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A numerical investigation of the connection between state of dispersion and percolation and its effect on the elastic properties of 2D random microstructures

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ABSTRACT

The present work is dedicated to a numerical investigation of the connection between state of dispersion and percolation and its effect on the elastic properties of 2D random microstructures. The main objective consists in checking out the link between percolation and mechanical response in the context of a heterogeneous medium the reinforcements of which are not homogeneously dispersed. Besides, the influence of the stiffness of inclusions is also investigated since this could impact on the percolation effects. For these purposes, large samples of volume elements are generated according to the Monte Carlo method. We consider the low cost framework of 2D random grids which enables large and in-depth investigations. Besides, the spatial distribution of heterogeneities is simulated with the help of the 2-scale Boolean scheme of disks which is a powerful tool for modelling and studying several states of dispersion. The numerical results highlight beneficial mechanical reinforcements for a heterogeneous dispersion when the percolation phenomenon is enhanced. This improvement is highly sensitive to the stiffness of heterogeneities.

1. Introduction

The effective behaviour of heterogeneous composites is closely related to the percolation phenomenon. This appears when the concentration of heterogeneities is sufficiently important and contacts are made easier. Pathways which are formed by a set of connected inclusions, then enable the diffusion of properties within the microstructure. As a result, a sharp jump is observed in effective properties at a critical area or volume fraction which is called percolation threshold. From a statistical point of view, this is the density of inclusions for which the percolation probability is 50%. In electricity and heat transfer fields, the percolation phenomenon is well-known and actually leads to a beneficial increase of properties as exhibited by numerous experimental measurements [1,2]. Classical power-law models provide convenient predictions of properties for conductivity problems. These depend on the properties of the medium, the percolation threshold and a percolation exponent which have to be determined according to the material configuration [3–5]. The binary behaviour of the conductivity leads to estimate effective properties as follows. Below the percolation threshold the conductivity is zero, above the percolation threshold the conductivity is predicted by the power-law model.

In the mechanical framework, classical power-law models are not sufficient to predict effective properties. Indeed the non-diffusive behaviour of the constitutive equations of elasticity leads to a more complex dependence. In this context, the predominant parameter is not the percolation threshold anymore but the area or volume fraction of heterogeneities. Thus, a network of unconnected stiff inclusions can reinforce a matrix with lower properties. However, in composites [6–8] and nanocomposites [9] field, an increase in mechanical properties was numerically and experimentally verified and connected to the percolation phenomenon which suggests non-negligible percolation effects. Furthermore, uncharacteristic percolation effects were sometimes observed at very low volume fraction. Fralick et al. [10] investigated these effects and the hypothesized role of a connected interface phase. However, other microstructural parameters such as the dispersion of heterogeneities, the stiffness of the material and the shape of inclusions could also impact on the percolation response. Classically, elastic coefficients are predicted using micromechanics models such as the Mori–Tanaka (MT) one [11] or bounds such as Hashin–Shtrikman (HS) ones [12]. Thus, the MT model takes into account the geometry of heterogeneities but is only valid for low densities due to percolation effects. Conversely, the phenomenological series–parallel model [13] is an improved power-law model which is only based on the percolation

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threshold and percolation exponents. That is why, this only provides predictions for an area or volume fraction of inclusions higher than the percolation threshold.

A full investigation for which both percolation and geometry are taken into account whatever the density of heterogeneities, necessitates a numerical approach. Generally the modelling is based on the generation of representative volume elements (RVE) and effective properties are estimated using a numerical technique such as the Finite Element Method (FEM). The RVE enables to describe complex microstructures for which several morphological parameters are taken into account. In the present context, we focus our investigations on the distribution of heterogeneities. We consider several states of dispersion in the sense that multiscale random distributions are studied. We distinguish two cases. First, the well-established case of a homogeneous dispersion for which a classic random distribution is considered. Second, the case of a 2-scale random distribution for which the dispersion is heterogeneous. The material heterogeneity can be characterised by the formation of agglomerates or voids. From an experimental point of view, agglomerates reduce the surface bonding between the inclusions and the matrix in such a way that the percolation phenomenon is disadvantaged. Thus, they act as stress concentrators which thwart the reinforcement of the composite material [14,15]. Several numerical studies arrived at the same conclusions [16,17]. However, as described by Jeulin and Moreaud [18–20], the material heterogeneity can also be characterised by an arrangement of agglomerates at different scales. In this case, the composite is homogeneous at the microscopic scale and void areas and aggregates are only observable at the mesoscopic scale. Thus, the percolation phenomenon is advantaged and potentially related to a beneficial improvement of mechanical properties. This issue was recently investigated by Leclerc and Karamian [21] in the framework of random fibre composites. Nevertheless, even though low percolation thresholds were exhibited, no mechanical reinforcement was observed by the two authors.

