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Mechanical modeling of incompressible particle-reinforced neo-Hookean composites based on numerical homogenization

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ABSTRACT

In this paper, the mechanical response of incompressible particle-reinforced neo-Hookean composites (IPRNC) under general finite deformations is investigated numerically. Three-dimensional Representative Volume Element (RVE) models containing 27 non-overlapping identical randomly distributed spheres are created to represent neo-Hookean composites consisting of incompressible neo-Hookean elastomeric spheres embedded within another incompressible neo-Hookean elastomeric matrix. Four types of finite deformation (i.e., uniaxial tension, uniaxial compression, simple shear and general biaxial deformation) are simulated using the finite element method (FEM) and the RVE models with periodic boundary condition (PBC) enforced. The simulation results show that the overall mechanical response of the IPRNC can be well-predicted by another simple incompressible neo-Hookean model up to the deformation the FEM simulation can reach. It is also shown that the effective shear modulus of the IPRNC can be well-predicted as a function of both particle volume fraction and particle/matrix stiffness ratio, using the classical linear elastic estimation within the limit of current FEM software.

1. Introduction

A fundamental problem for particle-reinforced composites (PRC) is to predict the overall mechanical behavior of the composite based on the mechanical properties of the constituents and the microstructure of the composites. Guth (1945) extended Einstein's linear estimate originally developed for viscous fluid and proposed a second order polynomial to predict the small strain Young's modulus of (rigid) particle-filled solids. Kerner (1956) designed an averaging procedure to estimate the effective shear modulus and bulk modulus of the PRC. Hill (1965) proposed a self-consistent model to estimate the effective shear modulus of the PRC. The three-phase model developed by Christensen and Lo (1979) gives a very good prediction of the PRCs effective shear modulus (Segurado and Llorca, 2002). Torquato (1998) derived accurate expressions for the bulk and shear moduli of the PRC based on a third-order approximation. Although a few studies investigated some special microstructures such as cubic arrays of spheres (e.g., Cohen, 2004), most papers in the literature have focused on macroscopically isotropic composites with randomly distributed particles. Besides the direct estimation of the effective moduli of the PRC, some rigor-

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ous bounds for the elastic properties of the PRC have been obtained from variational principles (e.g., Hashin and Shtrikman, 1963). Another approach to investigate the "overall" mechanical behavior of the PRC is to solve the boundary value problems for a representative volume element (RVE) model of the composite numerically (Michel et al., 1999). Drugan and Willis (1996) showed that a small size RVE model can predict accurately the mechanical response of the PRC. Segurado and Llorca (2002) provided a comprehensive numerical study of the mechanical properties of the linear elastic PRC using multi-particle RVE models.

Although the mechanical properties of the PRC in infinitesimal strain have been investigated extensively, their mechanical behavior in the finite deformation regime is still not well-understood due to the intrinsic difficulties related to the geometrical and material nonlinearities. Hill (1972) proposed a set of macroscopic variables for constitutive modeling of composites in finite deformation. Based on that, Ogden (1974) derived an approximate expression for the overall bulk modulus of the PRC with second-order isotropic compressible elastic constituents under finite strain. Hashin (1985) studied the response of hyperelastic PRC under hydrostatic loading. Imam et al. (1995) derived the second order elastic field for incompressible hyperelastic composites with dilute inclusions, which was then employed to estimate the overall moduli of the PRC. Although recently several research groups have investigated hyperelastic composites with inclusions in two dimension (which physically implies composites with aligned fiber reinforcement) and some related boundary value problems are solved analytically (e.g., deBotton et al., 2006; Guo et al., 2008; Guo et al., 2006; Lopez-Pamies, 2010), analytical solutions for three-dimensional PRC model under general homogeneous displacement boundary conditions are far more difficult. Castaneda (1989) proposed a self-consistent approach to predict the shear modulus of incompressible particle-reinforced neo-Hookean composites (IPRNC). Bergstrom and Boyce (1999) used the concept of strain amplification under large strain to estimate the shear modulus of incompressible neo-Hookean composites filled with rigid particles. Because these two models are not based on an accurate approximation of the elastic fields, it is not surprising to find that they don't provide good estimates of effective shear modulus of IPRNC with moderate particle volume fractions. Recently Avazmohammadi and Castaneda (2012) developed a tangent second-order (TSO) method to investigate the macroscopic response of PRC in finite deformation and an explicit formula is derived to approximate the strain energy of incompressible neo-Hookean composites reinforced with rigid particles.

