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%). 27 equal-sized sphere particles were randomly distributed in the RVE and periodic boundary conditions (PBC) have been implemented. Four types of finite deformation (uniaxial tension/compression, simple shear and general biaxial deformation) have been studied by means of finite element (FE) simulations. Results show that a simple incompressible neo-Hookean model can be used to predict the mechanical responses of the IPRNC, and the effective shear modulus of the IPRNC obtained from the FE simulations agrees well with the classical linear elastic estimation.

2. Numerical Simulation of RVE Models

The simplest hyperelastic particle-reinforced composite is considered here. The mechanical properties of both the matrix and the reinforcement are described by incompressible neo-Hookean models, however the exact solution for a three-dimensional PRC model under general deformation is still not available in the literature. 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.

A number of RVE models with periodic microstructures have been created to represent neo-Hookean composites consisting of one neo-Hookean elastomer embedded with randomly distributed equal-sized spherical neo-Hookean particles. Four types of finite deformation (uniaxial tension/compression, simple shear and general biaxial deformation) have been simulated, all using RVE models with the PBC enforced. Results show that the overall mechanical response of such neo-Hookean composites can be well-predicted by another simple neo-Hookean model and the effective shear modulus of the IPRNC obtained from the FE simulations agrees well with the classical linear elastic estimation.
Here $\mu$ is the shear modulus and $I_1 = \text{tr}^{}(\mathbf{C})$ represents the first invariant of the right Cauchy-Green deformation tensor $\mathbf{C} = \mathbf{F}^T \mathbf{F}$ where $\mathbf{F} = \partial x/\partial X$ is the deformation gradient.

The commercial software DIGIMAT 4.1 has been used to generate the RVE models and a typical RVE model’s microstructure is shown in Fig. 1. In this model, 27 equal-sized spherical particles are randomly distributed in a unit cube and some particles are divided by the surface to accommodate the PBC. In order to achieve a series of particle volume fractions $c$, the sphere size was changed accordingly; when $c$ equals 0.05, 0.1, 0.2 and 0.3, the diameter of the sphere $d$ is 0.1524, 0.1920, 0.2418 and 0.2768, respectively. To make the meshing procedure of the microstructure easier, the distance between any two spheres was set to be larger than $0.1d$ when $0.2c \leq$ and larger than $0.05d$ when $c = 0.3$.

Fig.1. The microstructure of a typical RVE model.

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 [7]. The RVE models were meshed using quadratic tetrahedral elements (type C3D10MH in ABAQUS [8]). There are around 80,000 elements and 100,000 nodes in a typical RVE model. The PBC [9] 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 $\mu_m$ and $\mu_r$ respectively (here only the stiffness ratio $\mu_r/\mu_m$ 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.

3. Results

3.1 RVE size in finite deformation

Drugan and Willis [10] 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 [11]. Our current simulation results show that in the finite 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.

3.2 Isotropy of the RVE models
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 [11]. In addition, direct FE simulations were also employed to check the mechanical isotropy of the RVE models as follows: First, the nominal stress vs. strain curves of an RVE model \((c = 0.2, \mu_i/\mu_n = 10)\) under uniaxial tension along each of the three orthogonal coordinate directions were produced and were plotted in Fig. 2. The stretch ratio \(\lambda\) reaches about 1.5 before convergence problems occur. The three curves are almost identical. Motivated by Castaneda [2] and Bergstrom and Boyce [12] who both proposed the use of an incompressible neo-Hookean model to estimate the response of IPRNCs, the strain energy, \(W\), computed from these simulations has been plotted against \(I_1 - 3\) in Fig. 3. A linearly proportional relationship is observed and the data are well-fitted by the equation: \(W = 0.7440(I_1 - 3)\) (the least square regression coefficient, \(R^2 = 0.9999\)). This implies that the effective shear modulus of the IPRNC is \(\mu_i = 1.4880\). For comparison, the theoretical nominal stress-strain curve computed from the fitted strain energy function is also plotted as a dotted line in Fig. 2, and is seen to be almost identical to the directly calculated stress results.

