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Probabilistic effective characteristics of polymers containing rubber particles of Gaussian random diameter

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A B S T R A C T

This study is focused on the problem of statistical distribution of the size of rubber particles as fillers in elastomeric composites. This distribution (average diameter of the injected particles) is assumed to be Gaussian and uniquely defined by its mean value as well as standard deviation. The basic probabilistic parameters of the effective elasticity tensor of the entire elastomer are under consideration by using of the homogenization method. The basic computational ideology is based on strain deformation of the Representative Volume Element under uniaxial and biaxial loads. This deterministic method is enriched with the generalized stochastic perturbation technique and also by semi-analytical strategy, which are used together with the system ABAQUS® as the Stochastic Finite Element Method (SFEM) serving for a solution of the homogenization problem for such a composite. The basic stochastic characteristics of the homogenized elasticity tensor and its deterministic sensitivity coefficients are verified with such coming from analytical deterministic homogenization method extended towards random case in the computer algebra system MAPLE®. The computational study contains additionally computational error analysis as the homogenization problem is solved here with tetrahedral and hexahedral 3D solid finite elements with linear as well as with parabolic shape functions and their meshes with different densities.

1. Introduction

Sensitivity analysis and uncertainty modeling of composite materials has been an attractive and interesting area of investigations since many years [4,7,11,9] considering especially optimization of the constituents composition, their shape and spatial distribution [10]. One of the fundamental mathematical methods is homogenization theory applied to replace original composite by an equivalent and statistically homogeneous medium (not necessarily isotropic). There are some relatively simple algebraic expressions for these homogenized material characteristics available in the literature [3,17,19], some asymptotic solutions of the so-called homogenization problem [2,21,5] with the additional probabilistic extensions [11] and also deformation energy driven estimates for the effective material tensors [14,15] – all with a variety of specific applications to the engineering problems, cf. [8]. Taking into account probabilistic modern aspects of homogenization method one may find Monte-Carlo simulation [4,11,12], Karhunen–Loeve and polynomial chaos realizations [22], lower [20] and higher [13] order stochastic perturbation techniques as well as some semi-analytical methodology [12]. A very interesting study in the above context is a composite including rubber phase (in the form of distributed spherical particles here) due to the well-known incompressibility of this material and also to the Mullins effect [16] or cavitation phenomenon [6]. An application of the probabilistic methods to the homogenization problem of a composite including polymeric matrix and rubber particles has been successfully resolved in [14] and is available for uncertainty in material characteristics of its both constituents. Let us note that solutions to the mechanical problems with material uncertainty (for example Gaussian) are widely accessible. Amore challenging computational problem would be the shape or geometry uncertainty, stochastic waviness of the boundary (interface or interphase), especially in the area of composite materials (also for the functionally graded materials – FGMs), and even stochastic geometrical imperfections or support location/direction in traditional

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** The first Author would like to dedicate this work to his teacher in computational mechanics, prof. Michał Kleiber from the Institute of Fundamental Technological Research in Warsaw, Poland on the occasion of his 70th birthday.

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civil engineering structures. Numerical difficulty in this case (while using the Finite Element Method) is a need of re-meshing of computational domain exhibiting uncertain geometrical dimensions or stochastic shape fluctuations. This must be done for both classical Monte-Carlo simulation strategy and also for the modern fast computational techniques like the stochastic perturbation method. Considering this fact, the FEM numerical error problem associated with the mesh generation has to be resolved and probabilistic methodology is to be based on automatic mesh generator having the parameters as similar as it is possible in each separate experiment – to avoid mesh sensitivity of such a stochastic solution.

This work addresses the determination of the first four probabilistic moments of the effective elasticity tensor components of elastomers filled with rubber particles of Gaussian random diameter. Homogenization method is based upon the deformation energy of the Representative Volume Element (RVE) under uniaxial and biaxial stretches [14] calculated via the Finite Element Method (FEM), so that we are able to study the influence of the finite element type (tetrahedral and hexahedra), order (linear and parabolic) and the total number on the accuracy of the deterministic solution. Further, we apply the Response Function Method (RFM) [13] to recover polynomial responses of homogenized tensor to the particle diameter and to use these responses in the semi-analytical as well as in stochastic perturbation-based tenth order computations of basic probabilistic characteristics of this tensor. The majority of our numerical approach is that it is dual and enables to determine all the basic probabilistic characteristics of the effective tensor as the explicit functions of the input parameter uncertainty level (unlike in the Monte-Carlo simulation scheme and also in Karhunen–Loeve or polynomial chaos expansions). The RFM implementation significantly varies from its all previous applications because each FEM experiment with the new modified value of particle radius R needs the brand new mesh generation for the entire RVE. Therefore, automatic meshing for all the finite element types and their orders is done for all discrete values of this R with the same parameters to avoid any mesh sensitivity in this study (mesh adaptation is postponed in this initial study). Moreover, it needs to be mentioned that these semi-analytical and also perturbation-based techniques are used in conjunction with the widely available analytical formulas for the effective elasticity tensor (implemented in the computer algebra system MAPLE); the remaining two methods are implemented with the Stochastic Finite Element Method (modification of the system ABAQUS). Computer analysis provided verifies qualitatively and quantitatively the influence of random fluctuations of the rubber particle size (frequently observed in engineering practice not only in case of rubber fillers) on the basic statistics of the effective characteristics of the elastomer and may be further extended towards nonlinear case studies. This influence is verified also in a deterministic way – by computations of the normalized sensitivity coefficients of $C_{ijkl}^{(eff)}$, because first order partial derivatives are computed by the way during stochastic Taylor expansion for the SFEM.