The numerical studies of hyperelastic composites available in the literature are also mainly limited to two-dimensional problems of composites with aligned fibers or voids (e.g., Guo et al., 2008; Moraleda et al., 2007, 2009; Tang et al., 2012a, b), though Bergstrom and Boyce (1999) used simple 2D axisymmetric models to simulate IPRNC under uniaxial deformation. Three-dimensional RVE modeling in finite deformation is only investigated for single-fiber unit cell (Guo et al., 2007). To the best of the authors' knowledge, there is no comprehensive numerical study of the PRC under finite deformation published in the literature.

Because it is difficult to predict the mechanical response of the PRC under general finite deformation theoretically due to the related geometrical and material nonlinearities, this study employs the numerical homogenization approach to investigate the mechanical behavior of the simplest hyperelastic PRC under general finite deformation, in which the mechanical properties of both the matrix and the reinforcement are described by an incompressible neo-Hookean model respectively. In this paper, three-dimensional RVE models are created to represent the neo-Hookean composite which consists of one incompressible neo-Hookean elastomer embedded with another randomly distributed equal-sized spherical incompressible neo-Hookean particle reinforcement. Commercial finite element analysis software ABAQUS is employed for the numerical simulations of the RVE models. Periodic boundary conditions (PBC) are implemented in the RVE models when general finite deformation is applied to the RVE models. The numerical results show that the overall mechanical responses of the IPRNC can be well predicted by another simple incompressible neo-Hookean model. The simulation results also suggest that the classical linear elastic estimation (Christensen and Lo, 1979) can be used to predict the effective shear modulus of the IPRNC with different particle volume fraction and different particle/matrix stiffness ratio.

The structure of the paper is as follows: In Section 2, the IPRNC to be investigated is described and the theoretical basis of the numerical homogenization in finite deformation (Hill, 1972; Ogden, 1974) is also introduced. In Section 3, the RVE models are developed for numerical simulations using finite element method (FEM) and some related issues (e.g., isotropy of the RVE models, FEM mesh) are discussed. The results of the RVE simulations are presented and investigated in Section 4. The effective modulus of the hyperelastic composites is also compared with classical linear elastic estimation. Some concluding remarks are given in Section 5.

2. Particle-reinforced neo-Hookean composites and theoretical basis of numerical homogenization

First of all, some basic concepts in continuum mechanics need to be introduced. For a continuum solid, the deformation gradient is defined as $\mathbf{F} = \partial\mathbf{x}/\partial\mathbf{X}$, where $\mathbf{X}$ and $\mathbf{x}$ denote the positions of a typical material point respectively in the original (undeformed) and deformed configuration of the solid, respectively. The mechanical behavior of an isotropic hyperelastic material can be determined by its strain energy function (per unit volume in the original configuration) $W = W(\mathbf{F})$. If the material is compressible, the nominal stress $\mathbf{P}$ can be obtained as

$$\mathbf{P} = \frac{\partial W(\mathbf{F})}{\partial \mathbf{F}}, \quad P_{ij} = \frac{\partial W}{\partial F_{ij}}, \tag{1}$$

while for an incompressible material, it reads

$$\mathbf{P} = -p\mathbf{F}^{-T} + \frac{\partial W(\mathbf{F})}{\partial \mathbf{F}}, \tag{2}$$