Next the strain energy, \(\bar{W}\), computed from three uniaxial compression simulations were predicted and are plotted against \(I_1 - 3\) in Fig. 4. Again this shows a linearly proportional relationship (the compression stretch ratio \(\lambda\) reaches around 0.55) that can be fitted by the equation \(\bar{W} = 0.7514(I_1 - 3)\) (with \(R^2 = 0.9999\)). The relative difference between the effective shear moduli of the IPRNC predicted by the uniaxial tension and uniaxial compression simulations is less than 1% (within the range of error caused by the FE simulation itself), which suggested that a single incompressible neo-Hookean model might be able to predict the mechanical behaviour of a given IPRNC RVE under general finite deformation.

In light of these positive results on a single RVE, the same procedure was applied to all 16 RVE models to examine their isotropy also. Results showed that for every RVE, their response under uniaxial tension or compression along different directions could, in each case, be well-described by a unique incompressible neo-Hookean model. Further, the difference between the effective shear moduli predicted by the various tension and compression simulation cases for any given model was found to be well below 2%. In this way the mechanical isotropy of the 16 RVE models was confirmed.

3.3 General deformation
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 \((\lambda_1, \lambda_2)\), (note that \(\lambda_3 = \lambda_1\lambda_2\) due to the incompressibility constraint). Thus, the overall strain energy function can be written as \(W = \bar{W}(\lambda_1, \lambda_2)\). Alternatively, when the invariant approach is used, the overall
strain energy function can be represented as 
\[ \overline{W} \equiv \overline{W}(I_1, I_2) , \quad \text{where} \quad I_2 = \frac{1}{2} \left[ (trC)^2 - trC^2 \right] \] is the second invariant of the right Cauchy-Green deformation tensor \( C \).

A series of general biaxial simulations have been conducted using an RVE model \((c = 0.2, \mu / \mu_m = 10)\). 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 plotted against the function \(I_1 - 3\) in Fig. 5. The results can be well-fitted by the linear function 
\[ \overline{W} = 0.7476( I_1 - 3 ) \quad ( R^2 = 0.9999 ) \]. The effective modulus of the IPRNC is \(\mu_t = 1.4952\). This result closely matches results predicted from the uniaxial tension and uniaxial compression simulations and shows that the mechanical behaviour of the IPRNC under general finite deformation can be predicted by an incompressible neo-Hookean model.

### 3.4 Composites embedded with rigid particles

For the case of composites reinforced by rigid particles, each particle or indeed, each component of a particle (for some particles were partitioned by the RVE surface, was defined as a rigid body using the nodes on the matrix-particle surface. Hence, there was no need to discretise the particles into finite elements. Further if a spherical particle crossed the RVE surface, the translational and rotational degrees of freedom (d.o.f.s) of those components were properly constrained to make sure the PBC was satisfied on the RVE surface. As before, 4 types of finite deformation have been simulated using an RVE model \((c = 0.05)\) and the computed strain energy \(\overline{W}\) was found to fit closely a linearly proportional relationship, 
\[ \overline{W} = 0.5695(I_1 - 3) \quad ( R^2 = 0.9999 , \text{and relative error well below } 2\% ) \]. Therefore the effective shear modulus of the RVE model is predicted as \(\mu_t = 1.1390\). The effective shear moduli of three other RVE models with \(c = 0.05\) have been obtained through the same procedure and they too closely produce the value of \(\mu_t = 1.1390\) (relative error less than 2%). Similarly, FE simulations have been performed to compute the effective shear moduli of other RVE models with \(c = 0.1, 0.2\) and \(0.3\), respectively. These effective shear moduli are plotted against the classical linear elastic estimation [13] in Fig. 6, which again shows very good agreement.

