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Uncertainty in effective elastic properties of particle filled polymers by the Monte-Carlo simulation

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ABSTRACT

The main issue of this paper is to present statistical computational procedure for a determination of the effective elastic parameters for polymers filled with rubber particles. The homogenized elasticity tensor components are derived both as the variational upper and lower bounds as well as the solution for the cell problem on the composite Representative Volume Element. Probabilistic simulation is provided using both Monte-Carlo simulation technique and the generalized stochastic perturbation technique implemented in the symbolic computer algebra system MAPLE and, separately, together with the FEM-oriented code MCCEFF. Finally, up to fourth order probabilistic moments and coefficients of the homogenized tensor for the elastomers are computed as functions of the polymer's and particles' Young's moduli coefficients of variation. This study gives the basis for further homogenization-based experiments, where the hyperelastic constitutive model will replace the classical Hookean one applied here.

1. Introduction

An uncertainty of material, physical and even geometrical parameters [1,2] in polymers and especially elastomers [3,4] is intuitively natural. A random dispersion of the particles, unstable thermal manufacturing processes, reinforcing and filling particles distribution as well as agglomeration and polimerization processes make the standard deviations of material characteristics really very important. The second crucial problem in a computational mechanics of these continua is a number of physically different scales – from atomic and molecular through micro and meso up to sometimes the very sophisticated macro-scale, where the elastomer-based structures may have very complex shapes – also in various geometrical scales like the automobile tires, for instance. This complexity of both material and geometrical multiscale character undoubtedly leads to the usage of some simplifications like the homogenization method, which appeared yet to be very efficient in modeling of various composites, including the metal matrix composites (MMC) at least [5,6]; considering above, we would recommend its probabilistic version. Because the preliminary character of this study is related to elastomers, we engage mainly the crude version of the Monte-Carlo simulation method [2,7] providing up to the first fourth order statistics of the homogenized elasticity tensor, which on further stage of these studies will be replaced with some linear viscoelastic homogenization model. The new problem with elastomers, in the context of the homogenization method availability and application, is the fact that the Young's moduli of the filler particles is a few times smaller than that of the matrix, while usually this interrelation between the reinforcing particles or short/long fibers [8] and the matrices was quite inverse. It is quite natural to apply the Finite Element Method (FEM) to model the complexity and various scales in composite materials. However, spatial modeling of the Representative Volume Element (RVE) may include single particle/fiber with the surrounding matrix by the classical 2D or 3D finite elements and, on the other hand, Voronoi tessellations and the corresponding irregular finite elements to mesh the specimen with many particles/fibers as well [9]. Usually, after solving the FEM cell problem, this solution is contrasted next with the well known analytical approximations as well as the upper bounds on the effective tensor [10]. An interesting mathematical aspect here is the fact that the Poisson's ratio in case of the rubber particles analyzed here equal to about 0.49. It reaches almost its physical limit and that is why Young's moduli of both composite phases are randomized by only.

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A significant time consumption in the Monte-Carlo analysis suggests an application of another numerical technique, which is in our case the generalized stochastic perturbation technique [2,11] (one may propose alternatively a multiscale spectral stochastic method [12]). Contrary to its previous applications, now the full tenth order and multiparametric version was introduced to check its efficiency at different random dispersion levels for the Gaussian variables. The numerical results obtained confirm that the effective elasticity tensor have Gaussian distribution also for the elastomers and that the multiparametric generalized stochastic perturbation technique returns the homogenized tensor's moments quite close to their estimation-based counterparts.

It needs to be outlined that the analysis presented below is the next introductory step, after the work published in [13], to develop full probabilistic homogenized stress–strain relationship for the polymers filled with rubber particles. It was just demonstrated that various theories concerning effective shear modulus for both linear elastic and inelastic ranges may be successfully randomized using analytical, simulation and perturbation-based computational tools, and now we provide analogous studies for the elasticity tensor. According to numerous experimental validations, such a non-linear homogenized constitutive law should account for the Mullins' effect [14], however it cannot be reliably implemented without a full prior knowledge about up to the fourth central probabilistic moments of the homogenized constitutive law in linear elasticity. The second, pure computational issue, is a choice of a probabilistic numerical technique to accomplish this goal, because the Monte-Carlo simulation approach, even if treated as almost exact estimation of the results, may be enormously time consuming one for the viscoelastic multiscale problems. Finally, having implemented probabilistic effective constitutive law in the nonlinear range one does not need any further multiscale FEM modeling to perform the reliability analysis for the elastomers, where a limit function based on maximum stresses or admissible deformations may be the basis for the reliability index computations. Alternatively, one could provide the durability studies (quite analogous to these proposed in [13]), where stochastic fluctuations in the system parameters may lead to a determination of the structural element lifetime statistical parameters.

