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On the isotropy of randomly generated representative volume elements for fiber-reinforced elastomers

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ABSTRACT

The isotropy of different numerical simulations of fiber reinforced elastomers has been explored by explicitly applying stretch in different loading directions, in models with representative volume elements (RVEs) spanning a wide range of fiber volume fractions and system sizes. The results show that the homogenized response is not the same for all loading directions, and that the corresponding dependance takes the form of a sine. The anisotropy decreases with the RVE size, and so it can be used to asses if the scales can be separated in a given model. Considering the average response over all loading directions greatly reduces the variation between different RVEs, which can be used to improve the accuracy of the simulations in a way that is significantly more efficient than increasing the size of the RVE. The simulations have also shown a good correlation between the isotropy of each representative volume element at low and high values of the applied stretch. The result of linear simulations can therefore be used as an efficient indication of the anisotropy expected at high deformations.

1. Introduction

Fiber-reinforced composites are widely used in industry due to their high stiffness-to-weight and strength-to-weight ratio. In addition to their application as structural elements, in recent years new elastomer-based composites have been proposed in systems that exploit the mechanics of large deformations, with examples ranging from strain sensing [32] to deployable structures [18] and shape memory composites [7]. This new set of constituent materials, loading conditions and application requirements have made necessary the development of new tools to predict the mechanical response of fiber composites in the nonlinear regime [27].

A set of such tools are analytical homogenization techniques. Following the pioneering work of Ponte Castañeda [26], several studies have provided increasingly refined homogenization models for the nonlinear behavior of fiber-composites [3,4,21,1,20]. However, this is a very complicated problem, where the possibility of obtaining simple closed form solutions is limited to a certain set of constituents and microstructure geometries. In addition, such models can only provide the homogenized response, and are unable to study the microscopic strain and stress fields.

The other option is numerical-based homogenization [22], which is widely used in the study of both linear and nonlinear composites [10,13,2,31]. This approach is based on the existence of a representative volume element (RVE) in which the microstructure and size are such that its overall response is the same as that of the real material. This is called separation of scales between the microscopic and macroscopic scales, and is only strictly true in the case in which the size of the RVE is mathematically infinite, that is, extremely large compared to the fiber dimension. The main problem is, therefore, establishing the minimum element size that provides a sufficiently accurate prediction of the response of the ideal composite, as well as bounding the associated error [28]. Several authors have provided estimates for this critical size in the case of composites with linearly elastic properties [5,11,14]. In the case of nonlinear composites, the critical size of the RVE depends not only on the source of nonlinearity, but also on the criteria used to establish if the different realizations of the RVE, with increasing size, have converged to the behavior of the ideal, infinite composite [15,30,25,8,9,23,12], the most common being the convergence of the homogenized mechanical response, that is, the macroscopic average stiffness, as the model size increases.

Another possible criteria is the requirement that, since a composite of infinite size and random microstructure must be isotropic, the response of the numerical model should be isotropic too. Deviations from this ideal behavior are therefore a numerical artifact

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due to the finite size of the model. The RVE size is considered to be sufficiently large, then, when its mechanical response is close to isotropic. This is commonly assessed by looking at the coaxility of the strain and stress tensors [19]. However, and to the author's knowledge, there are no published studies in which the isotropy is explicitly explored by systematically varying the loading direction. This provides a direct measure of the RVE anisotropy, that can be explored as a function of its size and fiber volume fraction. The fact that the level of isotropy of a given microstructure might change as the applied loading increases, as it happens with nonlinear composites, has also seldom been addressed in the existing literature.

The goal of this work is to study the isotropy associated to the RVE size at low and high strains, as well as the relationship between isotropy and convergence of the homogenized response as the size of the RVE increases. We will focus on two-dimensional RVEs, with parallel fibers, that are transversely isotropic in the plane perpendicular to the fiber direction. There are two main reasons to choose this simplified geometry. First, it is a particularly interesting case since the mechanical properties are dominated by the matrix, and the evolution of the fiber arrangement as the loading increases significantly affects the nonlinear response. Second, we will make use of the fact that the response of an incompressible material under plane strain can be defined with only two parameters, namely the principal stretch, λ, and the angle of the corresponding principal direction, θ, in order to explicitly explore the isotropy of the RVEs: for all realizations of our model, the same value of λ will be applied at several values of θ, which provides the homogenized stiffness as a function of the loading direction. The numerical model will be presented in Section 2. The results for small and large strain loading will be presented in Section 3, followed by a summary and discussion of the main findings in Section 4.

2. Computational model

Numerical homogenization is performed through a series of finite element simulations with the commercial package Abaqus. The RVEs are loaded applying a macroscopic deformation gradient $\overline{\mathbf{F}}$ through a combination of dummy nodes and periodic boundary conditions. The total strain energy of each RVE is used to calculate a homogenized strain energy density $\overline{W}$:

$$\overline{W} = \frac{\int_{A_f} W_f dA_f + \int_{A_m} W_m dA_m}{A_f + A_m} \tag{1}$$

where W_i and A_i are the strain energy density and area of either fiber, f, and matrix, m. The rest of this section provides details on the parameters, microstructure and boundary conditions of the model. A very similar model has been verified with experimental results of carbon fiber composites with a soft silicone matrix [17].