2. Mathematical model of the composite

Let us consider a statistically heterogeneous and bounded continuum $\Omega \subset \Re^3$ with no initial stresses and strains consisting of spherical rubber particles statistically uniformly distributed into the homogeneous polymeric matrix (Fig. 1). We assume a perfect contact in-between these two constituents throughout all the interfaces and also a lack of any contact of any two neighboring particles. The rubber and polymer phases work both in the linear elastic regime and their material characteristics are uniquely defined by their Young's moduli and Poisson's ratios and they are given in a deterministic manner. We assume that the filler particles have random Gaussian size distribution defined by the expectation and standard deviation of their radii, namely $E[R]$ and $\sigma(R)$. These operators are traditionally defined as [1,13] as

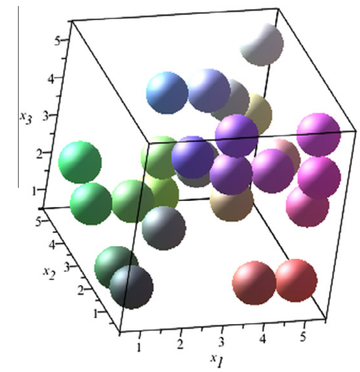

Fig. 1. Idealization of the polymer with rubber particles.

$$E[R] = \int_{-\infty}^{+\infty} R\, p_R(x)\, dx, \tag{1}$$

and

$$\sigma(R) = \sqrt{Var(R)} = \left\{ \int_{-\infty}^{+\infty} (R - E[R])^2\, p_R(x)\, dx \right\}^{\frac{1}{2}}, \tag{2}$$

where $p_R(x)$ is the probability density function assumed to have the form

$$p_R(x) = \frac{1}{\sigma(R)\sqrt{2\pi}} \exp\left(-\frac{(x - E[R])^2}{2\sigma^2(R)} \right). \tag{3}$$

We use further also skewness and kurtosis classically introduced in probability theory in the following form (Monte-Carlo simulation explores a variety of estimators, whose accuracy depends on the few parameters):

$$\beta(R) = \frac{\mu_3(R)}{\sigma^3(R)}, \quad \kappa(R) = \frac{\mu_4(R)}{\sigma^4(R)} - 3, \tag{4}$$

which equal both to 0 for Gaussian variables and where

$$\mu_m(R) = \int_{-\infty}^{+\infty} (R - E[R])^m\, p_R(x)\, dx, \tag{5}$$

denotes the mth central probabilistic moments of the variable R for any natural number m. The main goal of further considerations is to determine the basic probabilistic material characteristics of the equivalent homogenized medium and we introduce for this purpose the Representative Volume Element (Fig. 2) consisting of a single rubber particle within the surrounding polymeric matrix in the form of a cube (due to the same importance of all directions related to Cartesian coordinates which is affected by statistical isotropy of the matrix and the whole composite themselves). We determine

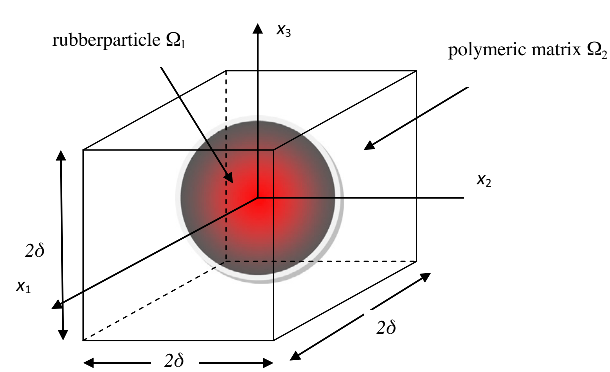

Fig. 2. The Representative Volume Element of the elastomer.