A HYPERELASTIC MODEL OF PARTICLE-REINFORCED NEO-HOOKEAN COMPOSITE

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Summary 16 three-dimensional representative volume element (RVE) models have been generated to represent incompressible particle-reinforced neo-Hookean composites (IPRNC) with different volume fractions of reinforcements (5%, 10%, 20% and 30%). Four types of finite deformation (uniaxial tension/compression, simple shear and general biaxial deformation) were studied by means of finite element (FE) simulations. Results show that a simple incompressible neo-Hookean model can be used to predict the responses of the IPRNC.

The mechanical properties of particle-reinforced composites (PRC) in the infinitesimal strain regime have been investigated extensively. In contrast their mechanical behaviours in the finite deformation regime are still poorly-understood due to the intrinsic difficulties related to geometrical and material nonlinearities. In this paper, the numerical homogenisation approach is employed to investigate the mechanical behaviour of the simplest hyperelastic PRC under general finite deformation; the mechanical properties of both the matrix and the reinforcement are described by incompressible neo-Hookean models.

The simplest hyperelastic particle-reinforced composite is considered here. The mechanical properties of both the matrix and the reinforcement are described by an incompressible neo-Hookean model, whose strain energy function is written as $W = \mu(I_1 - 3)/2$. Here μ is the shear modulus and I_1 represents the first invariant of the right Cauchy-Green deformation tensor $\mathbf{C} = \mathbf{F}^T\mathbf{F}$ where $\mathbf{F} = \partial\mathbf{x}/\partial\mathbf{X}$ is the deformation gradient.

The commercial software DIGIMAT 4.1 has been used to generate the representative volume element (RVE) models. In each RVE model, 27 equal-sized spherical particles are randomly distributed in a unit cube and some particles are divided by the surface to accommodate the periodic boundary condition (PBC). In order to achieve a series of particle volume fractions $c = 0.05, 0.1, 0.2, 0.3$, the sphere size is changed accordingly. To make the meshing procedure of the microstructure easier, the distance between any two spheres was set to be larger than $0.1d$ when $c \le 0.2$ and larger than $0.05d$ when $c = 0.3$.

The commercial FE software ABAQUS has been used to mesh the RVE models and to carry out the simulations. In order to apply the PBC, a periodic mesh was generated for all RVE models. The RVE models were meshed using quadratic tetrahedral elements (type C3D10MH in ABAQUS. There are around 80,000 elements and 100,000 nodes in a typical RVE model. The PBC were applied throughout the numerical simulations. Matrix and particle reinforcements were modelled as incompressible neo-Hookean materials and the matrix-particle interface assumed to be perfectly bonded, which means that there is no relative movement on the interface during the simulation. The shear moduli of the matrix and the particle are denoted by μ_r and μ_m respectively (here only the stiffness ratio μ_r/μ_m rather than the absolute values of the moduli matters). When the composite is assumed to be isotropic and homogeneous, the only parameters needed for consideration are the stiffness ratio and the particle volume fraction c.

Four types of finite deformation have been simulated including: uniaxial tension, uniaxial compression, simple shear and general biaxial tension. For each simulation, the deformation was applied until convergence could no longer be achieved. Because of the material and geometrical nonlinearities, as well as severe mesh distortion in the matrix necking zones between spherical particles, convergence is usually very challenging (particularly when the stiffness contrast between the particles and the matrix is large). A typical simulation takes about 4-7 days on a HP Z600 workstation with 16 GB of RAM and 12 CPU cores.

To check whether the standard mesh was good enough to predict the response of the RVE models accurately, the mesh of one of the RVE models ($c = 0.2$) was refined; more than 170,000 elements and 200,000 nodes were used in the refined mesh. Uniaxial tension along the X_1 axial direction was simulated using both the 'standard' and 'refined' meshes. The stress-strain curves from the two simulations are identical, which implies that the standard mesh is able to predict the mechanical response of the RVE model at almost the same level of accuracy as the refined mesh (though the model with the refined mesh could simulate larger value of uniaxial tensile stretch). Hence the 'standard' mesh was subsequently used in all the numerical simulations reported here due to limitations on computing resources.

Drugan and Willis [1] showed that within the framework of linear elasticity, a small size RVE model can well-represent the macroscopic behaviour of many composites with reinforcements. This has been verified by the numerical simulations of RVE models for the linear elastic PRC [2]. Our current simulation results show that in the finite

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deformation regime, a small size RVE model can still be used to obtain accurate results (with a few percent error) similar to the linear elastic case. To verify the isotropy of the RVE models, the positions of the centroid of the particles and their moment of inertia were first examined using the same procedure as suggested in [2]. In this way the mechanical isotropy of the 16 RVE models was confirmed.

From the macroscopic point of view, any general deformation for a homogeneous isotropic incompressible hyperelastic material can be treated as a biaxial deformation along the principle directions. Therefore, any general deformation can be represented by the two principal stretches (λ_1, λ_2), (note that $\lambda_3 = 1/(\lambda_1\lambda_2)$ due to the incompressibility constraint). Thus, the overall strain energy function can be written as $\overline{W} \equiv \overline{W}(\lambda_1, \lambda_2)$. Alternatively, when the invariant approach is used, the overall strain energy function can be represented as $\overline{W} \equiv \overline{W}(I_1, I_2)$, where I_2 is the second invariant of the right Cauchy-Green deformation tensor $\mathbf{C}$.

A series of general biaxial simulations have been conducted using an RVE model ($c = 0.2$, $\mu_r/\mu_m = 10$). The stretch ratio between the principal directions X_1 and X_2 defined as $(\lambda_2 - 1)/(\lambda_1 - 1)$ was set as -0.4, -0.2, 0, 0.2, 0.4, 0.6, 0.8 and 1. The strain energy results, $\overline{W}$, computed from the FE simulations of: each of the general biaxial deformations, the uniaxial tension and uniaxial compression and also for simple shear, are related against the function $I_1 - 3$. The results can be well-fitted by the linear function $\overline{W} = 0.7476(I_1 - 3)$ ($R^2 = 0.9999$). This result shows that the mechanical behaviour of the IPRNC under general finite deformation can be predicted by an incompressible neo-Hookean model.

Four different particle/matrix stiffness ratios are studied in the FE simulations: $\mu_r/\mu_m = \infty$ (i.e., rigid particles), 100, 10, 0.5, to investigate the effect of stiffness ratio between the particle and the matrix. The following four types of finite deformations are simulated: uniaxial tension and compression along coordinate axial directions and random directions, simple shear, and general biaxial deformation. All the simulation results (i.e., RVE with any particle volume fraction, any particle/matrix stiffness ratio and any loading case) show that the average strain energy $\overline{W}$ is proportional to $I_1 - 3$, which suggests that the overall behavior of the IPRNC can be well modeled by an incompressible neo-Hookean model. The effective shear moduli μ_c of the IPRNCs are obtained by fitting the strain energy data from the numerical simulation results. Because the dispersion in the values of the obtained moduli is remarkably small in all cases, the numerical results can be considered as a very close approximation to the "exact" effective shear moduli of the IPRNC. They are compared with three theoretical models: the self-consistent estimate, SCE [3], the strain amplification estimate for composites with rigid particles, SAE [4], and the classical linear elastic three phase model, TPM [5]. It is found that the TPM provide very accurate approximation to the numerical results (maximum relative difference less than 5.1%) though it is developed for linear elastic PRC. Even though the SCE and the SAE are proposed for neo-Hookean composites, they overestimate the effective shear modulus of the IPRNC when the particle volume fraction $c > 0.1$.

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