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► To cite this version:

Sami Ben Elhaj Salah, Azdine Nait- Ali. Effect of aggregation phase on the elastic properties of a heterogeneous material. 2019. hal-02189841

HAL Id: hal-02189841

<https://hal.science/hal-02189841>

Preprint submitted on 22 Jul 2019

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Effect of aggregation phase on the elastic properties of a heterogeneous material

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Abstract

In this study, the technique of homogenization and morphological analysis is used in order to quantify the relationship between two morphologies of voided material: two types of structures are considered. Each one is characterized by a scale which was observed. Structure 1 is an elastic matrix containing a random distribution of spherical inclusions corresponds to a smallest scale (microscopic scale). Structure 2 is a composite material consisting of spherical inclusions distributed randomly in an elastic matrix corresponds to a largest scale (mesoscopic scale). A well-known mathematical morphology technique is used in this investigation. The parameters of mathematical morphology, such as *covariance*, are determined and presented the relationship between the parameters of the two structures. All the obtained results suggest us to define a new concept called "the equivalent morphology". This concept is to replace the first composite containing inclusions with radius R1 by other fictif material containing inclusions with radius R2 that was expressed as a function of the parameters derived from the analysis of the initial morphology. These two composites 1 and its equivalent morphology 2 give the same effective elastic properties, but not necessarily with the same size of the deterministic representative volume element, DREV.

Keywords: Heterogeneous material, Inclusion, Covariogram, Equivalent morphology concept, Elastic properties, Homogenization, Tomography

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1. Introduction

Sectors were developed, like aeronautics or space require the development of more efficient materials. Composites, with their various mechanical properties, are materials that improve the quality of the face material to some use (lightness, stiffness to a force, etc.). However, their morphological characteristics and mechanical behavior attached to each phase are difficult to be modeled in this class of materials.

In the following, only a voided material with random distribution of spherical inclusions in an elastic matrix under a displacement are considered. Thus, in this context, much progress has been made in characterizing the microstructure of statistically homogeneous two-phase random media, via covariance and integral range(IR). This is the case of Torquato [1], Jeulin and Ostoj-Starzewski [2], for two-phase heterogeneous media, Kanit et al. (2003) [3] for Voronic mosaics, Kanit et al. (2006) [4] for ice cream, Willot and Jeulin [5] for porous materials, Jean et al.[6] for elastomer materials, Jeulin [7] for 3D composite materials and Painbon et al. [8] for two-phase heterogeneous media with overlapping and non-overlapping spherical particles. We studied voided structures by measurements on 3D images [9], such as the covariogram [10] and [11] which allows us to have maximum of microstructural information for the materials studied and permits us to have a good morphological description. Many morphological information can be determined from this statistical analysis method as the volume fraction, the isotropy or the ergodicity of the distribution of inclusion. The aim of this paper is to expand the concept of the equivalent morphology, thus, by using the data derived from this statistical analysis and the analytical estimation for the effective elastic properties. Hashin and Shtrikman [12] - [13] proposed a more efficient framework and several homogenization techniques for two-phase materials named Hashin Shtrickman Bounds or known as up-scaling. It is based on solving a problem of inclusions embedded in a finite homogeneous matrix. We can define an equivalent heterogeneous composite made of two phase as well. Then, an optimization by an ellipsoidal model will be proposed. Finally, numerical and analytical results will be compared with the experimental for an EPDM under a diffusion of hydrogen, but in this case we will only focus on the mechanical approach and not on the phenomeno of diffusion . Indeed, under a decompression, the damage on these materials involves the nucleation and growth of spherical cavities.

2. Morphological characterization

We introduce the basic elements retained to characterize the morphology of random microstructures. The morphological tools for these aspects are the covariance.

2.1. covariance

The covariance is very useful characteristics for the description of the size, shape and spacial distribution of a given particle. Covariance $C(x, x+h)$ [14]-[15] and [16] is defined by the probability P for two points, separated by the vector h , to belong to the same stationary random set B . We have:

$$C(x, x + h) = P\{x \in B, x + h \in B\} \quad (1)$$

See [11] that the covariogram can be used in dynamic case. Such a function corresponds to the probability to intercept other particles at a distance h from a reference particle.

More particular properties of the covariogram are listed blow.

(P1) : It can be noticed first that the volume fraction of set B is directly given by covariogram for $h=0$: $C(h)=p$.