However, this work suffered of two main limitations related to the complexity of the framework of random fibre composites. First, the effects of contrast, i.e., the effects related to the ratio between the properties of the inclusions and those of the matrix, were not taken into account. Second, the simulation of the heterogeneous medium by the 2-scale Boolean scheme of disks [20] was limited to a scale factor of 4. This parameter describes the scale of agglomeration so that a low value, typically lower than 5, leads to individual agglomerates, and a high value, greater than 5, leads to a 2-scale arrangement of agglomerates. Thus, the scale factor was not really investigated and only very small beneficial improvements in percolation threshold were observed. In the present work, we propose to enlarge this previous study to a full range of contrasts between 10 and 10^7 and higher scale factors up to 20. Our main objective is to provide some responses on the issue of the connection between percolation and effective properties in the context of a heterogeneous dispersion. We expect to exhibit both advantageous reinforcements and contrast effects for a heterogeneous state of dispersion. For this purpose, we consider a simple modelling for which a low calculation cost is required. A very large number of volume elements (VE) are generated by Monte Carlo random draws [22,23] so that accurate results in both percolation thresholds and effective properties can be obtained. 2D random microstructures are built with the help of a structured grid of cells for which the heterogeneities are represented by a set of randomly drawn cells. The heterogeneous dispersion is simulated using the 2-scale Boolean scheme of disks which enables a 2-scale modelling for which the first scale corresponds to the agglomerates, and the second scale to the heterogeneities. For practical purposes, patterns are periodic. This assumption enables a direct use of the double-scale homogenisation [24,25] which is a powerful tool for estimating elastic properties whatever are both contrast of properties and complexity of the microstructure. To end up, percolation thresholds are assessed via the depth-first search (DFS) algorithm which is improved by a dichotomous and recursive approach [21].

The present paper is outlined as follows. Section 2 describes the generation of random microstructures via the Monte Carlo method. Section 3 is dedicated to the numerical method for assessing percolation thresholds. Section 4 presents the double-scale homogenisation process which leads to the effective elastic properties. A detailed study is also performed for estimating the suitable VE dimensions in the framework of the Monte Carlo method. The last section is dedicated to results and discussion. We precise that from now on, the term “1-scale Boolean scheme” will designate a homogeneous dispersion, and the term “2-scale Boolean scheme” will designate a heterogeneous dispersion.

2. Microstructure modelling

2.1. RVE

Random microstructures are typically modelled with the help of an RVE. An RVE is a classic but powerful tool to model a material with heterogeneities. This is a representative pattern of the medium the size of which has to respect several criterions. Indeed, the RVE must be large enough to provide a large amount of information on the microstructure but small enough to remain elementary and limit the calculation cost in a finite element analysis (FEA) [22,26]. Two methodologies can be considered. First, one can generate a large RVE the size of which L is chosen such as no boundary effects or anisotropy can be observed. Typically L has to tend to infinity which is obviously not practically possible. Consequently L is often chosen between 10 times or 20 times a characteristic dimension δ of the heterogeneity. This is done to the detriment of the representativeness of the cell. Hence the use of a second methodology which consists of a random draw of a large number of small volume elements (VE). In this case, boundary effects are not negligible for one occurrence but tend to disappear when considering the whole sample. Thus, one pattern is not representative of the material while the whole sample is representative. This approach has two main advantages. First, this is more practical owing to the low dimensions of the VE. Second, even if small VE require a large number of realisations, the methodology is much more efficient, especially when L is less than 10 [27]. In such an approach the number of realisations n_r of the sampling process is estimated by a statistical approach based on the study of the variance parameter D_Z relatively to an effective elastic property Z. n_r and D_Z are then connected to Z by the relative error ε_{rel} which reads

$$\varepsilon_{rel} = \frac{1.96 D_Z}{Z\sqrt{n_r}} \tag{1}$$

However, the VE cannot be chosen too small and an accurate investigation of their dimensions has to be performed. The most common process is studied and described in [22]. It consists in generating a sample for which the VE dimensions are minimal, i.e., 2 or 3 times the dimension of the heterogeneity, and testing the validity of the results according to statistical tools. Two possibilities exist, either results are valid and the VE dimensions are determined, or results are not accurate enough and the process is repeated for larger VE as many times as necessary for getting a good accuracy.