = 24.504h_2f + C_1h_f + C_2\ h_1f / 2 + C_3h_1f / 4 + L + C_8h_1f / 128$ (2.2)

where C1 to C8 are constants and can be determined by standard calibration procedure. The final Therefore, the specimen's hardness *H* and elastic modulus *Es* will be obtained from this set of equations.

2.2 Analytical Modeling Stiffness Of Nanocomposites

It is well known that composite materials have advantages over traditional materials.

Nanocomposites, where nano-sized reinforcements (fillers) are dispersed in the base material (matrix), offer a novel class of composites with superior properties and added functionalities [39- 62]. Although the applicability of continuum mechanics (including micro mechanics) to nanocomposites has been subjected to debate [59,63], many recent works directly applying continuum mechanics to nanostructures and nanomaterials have reported meaningful results and elucidated many issues [64-73].reviewed.

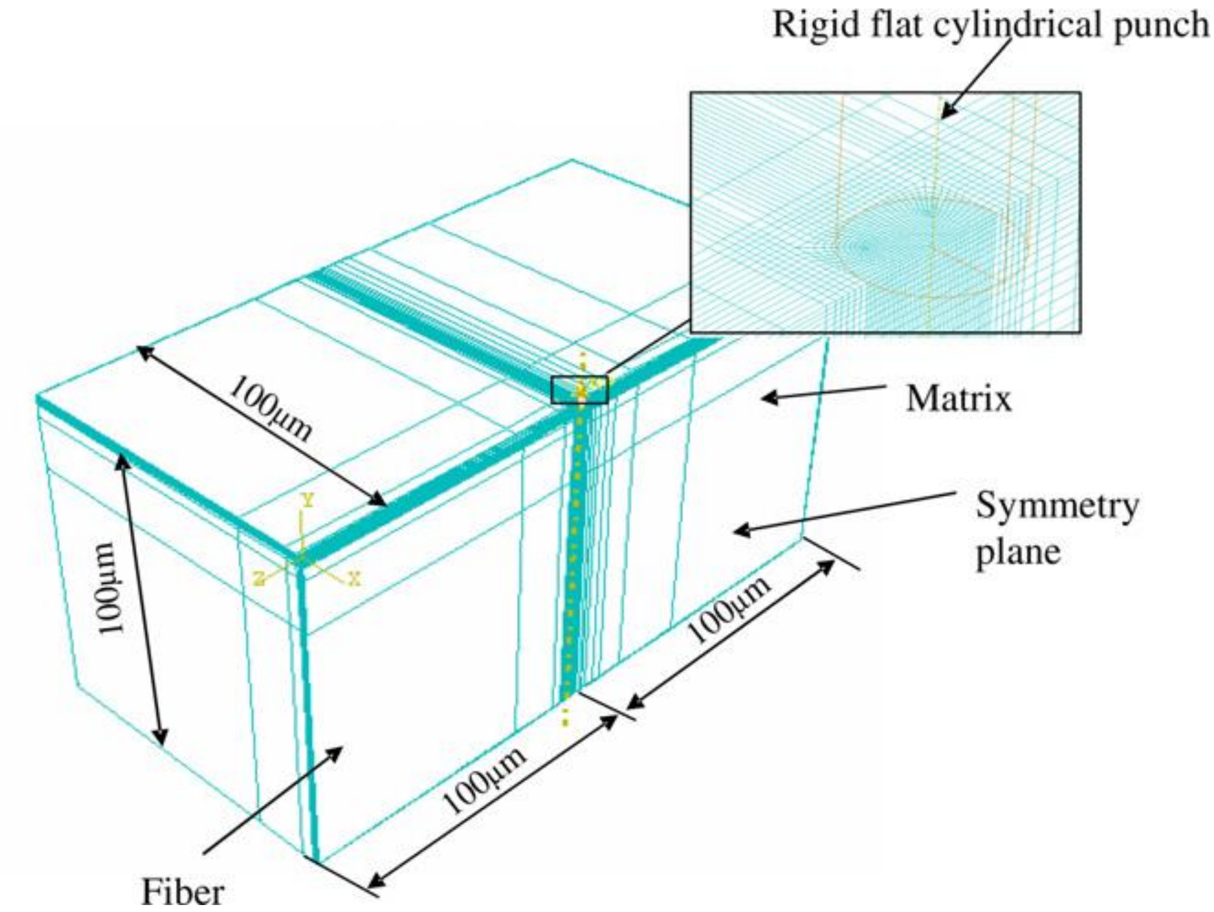


Figure3. Illustration of a three dimensional nanoindentation finite element model [18]

They are cylinder-like nanofibers(nanotubes), flake-like (disk-like) platelets (nanolayers, nanoclays), and spheroid-like particulates, refer to Figs. 1 and 2. For the fiber-reinforced nanocomposites, there are two cases depending on the orientation of the fibers, i.e. aligned fibers and randomly oriented fibers, see Fig. 6 below. The popular micromechanical models for prediction of modulus of elasticity are summarized and discussed in the following:

2.2.1 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 [74] got the effective modulus in the fiber direction as:

$EL = \varphi E f + (1-\varphi)Em$

Reuss [75] 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: 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 is the parallel coupling formula, and it is also called the “rule of mixtures”, whereas 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

Schematics of nano composites: (a) with aligned fibers; (b) with randomly oriented fibers; (c) with aligned platelets; and (d) with randomly oriented particulates . Note that in these formulas, only three parameters are involved, i.e. modulus of the fiber and the matrix, and the fiber volume fraction.