(P2) : If the events $x \in B$ and $x+h \in B$ become independent as the magnitude of h tends to the higher values, moreover, $C(h)$ converges to an asymptotic theoretical value equal to p^2 , then the probability distribution is ergodic, meaning that the inclusions distribution statistic is homogeneous, so whatever the draw, the macroscopic behavior will be the same and the occurrence probability is the same at any point of the volume.

(P3) : If the horizontal asymptote values is the same for all direction, the microstructure is isotropic at the macroscopic scale. But values can be different depending on the direction. In this case, the material is anisotropic.

(P4) : The first intersection between $C(h)$ and the asymptote corresponds to the correlation length in the z direction, for example $Dc(z)$. It is also called Integral Range by some authors [3]. It is defined by:

$$Dc(z) = \min_{h \in \mathbb{R}^*} \{Cz(h) - p^2 = 0\} \quad (2)$$

This distance corresponds to the maximal distance of statistical influence of the inclusion phase B. It provides information about the minimal size of the domain over which the volume is statistically representative. If the heterogeneous medium contains clusters of inclusions, $Dc(.)$ provides an estimate of the statistical average size of the cluster in each direction. If $Dc(.)$ is constant regardless of the direction, the material is isotropic at this scale [3]

2.2. Equivalent morphology concept

At a microscopic scale, the characteristic variables which are derived during the analysis of the initial morphology, allow us to define the concept of equivalent morphology. This concept represents a composite with inclusions corresponds to a mesoscopic scale, statistically equivalent to the original structure. It means replacing each cluster by one effective inclusion whose parameters are given in terms of the different distances from where any phase affects the neighborhood. It is called correlation length. In our case, it should be noted that the equivalent material will follow the same law of distribution of clusters in the original material. Thus, we are able to consider the assumption of ergodicity. Then, an optimization by an ellipsoid is realized in order that the mechanical fields around these iclusters are similar to the inclusions presented in the original material. The spherical and ellipsoid models (original and equivalent morphologies) are given in Fig.1 and 2.

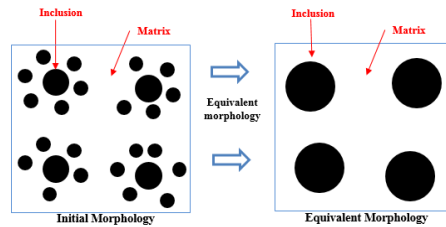


Fig. 1. Concept of equivalent morphology: spherical model

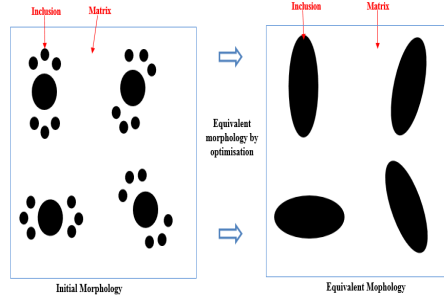


Fig. 2. Concept of equivalent morphology: ellipsoidal model

Many different data can be estimated from this statistical analysis method through the covar-iogram for the initial images. In this part, only the correlation lengths $Dc(.)$ are considered. In Fig.3, it seems that we increased gradually the number of the clusters in our matrix in order to come closer to reality and have a significant results in the equivalent morphology.

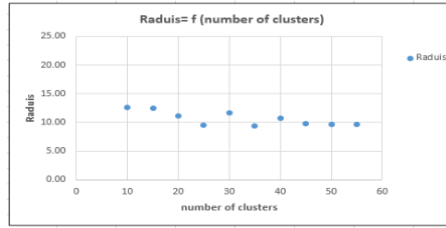


Fig. 3. Variation of raduis of the inclusion in the equivalent morphology

After the presentation of the basic morphological parameters, these available notions are used to characterize the geometry and the morphology of random composite. The objective of this paragraph is to find a relationship between the morphological parameters of initial and equivalent morphology. This relationship is used to define the concept of equivalent morphology in the two types of model: spherical and ellipsoidal. They are mentioned in the following equations:

$$\text{spherical model : } Requ = \frac{\langle Dc \rangle}{6} \quad (3)$$

$$\text{ellipsoidal model : } \begin{cases} Rmax &= \frac{Max\{Dc(.)\}}{2} \\ Rmin &= \frac{Min\{Dc(.)\}}{2} \end{cases} \quad (4)$$

The obtained results, based on laws of mathematical morphology that the error between the two microstructures examined on a macroscopic scale (Asymptote) is insignificant and does not overpass 2 percent. However, we noted that there is a slight increase on a local scale (Correlation lengths) because the inclusions are empty. Also, it is due to the morphology of local field. Thus it appears that there is a small oscillation because the clusters are the same in the original material with meadows of rotation. Using this condition, the equivalent morphology concept can be proposed for the voided materials. Figures 1 and 2 describe schematically this concept that consists to replace

the structure containing clusters by structure just containing inclusions. These two structures give the same elastic properties but not necessary the same DREV.

