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Catching the time evolution of microstructure morphology from dynamic covariograms

Évolution temporelle de la morphologie de la microstructure à partir d'un covariogramme dynamiques

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ABSTRACT

In micromechanical modelling, covariograms are often used as a statistical analysis to estimate the features or morphological Representative Elementary Volumes (REV), from representative pictures of the initial microstructure (i.e. static covariogram). The aim of this article is to present an extension of the method to the time evolution of the microstructure, through the idea of dynamic covariogram built up of successive pictures of the microstructure along time. The possible enhanced evolution of covariogram parameters is analyzed first from a general point of view. It is then illustrated on the cavitation damage occurring during decompression in rubbers exposed to diffusing gas.

RÉSUMÉ

En micromécanique, la construction de covariogramme est utilisée pour renseigner la notion de volume élémentaire représentatif morphologique, à partir d'images représentatives de la microstructure initiale. L'objet de cet article est de présenter une extension de cette notion à l'évolution temporelle de la microstructure au cours du temps, via la notion de covariogramme dynamique, issue d'images successives de la microstructure au cours du temps. L'évolution possible des différents paramètres du covariogramme est analysée de manière standard, puis illustrée à partir de l'endommagement par cavitation observé dans les élastomères sous décompression après exposition à un gaz diffusant.

1. Introduction

In micro-mechanics, a rigorous definition of the Representative Elementary Volume (REV) is needed, either for analytical modeling or for full-field numerical simulations. REV implies to be representative of both the microstructure morphology and the mechanical properties. Only the morphological aspect is addressed here. Microstructure within the morphological

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REV can be more or less finely defined. Basic descriptions are often based on the volume fraction of components only, but more sophisticated descriptors can be used too, for instance the size distribution of inclusions or porosity, or the shape factor distribution in case of anisotropic particles. The REV description can be based on stochastic considerations. When inclusions are stochastically distributed, the REV is called DREV, standing for Deterministic Representative Elementary Volume. A fine morphological description of the REV can be obtained using image analysis through covariogram [4–6]. Many different data can be estimated from this statistical analysis method, among which the size of the REV, the number of included phases, the isotropy or the ergodicity of the distribution of inclusions. Such a concept has been widely used so far, almost systematically to static cases, i.e. to images of the initial microstructure. The covariogram analysis is used to identify parameters of the schematized microstructure or generate numerical models, in analytical or full-field numerical models respectively. Microstructure morphology is not updated during the simulation. The aim of this paper is to extend this approach to so-called dynamic cases, i.e. situations for which the microstructure evolves with time, like during damage processes for instance. Indeed, the REV changes occurring during the damage process can be tracked through the evolution of covariograms parameters deduced from successive snapshots of the microstructure. In the following, only heterogeneous materials made of two phases will be considered. The article is divided into two parts. The first part briefly describes useful parameters displayed by covariograms. The second part is dedicated to the mechanical interpretation of these parameter evolutions. As a first example about material cracking, it is explained how privileged cracking directions and/or evolution of these directions can be pointed out from REV evolution. A second example deals with the ability of covariograms to highlight damage evolution during cavitation damage occurring during transient diffusion loadings.

2. Covariogram parameters obtained from a single picture of the initial microstructure (static case)

This first section briefly reminds the statistical framework of covariogram analysis and introduces relevant parameters that can be deduced for microstructure description. The same parameters will be further considered in the dynamic case, to highlight the physical interpretation of complex transient phenomena.

No difference is made between R^3 and the three-dimensional Euclidean physical space equipped with an orthogonal basis denoted by (e_1, e_2, e_3). Let us consider the set $\Omega \in R^3$ and $X := \cup_{i \in \mathbb{N}} X_i \subset \Omega$ with X_i connex family set. For every $z \in \mathbf{Z}^2$, the operator $\tau_z : \Omega \to \Omega$ by $\tau_{-z} X := X + z$ is defined. Vector z corresponds to a direction of study. The probabilistic set X is equipped with the trace σ-algebra A of standard product σ-algebra on $\mathbb{R}^3$. Then, the probability space $(\Omega, A, \mathbf{P})$, with P a probability measure, can be defined. The covariogram describes the probability that both events X and $\tau_{-z} X := X + z$ occur simultaneously. In direction z, Eq. (1), the covariogram function is defined by:

$$\begin{aligned} & C : \mathbb{R}^3 \to \mathbb{R} \\ & z \to C(z) \\ & C(z) = \mathbf{P}\{x \in X \cap \tau_{-z} X\} \end{aligned} \tag{1}$$

Covariogram can be viewed as a concept close to pair-correlation functions. Such a function corresponds to the probability to intercept other particles at a distance h from a reference particle. It is obtained by growing a sphere of radius h from this reference particle. Firstly, pair-correlation function is not calculated for a given direction and is thus unable to quantify anisotropy. Secondly, unlike covariogram, pair-correlation function provides representative information if it is independent of the choice of the reference particle, i.e. in case of a homogeneous distribution. Covariogram is thus a more general tool for quantification of microstructure morphology.

It can be pointed out easily from this definition that if the material is periodic, then the function $C(\cdot)$ is periodic too. When applied to image analysis, if noting I the characteristic function of pixel x (i.e. $I(x) = 1$ if $x \in X$ and 0 otherwise), the definition of the covariogram becomes (Eq. (2)):

$$C(z) = \int_{\Omega} I(x) \cdot I(x+z) \, \mathrm{d}x \tag{2}$$

In this work, the calculation of covariograms is based on the Fast Fourier Transform (FFT). Therefore, it allows us to work in a frequency space, and therefore, the medium is considered infinite.

For easier reading, the evolution of the covariogram according to any direction z is noted $C_z(\cdot)$. For a heterogeneous bi-phasic medium like that depicted in Fig. 1—left, the domain X can be associated with one phase, e.g., with inclusions. It is then possible to get statistical data related to this phase. For instance, the right part of Fig. 1 displays covariograms along the horizontal (X) and vertical (Y) directions. Curve shapes are classical for such a microstructure.

More particular properties of the covariogram are listed below.

$(\mathcal{P}_1)$ – It can be noticed first that the volume fraction of phase X is directly given by the covariogram for $h = 0$:

$$C_z(0) = \mathbf{P}\{x \in X\} := f_X$$

with f_X the volume fraction of X in the medium Ω.

$(\mathcal{P}_2)$ – If an horizontal asymptote line exists when h tends to the higher values, moreover with a value $C(z) = f_X^2$, then the probability distribution is ergodic, meaning that the distribution is homogeneous. The occurrence probability is the