2.2.2 Hashin and shtrikman upper and lower bounds (H-S model)

Hashin and Shtrikman [75,77] 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.

2.2.3 Halpin-Tsai model (H-T model)

For aligned fiber-reinforced composite materials, Halpin and Tsai [78-81] developed the equations for prediction of elastic constants based on the work of Hermans [82] and Hill [83]. The H-T model is a semi-empirical model, and the longitudinal and transverse moduli

2.2.4 Hui-Shia model (H-S model)

Mori and Tanaka [84] developed analytical expressions for elastic constants based on the equivalent inclusion model of Eshelby [85]. Taya and Mura [86] and Taya and Chou [87] used Mori-Tanaka approach to predict the longitudinal modulus of fiber-reinforced composites, Weng [88] and Tandon and Weng [89] 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 [89], Hui and Shia [90] and Shia et al. [91] 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.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. For example,

refer to Fig. 2, $\alpha = l / d$ for nanotube, $\alpha = t / D$ for nanoplatelet, and EL will be along axis 3,

and ET will be along axis 1 (or 2).

3. LITERATURE REVIEW

3.1. Bao Le Technische Universität Berlin, Xiangyu Teng Newcastle University ,”A Review on Nanocomposites. Part 1: Mechanical Properties”

Micromachining of nanocomposites is deemed to be a complicated process due to the anisotropic, heterogeneous structure and advanced mechanical properties of these materials associated with the size effects in micromachining. It leadstopoorer machinability in terms of high cutting force, low surface quality and high rate of tool wear. In part 1 of this two-part review paper, a comprehensive review on mechanical properties of various nanocomposites will be presented while the second part of the paper will focus on the micro-machinability of these nanocomposite materials.

Keywords: nanocomposites; micromachining; manufacturing; materials; mechanical properties

3.2. M Vinyas1, S J Athul, D Harursampath1, Mar Loja,and T Nguyen Thoi"A comprehensive review on analysis of nanocomposites: from manufacturing to properties characterization"

The study of nanocomposites in its diverse scientific fields has increased dramatically over the years with numerous theoretical and experimental techniques emerging and redefining the process of synthesis, analysis and cost control methodologies of nanocomposites. The present review is an attempt to identify the various methodologies, techniques, theories and formulations that are used in nanocomposite technology. As an overall qualitative appreciation it is possible to conclude that the diversity of processes involved in the manufacture and analysis of nanocomposites, impacts them differently, influencing their physical nature, chemical behaviour, biological interactions, optical properties and production costs which consequently may introduce some constraints to their application. Hence, a critical review on the best methodology would remain inconclusive. This work intends to collect and relate publications on different fields of the nanocomposites technology and application fields, aiming at contributing to achieve a wide perspective of different aspects of the nanocomposites processes and theories and with this, being an aid to ease and raise the production and analysis of nanocomposites to a higher level.

3.3. Marino Quaresimin , Marco Salviato, Michele Zappalorto ,"Strategies for the assessment of nanocomposite mechanical properties"

The assessment of nanocomposite mechanical properties is a challenging task. Due to their hierarchical structure, which spans from nano to macro length-scales, a different way of thinking from traditional approaches is needed to account for the characteristic phenomena of each length-scale and bridge their effects from the smaller scale to the macroscale. In the present work, some important issues of nanocomposite modelling are discussed. Then, a classification of the available modelling strategies is proposed, according to the scale from which the problem is addressed. This comprehensive analysis is thought as a necessary tool for the development of new effective approaches