3. Material, Microstructure and conditions

3.1. Loading condition

The boundary condition is a main challenge in modeling a structure by finite elements and it is the application of a force and/or constraint. For the particular model, two types of boundary condition were applied. The first one is that the model is fixed in the bottom surface and subjected to a displacement in top one.

3.2. Morphology and Meshes

In this section we presented our 3D model in the context of the linear elasticity. It is a two-phase heterogeneous material with an elastic matrix containing a random distribution of spherical inclusions. There is a distance between each two neighbor's center inclusions that avoids the connection between them. We compared two types of morphologies: The initial composite and the equivalent one. The finite element mesh, related to our model, is obtained by using the tetrahedral as type of elements with the free technique. All our composites are characterized by a volume of fractions of the inclusions phases.

3.3. Overall stress, strain and displacement

The first step in a numerical study is to create a geometry that represents the microstructure of the studied material. This geometry is a numerical representation of real microstructures. The finite element solver ABAQUS with its integrated interface of visualization and modeling (ABAQUS / CAE) is used to make our 3D model. Calculations were done using the finite elements code "Foxtrot" that was developed in the DPMM team and finally for the post-processing and visualization of our simulations, we had used Paraview with a VTK file as an input.

In the present work, the definition of overall mechanical quantities usually defined as averages of microscopic and mesoscopic ones, must be explicit, see [17]. Let V denotes the total volume. The porous material is subjected to a displacement. In order to compare the two composite 1 and 2, it is classical to define the overall stress and strain as the volume averages of the corresponding local stress and strain fields over a volume V so we can write :

$$\langle \sigma \rangle = \frac{1}{|V|} \int_V \sigma \, dx \quad , \quad \langle \varepsilon \rangle = \frac{1}{|V|} \int_V \varepsilon \, dx \quad (5)$$

An example of the obtained numerical results is presented respectively in Fig.5, 6 and 7. These figures show that the mechanical fields in the two morphologies are nearby. Then, based on the obtained numerical results, a comparison has been done in order to quantify the difference. According to the results in Fig.8, it seems that they are adequate in the macroscopic scale even the error does overpass 4 percent.