2.1. Geometrical and material parameters

We consider an idealized composite with cylindrical fibers of radius r, extending perfectly parallel in the X_1 direction and with a random distribution within the X_2–X_3 plane. The composite is therefore transversely isotropic, i.e. isotropic in the plane perpendicular to the fiber direction. The fiber volume fraction is V_f. In the simulations presented here we assume plane strain to reduce the geometry to a square two-dimensional RVE of side length $L_2 = L_3 = \delta r$, with $N_f = V_f\delta^2/\pi$ fibers. Assuming generalized plane strain yields the same results, since the extreme stiffness of the fibers with respect to the matrix prevents any stretching in the X_1 direction. A schematic of the model is shown in Fig. 1.

Both fiber and matrix are modeled as incompressible hyperelastic Neo-Hookean materials, with strain energy density $W_i = \mu_i/2(I_1{-}3)$, where μ_i is the linear shear stiffness of the component i and I_1 is the first invariant of the Cauchy-Green deformation gradient $\mathbf{C} = \mathbf{F}'\mathbf{F}$, defined in function of the principal stretches λ_i as $I_1 = \sum_{i=1}^{3} \lambda_i^2$ [24]. The bonding between both components is assumed to be perfect. The ratio of stiffness between fibers and matrix is taken so that the fibers behave as rigid, $\mu_f/\mu_m = 10000$. Linear quadrilateral elements CPE4H are used for both components, with hybrid formulation to account for incompressibility. An average element size of $0.1r$ has been chosen after a parametric mesh size study.

2.2. Boundary conditions and loading

Periodic boundary conditions are applied in all faces of the RVE using the command EQUATION in Abaqus. This requires the mesh to be identical in all opposite faces of the RVE. The conditions can be summarized as:

$$\begin{aligned} \mathbf{u}(L_2, X_3) - \mathbf{u}(0, X_3) &= \overset{2}{\mathbf{u}} \\ \mathbf{u}(X_2, L_3) - \mathbf{u}(X_2, 0) &= \overset{3}{\mathbf{u}} \end{aligned} \tag{2}$$

where $\overset{i}{u}_j = \overline{F}_{ij}L_j$, L_j is the length of the RVE in the j-th direction, and $\overline{\mathbf{F}}$ is the applied deformation gradient, $\overline{F}_{ij} = \partial x_i/\partial X_j$. Using the spectral theorem, the Cauchy-Green deformation gradient can be expressed as a function of the principal stretches λ_i and principal directions $\mathbf{n_i}$ as

$$\mathbf{C} = \sum_{1}^{3} \lambda_i \mathbf{n_i} \otimes \mathbf{n_i} \tag{3}$$

The condition of plain strain imposes $\lambda_1 = 1$, $\mathbf{n}_1 = [1\ 0\ 0]$. The additional restraint due to incompressibility implies that all possible deformations are defined by a single principal stretch, $\lambda_2 = 1/\lambda_3 = \lambda$, and a direction θ, $\mathbf{n}_1 = [0 \quad \cos\theta \quad \sin\theta]$ and $\mathbf{n}_2 = [0 \quad -\sin\theta \quad \cos\theta]$. Equation (3) is then used to calculate $\mathbf{C}$, and the deformation gradient is obtained solving the equation $\mathbf{F}'\mathbf{F} = \mathbf{C}$.

The components of $\overset{i}{\mathbf{u}}$ can therefore be obtained from the desired principal stretch and direction, and imposed to the model through auxiliary dummy nodes. However, imposing the four displacements often leads to numerical errors, since even small rounding errors result in a violation of the incompressibility condition. In practice, this is resolved by allowing free expansion in the X_3 direction. Analysis of the results show that the resultant displacement is basically equal to $F_{33}L_3$, as expected.

2.3. Fiber arrangement

For a given set of values of δ and V_f, the microstructure is fully described by the position of the center of the fibers within the RVE. These are obtained through a random sequential adsorption algorithm [6]. This is is a hard-core process, i.e. a Poisson process in which a limitation on the minimum distance between the centers is introduced: the positions are obtained randomly, and rejected if the distance to any of the already allocated fibers is less than a given limit. In this work, an unless noted otherwise, the minimum distance adopted is 1.1 times the diameter. Additionally, a fiber is also rejected if the distance between its center to the edge of the RVE is in the $[0.9r, 1.1r]$ interval. The goal of both conditions is creating a geometry that can be easily meshed.

It is possible that a given fiber distribution reaches a jammed configuration [29], in which no new fibers can be added without violating the non-overlap restriction. For this reason, if after 1000