### 3.5 Effect of particle/matrix stiffness ratio

#### 3.5.1 Particles 100 times stiffer than matrix

FE simulations have been conducted on the IPRNC with large but finite stiffness contrast between
particles and matrix ($\mu_r = 100$). Again the effective shear moduli were obtained by simulations of the four types of deformation on the RVE models. For an RVE model with $c = 0.1$, the strain energy, $\bar{W}$, obtained from the FE simulations of the uniaxial tension along the $X_1$ axial direction, the uniaxial compression along the $X_3$ axial direction, and the simple shear in the $X_1X_2$ plane can be well fitted by $\bar{W} = 0.6460(1 - 3I_1) \ (R^2 = 1\ , \ \text{and relative error is well below } 0.65\%)$, which implies $\mu_{r} = 1.2920$. The same simulations applied on three other RVE models with $c = 0.1$, showed consistent shear moduli with very small differences (well below 2%). A similar procedure was employed to compute the effective shear moduli of the other RVE models with $c = 0.05, 0.2$ and 0.3. These effective shear moduli are compared with the classical linear elastic estimation [13] in Fig. 6, which shows again a good agreement.

3.5.2 Particles 10 times stiffer than matrix

To explore the case where the particle stiffness is comparable to the matrix stiffness, a set of simulations was performed for $\mu_r = 10$. The same procedure was used and the numerical results are compared with theoretical formula from linear elasticity [13] in Fig. 6, excellent agreement is observed.

3.5.3 Matrix twice stiffer than particles

In simulations described previously, the particles have always been stiffer than the matrix. The opposite case (i.e., the matrix is stiffer than the particles) is considered here to fully examine the effect of stiffness contrast between the particles and matrix. In the simulations a small stiffness contrast $\mu_r = 0.5$ was used to make relatively large deformation possible in the numerical simulation (the convergence problem usually occurred at relatively moderate deformation in previous simulations, partly due to the large stiffness contrast, i.e. $\mu_r / \mu_m \geq 10$).

Several deformations including; uniaxial tension along the $X_1$ axial direction, uniaxial compression along the $X_3$ axial direction, and simple shear in the $X_1X_2$ plane were simulated in using an RVE model ($c = 0.3$). The resulting strain energy, $\bar{W}$ computed from the FE simulations s well-fitted by the function $\bar{W} = 0.4139(1 - 3)\ , \ \text{which indicates } \mu_r = 0.8274\ .$ Similar simulations were performed on three other RVE models with $c = 0.3$, and the effective shear moduli obtained were found to be consistent with this result (relative difference less than 2%). The effective shear moduli were then obtained from FE simulations on the other RVE models with $c = 0.05, 0.1$ and 0.2. They are compared with the classical linear elastic formula [13] in Fig. 6, where again an excellent agreement is achieved.
4. Conclusions

Three-dimensional RVE models have been employed to investigate the mechanical behaviours of IPRNCs, in which both the matrix and the particle reinforcement are incompressible neo-Hookean materials. In order to consider different particle volume fractions, \( c \), 16 RVE samples have been created with \( c = 0.05, 0.1, 0.2, \) and \( 0.3 \) (4 for each volume fraction value). The effect of stiffness ratio between the particle and the matrix has also been investigated. Uniaxial tensions and uniaxial compression simulations along different directions have been used for every RVE to verify isotropy.

The mechanical behaviours of the RVE models have been simulated using ABAQUS with PBC applied. Four different particle/matrix stiffness ratios have been studied, i.e., \( \mu_p / \mu_m = 0.5, 10, 100, \) and \( \infty \) (rigid particles). Four types of deformation: uniaxial tension, uniaxial compression, simple shear and general biaxial deformation have been used to explore the behaviour of the RVEs. All the results show that the strain energy \( \tilde{W} \) is proportional to \( I_1 - 3 \), which suggests that the overall behaviour of the IPRNC can be modelled by an incompressible neo-Hookean model. The numerical results show that the effective shear moduli \( \mu_e \) of the IPRNC computed from the FE simulations are in excellent agreement of the classical linear elastic estimation [13].

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References