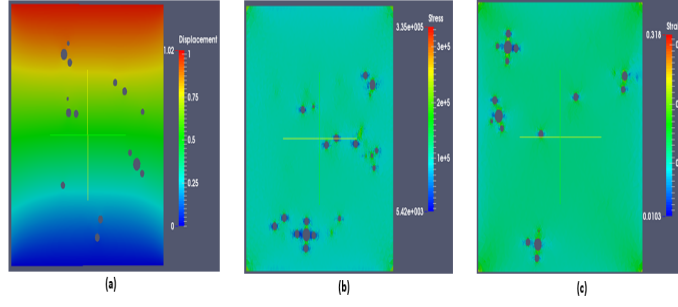


Fig. 4. Initial morphology: (a): displacement, (b): stress, and (c): strain

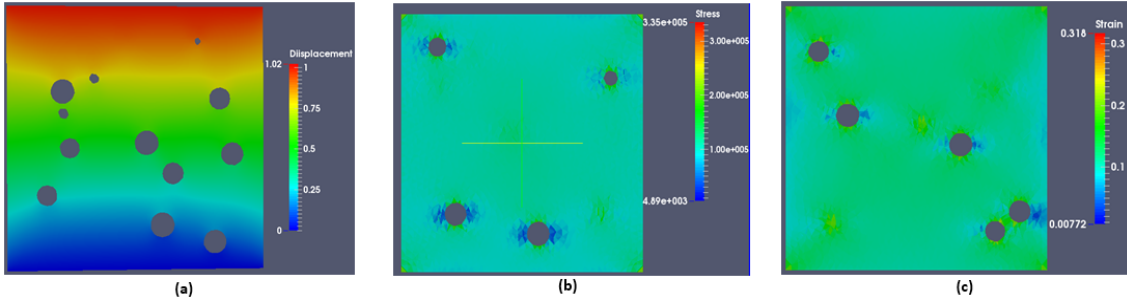


Fig. 5. Equivalent morphology: (a): displacement, (b): stress, and (c): strain

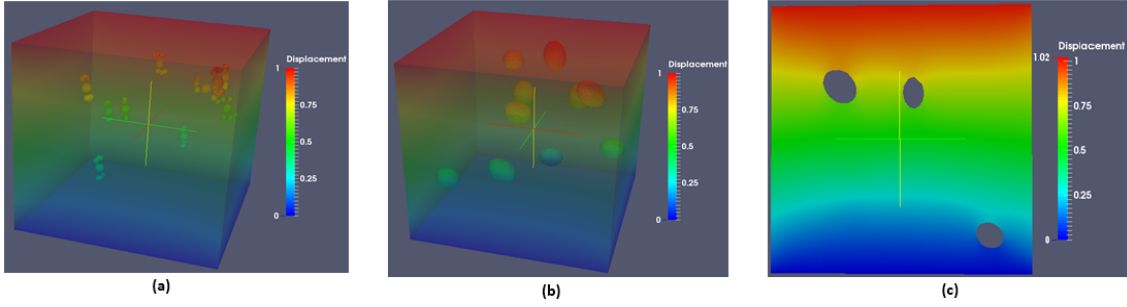


Fig. 6. Concept of equivalent morphology optimised by ellipsoidal model: (a): inial morphology, (b): equivalent morphology, and (c): cutting view

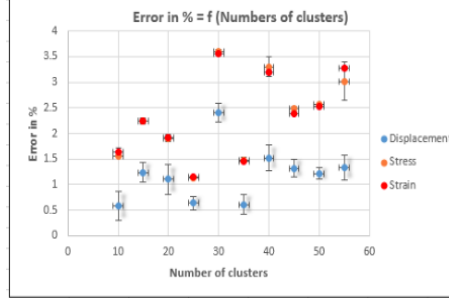


Fig. 7. Error between initial and equivalent morphology investigated in the macroscopic scale

4. Homogenization

In this part, several analytical homogenization techniques are used to estimate the effective linear elastic properties (ELEP), of three dimensional (3D) microstructures consisting of spherical inclusions distributed randomly in an elastic matrix.

4.1. Scales and structures

The present work with primary and secondary morphologies involves two different scales. The smallest (or microscopic) corresponds to composite 1 and the seconde one is the largest (or mesoscopic). The up-scaling procedure is able to modelize a heterogeneous material and estimates the linear elastic properties of voided material subjected to displacement on its top surface

4.2. Identification with Hashin-Shtrikman bounds

In the early age, effective properties in porous material are estimated by using an analytical technique of homogenous. Thus, they were derived from Finite Element Calculations. In this context, Hashin and Shtrikman [12] suggested a more useful framework for two phase materials named HS bounds. This technique aims to explain and solve the problem of a spherical inclusions randomly distributed in an elastic matrix. Compressibility and shearing ratios are associated to E and ν , so we can write:

$$K = \frac{E}{3(1 - 2\nu)} \quad (6)$$

$$\mu = \frac{E}{2(1 + 2\nu)} \quad (7)$$

Then, based on the homogenization process and using all the relations that are given bellow, we focus on estimating the values of young's modulus of equivalent inclusion. In this context we use the methode of optimisation based on the function of minimisation. It allows us to find the minimum of unconstrained multivariable function using derivative-free method. Fig.9 shows the procedure of the up-scaling technique.

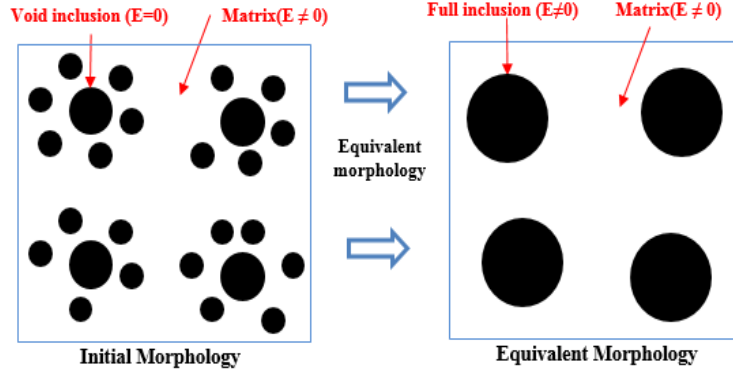


Fig. 8. Process of homogenization

$$\frac{1}{k^{HS} + k^*} = \frac{cm}{k^m + k^*} + \frac{cf}{k^f + k^*} \quad \text{with} \quad k^* = \mu^0 \quad (8)$$

