Modeling and simulation of mechanical properties of nano-particle filled materials

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Abstract
With the recent advances in nanoscale science and engineering, materials containing reinforcement with superior mechanical properties can be found in many advanced products. The accurate prediction of the mechanical properties of this class of composite materials is important to ensure the reliability of the products. Characterization methods based contact probe such as nano-indentation and scratch tests have been developed in recent years to measure the mechanical properties of the new class of nanomaterials. This paper presents a constitutive modeling framework for predicting the mechanical properties of nanoparticle reinforced composite materials. The formulation directly considers the effects of inter-nanoparticle interaction and performs a statistical averaging to the solution of the problem of two-nanoparticle interaction. Final constitutive equations are obtained in analytical closed form with no additional material parameters. The predictions from the proposed constitutive model are compared with experimental measurement from nano-indentation tests. This constitutive model for nanoparticle reinforced composites can be used to determine the volume concentration of the reinforcing nanoparticles in nano-indentation test.

Introduction
Composite materials containing reinforcement with superior strength manufactured with nanotechnology have emerged in many applications. For example, carbon nanotubes have been utilized in field emission display as indicated in Dresselhaus and Avouris (2001). Thin coatings with nanoparticle-filled sol-gel have also become popular in many advanced products including the protective topcoat of recording films in optical storage disks (Malzbender et al., 2002). For the reliability of these advanced products, accurate predictions of the mechanical properties of this class of composite materials are important.

In many existing constitutive models for composite materials, the effects of interaction among reinforcing elements have been neglected mostly due to the following two reasons. First, the difference of the mechanical strength between the reinforcement and the original matrix material may not be too large. Secondly, the volume concentration of the reinforcement may not be high. With the advance in modern nanotechnology, these two assumptions are no longer valid because some materials produced with nano-scale material engineering can have superior mechanical strength than traditional materials. In addition, the size of the reinforcement material can be made very small with nanoscale material engineering and thus greatly increase the homogeneity of the final composite material. This allows the volume concentration of the reinforcement to be increased to achieve much better overall mechanical properties.
This paper presents a material modeling framework for composites with nanoparticles. The major advantage of the proposed model is that the effects of inter-nanoparticle interaction are captured into the constitutive model through statistical averaging on the solution of a two-particle interaction problem. Analytical closed-form formulations can be derived to predict the mechanical properties of nanoparticle reinforced composites. The constitutive equations are expressed in terms of the volume concentration of the nanoparticles and the material properties of the original matrix material and the reinforcing material. No additional material parameter needs to be introduced.

For simplicity of mathematical derivation, in this paper, all nanoparticles are assumed to be of equal size and bonded firmly to the matrix material. These two restrictions can be removed by considering the variation on the size of the nanoparticles and the strength of the interface between the nanoparticles and the matrix. However, the framework for the more general case will be basically the same as that for this simplified case.

The average field theory is summarized in section ‘Average field theory’. In section ‘Interaction of two spherical inclusions’ presents a micromechanics-based solution to the problem of two interacting particles embedded in elastic solid. The concentration factor tensors for nanoparticle composites are derived in section Concentration factor tensors. In section Effective elastic properties presents the constitutive equations for this class of nanocomposite. A comparison of the prediction in this study with experimental data from nano-indentation tests is shown in section ‘Comparisons with experimental results’. The paper is concluded in section ‘Conclusions’.

**Average field theory**

The determination of the exact internal local stress or strain field in a composite system is in general formidable due to the high degree of complexity of the arbitrary geometry and concentration of the reinforcing material. In many applications, it is sufficient to have the average of the field concerned. A method based on the averages of stress and strain fields was introduced by Hill (1963) to describe the effective properties of composite materials.

In the average field theory, a concentration factor is introduced to represent the relationship between the local field and the average of the global field. For example, the stress at any local point for a specific material phase is related to the average stress for the global composite system via the stress concentration factor. If only the average of the local stress field is required, upon averaging over the local material phase, we have the following relationship

\[ \bar{\sigma}_x = P_x : \sigma, \]  

where \( \sigma \) represents the stress tensor, the fourth rank tensor \( P_x \) is the volume averaged stress concentration factor tensor for phase \( x \), an over-bar represents the volume average of the corresponding quantity, and the subscript \( x \) denotes the material phase. Similar definition is made for the strain field.

\[ \bar{\varepsilon}_x = Q_x : \varepsilon, \]  

in which \( \varepsilon \) represents the strain tensor and \( Q_x \) is the volume averaged strain concentration factor tensor for phase \( x \).

From elasticity theory, the elastic stiffness and compliance tensors, \( C_x \) and \( D_x \), respectively, for material phase \( x \) relate the local average stress and strain fields according to the following two equations

\[ \bar{\sigma}_x = C_x : \bar{\varepsilon}_x, \]  
\[ \bar{\varepsilon}_x = D_x : \bar{\sigma}_x. \]

Similarly, the macroscopic elastic properties can be expressed by the following equations through the global elastic moduli

\[ \bar{\sigma} = C : \bar{\varepsilon}, \]  
\[ \bar{\varepsilon} = D : \bar{\sigma}. \]

Subscripts 0, 1, and * denote the matrix, nanoparticle, and overall composite material, respectively. Based on the definitions in Eqs. (1)-(6), the global effective elastic moduli are expressed in terms of the volume fractions, elastic moduli of the constituent phases, and the concentration factor tensors as shown in the following two equations

\[ C_x = C_x + \phi_\beta (C_\beta - C_x) \cdot Q_\beta, \]  
\[ D_x = D_x + \phi_\beta (D_\beta - D_x) \cdot P_\beta. \]