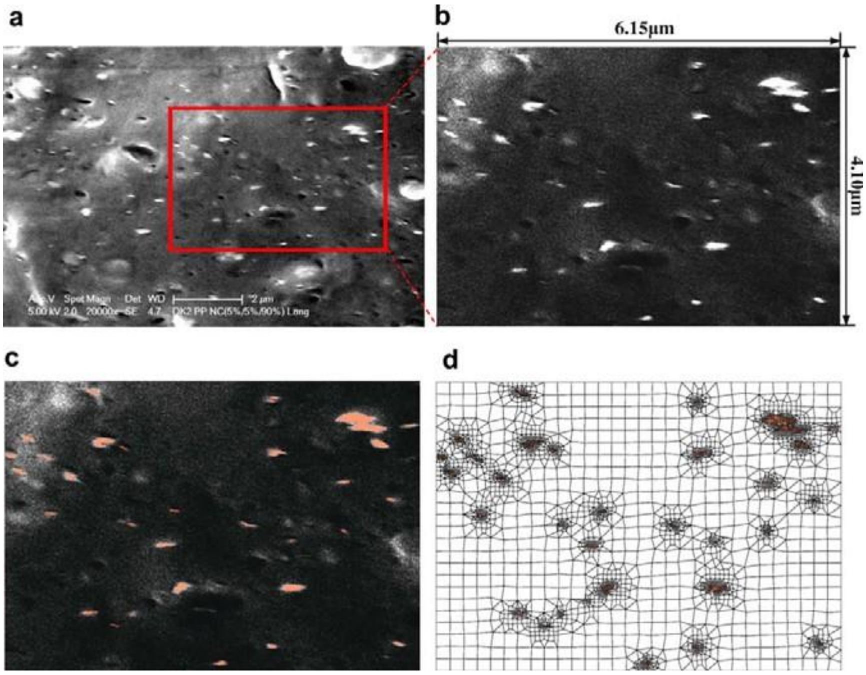
4.OBJECTIVES

1. To achieve the longstanding goal of predicting nanoparticles–nanocomposites–property relationships in material design and optimization
2. To study the various degrees in addressing many aspects of nanocomposites.
3. To develop new and improved simulation techniques at individual time and length scales.
4. It is important to integrate the developed methods at wider range of time and length scales,spanning from quantum domain to molecular domain, to mesoscopic domain, and finally to macroscopic domain, to form a useful tool for exploring the structural and mechanical properties, as well as optimizing design of nanocomposites.

5. METHODOLOGY

Finite Element Modeling: As a very general and powerful numerical analysis tool, finite element method was used to predict mechanical properties of composite materials started in early 1970s . Since then, various finite element models have been developed to characterize all kinds of composite materials . In 1991, Sumio Iijima, a Japanese scientist, discovered carbon nanotubes (CNTs) which possess exceptionally high stiffness and strength, as well as superior electrical and thermal properties. Soon after that CNTs were used as reinforcement in developing nanocomposite materials. In the past decade or so, there have been explosively experimental work and analytical work [e.g. 156-169], as well as finite element modeling work [e.g. 170-198] on developing, analyzing and characterizing CNT reinforced nanocomposites and other nanocomposites. 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.

Object-oriented modeling



In both multiscale RVE modeling and unit cell modeling, two basic assumptions are made. First, nanofillers can be idealized to simple geometries such as spheres, ellipsoids, cylinders, or cubes. And second, nanocomposites can be reproduced by assembling a large number of such RVEs (or unit cells). This can be a serious limitation when dealing with complex and highly heterogeneous nanocomposites. For example, for highly variable and irregular angular structure of fillers, using approximation of simple geometrical particles could not capture the complex morphology, size, and spatial distribution of the reinforcement. Therefore, 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.

The object-oriented modeling is a relatively new approach. 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 object- oriented finite element code, OOF [205, 206], developed by National Institute of Standards and Technology (NIST), has been extensively used in analyzing fracture mechanisms and material properties of heterogeneous materials [207-216] and mechanical properties of nanocomposites

6. CONCLUDING REMARKS

Specific challenges and the solution strategies are discussed in the following:

1. In either developing new or characterizing the current exist nanocomposites, a comprehensive approach should be adopted that integrates the experimental techniques with nanomechanics-based analytical explorations and computer modeling and simulation.

2. New computational tools are specially needed in the area of multiscale RVE modeling. The multiscale RVE modeling is in nature a “local-global” approach. In order to catch the local nano/micro characteristics, quantum mechanics or molecular dynamics needs to be explored. But the prediction of global macro-mechanical properties requires the continuum mechanics-based finite element method. How to transit from local to global becomes a research issue. Ogata et al. [198] proposed a way of combing quantum mechanics, molecular dynamics, and finite elements. In regions where the atoms obey the laws of continuum mechanics, the finite element method is used. However, in critical areas such as the extremity of a fracture, molecular dynamics and even quantum mechanics are required to obtain a more detailed study of the fracture process. The transition from the global to local levels involves a change of scale. Xiao and Belytschko proposed a way of improving the numerical compatibility between regions modeled by molecular dynamics and those modeled using the finite element method. The suggested method is introducing a broad transition region by superposing the finite element mesh of the continuum region on the atomistic structure of the molecular dynamics region. Clearly, there is still a lot of work needs to be done in connecting the local parameters to the global parameters.

3. In object-oriented finite element modeling, 2D modeling has been extensively used in nanocomposites [e.g. 8, 179], and there are also some works on 3D modeling [e.g. 178]. There are still issues to be resolved in 3D modeling, especially advanced object- oriented 3D finite element codes.

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