$$\frac{1}{\mu^{HS} + \mu^*} = \frac{cm}{\mu^m + \mu^*} + \frac{cf}{\mu^m + \mu^*} \quad \text{with} \quad \mu^* = \frac{k^0 \mu^*}{k^0 + 2\mu^0} \quad (9)$$

and there are two types of bounds for this technique:

- **HS Up-Bound:** $k^0 = k^m$ et $\mu^0 = \mu^m$
- **HS Down-Bound:** $k^0 = k^f$ et $\mu^0 = \mu^f$

With the results obtained by numerical simulation coupled with a process of homogenization, this paragraph is devoted to make a comparison in the mechanical field as displacement, stress and strain between the two composites under a displacement in the linear problem. Fig.9 shows an example of the results after a numerical simulation in Finite Element Code. Some results of this comparison are given in Fig.10. It seems that the results are suitable in macroscopic scale. Yet there was a small increase in stress level compared to strain and displacement. In other words, in this case we also decreased the properties' gradient. Thus the error in each mechanical field is constant because the clusters are distant and do not interact. Also, the same motif was repeated.

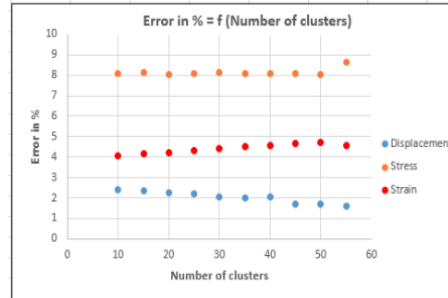


Fig. 9. Error between initial and equivalent morphology investigated in the macroscopic scale

5. Teste with EPDM Material

5.1. Tomograph and meshing of 3D images

This part is devoted to apply all our numerical simulations coupled with laws of mathematical morphology to a real elastomer EPDM subjected to a diffusion of hydrogen, used in the new energy. Thus, One of the best solutions available today to observe changes in the microstructure due to damage is High Resolution X-ray Computed Tomography (HRXCT) [18] [19]. It is not the purpose of the present paper to describe the tomography technique in detail. Many preceding papers have been published and can be referred to (see, for instance, the review in [20] and [21]) illustrate the principle of X-ray tomograph. Therefore, the mesh in initial structure is generated using the 3D pictures derived by this technique that converts the voxel in hexahedral elements, but in the case of the equivalent morphology, we have studied the convergence of mesh and using the required mesh by the tetrahedral elements.

5.2. Results and discussion

The obtained set of numerical results coupled with laws of mathematical morphology is used to quantify the difference between two different random structures of porous material. Two cases of real images will be analyzed and discussed.

The main objective of this work is to make a morphological simplification which allows us to replace one microstructure via another, named here equivalent morphology. Also it ensures shorter calculation times. Table 1 shows an example of two different 3D images of real materials treated and it is clear that the error in the stress field did not exceed 10 percent. Concerning the time calculations, we are able to optimize approximately 40 times.

Table 1. results of calculations

	Error $\langle \sigma \rangle$ in %	Time ratio
Example		
1	9,18	44
2	9,73	42

6. Conclusions

The main objective of this study is to quantify the difference between the two studied morphologies. The obtained results allow us to replace a composite containing clusters by other fictive composite containing inclusions that their radius was expressed as a function of the parameter (correlation lengths) derived from the analysis of the initial morphology. Thus a new concept is proposed and called "the concept of equivalent morphology". It was noted that these two morphologies have the same elastic properties, but not necessarily they have the same size of the deterministic representative volume element, DRVE.

Homogenization was considered the second main objective in this paper. In reality, it can currently consist of a step for some analysis of global behavior. Particularly, it is sensitive to the local responses of heterogeneous materials. As an example, the initiating of the damage by microcracks or composites microcavitation. Hence this work are also focuses on the prediction of the effective elastic properties of heterogeneous materials using a conventional analytical method of homogenizing called Hashin-Shtrikman Bounds. An extension of this study to other application (microstructures type, with pores having either different shape and containing an anisotropic material) will be discussed in the following works.

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