2. Homogenization method

Let us introduce a geometrical scaling parameter $\zeta > 0$ between the micro- and macroscale of the composite and introduce two coordinate systems $\mathbf{y} = (y_1, y_2, y_3)$ on the microscale of the composite and $\mathbf{x} = (x_1, x_2, x_3)$ on the macroscale (see Fig. 1 below). Traditionally, we introduce Y as the volume of the entire composite, while Ω stands for its Representative Volume Element (RVE) shown in the graph below. We consider the two-component

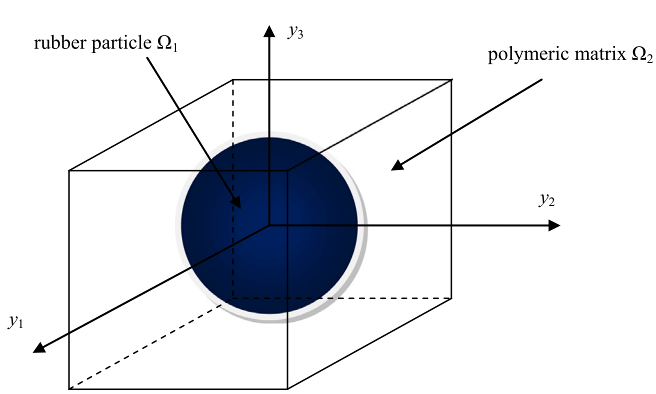

Fig. 1. Particle two-component composite's spatial idealization.

composite material with perfectly linear elastic and isotropic constituents that exhibit perfect contact in the microscale. An uncertainty would be considered in material characteristics of our composite, therefore the existence of the RVE has the same aspects as in prior deterministic models.

Let us denote the filler region by Ω_1, the matrix area by Ω_2 and the interface between them as Γ_{12}. Next, let us express any state function G defined on Y as

$$G^{\zeta}(\mathbf{x}) = G\left(\frac{\mathbf{x}}{\zeta}\right) = G(\mathbf{y}). \tag{1}$$

The linear elasticity problem for the periodic composite structure is given as follows:

$$\begin{cases} \frac{\partial \sigma^{\zeta}_{ij}}{\partial x_j} + F_i = 0 \\ \sigma^{\zeta}_{ij} n_j = p_i; \quad \mathbf{x} \in \partial Y_{\sigma} \\ u^{\zeta}_i = 0; \quad \mathbf{x} \in \partial Y_u \qquad i,j,k,l = 1,2. \\ \sigma^{\zeta}_{ij} = C^{\zeta}_{ijkl}(\mathbf{x}) \varepsilon^{\zeta}_{kl} \\ \varepsilon^{\zeta}_{kl} = \frac{1}{2}(u^{\zeta}_{k,l} + u^{\zeta}_{l,k}) \end{cases} \tag{2}$$

Assuming perfect interfaces between the matrix and the particles as well as no cracks and other defects into those constituents we solve this problem by introducing the bilinear form $a^{\zeta}(\mathbf{u}, \mathbf{v})$ [15,16]

$$a^{\zeta}(\mathbf{u}, \mathbf{v}) = \int_Y C_{ijkl}\left(\frac{\mathbf{x}}{\zeta}\right) \varepsilon_{ij}(\mathbf{u}) \varepsilon_{kl}(\mathbf{v}) dY, \tag{3}$$

and the linear one

$$L(\mathbf{v}) = \int_Y F_i v_i dY + \int_{\partial Y_{\sigma}} p_i v_i d(\partial Y), \tag{4}$$

in the following Hilbert space of admissible displacements defined on Y

$$V = \left\{ \mathbf{v} | \mathbf{v} \in (H^1(Y))^3, \mathbf{v}|_{\partial Y_u} = 0 \right\}, \tag{5}$$

$$\|\mathbf{v}\|^2 = \int_Y \varepsilon_{ij}(\mathbf{v}) \varepsilon_{ij}(\mathbf{v}) dY. \tag{6}$$

Then, the variational statement equivalent to the equilibrium problem (2) is to find $\mathbf{u}^{\zeta} \in V$ being a solution of the following equation:

$$a^{\zeta}(\mathbf{u}^{\zeta}, \mathbf{v}) = L(\mathbf{v}), \quad \mathbf{v} \in V. \tag{7}$$

Let us define the additional space of the admissible displacement functions $P(\Omega) = \left\{ \mathbf{v}, \mathbf{v} \in (H^1(\Omega))^3 \right\}$ periodic on the composite cell Ω. So that, we introduce the new bilinear form for any $\mathbf{u}, \mathbf{v} \in P(\Omega)$:

$$a_y(\mathbf{u}, \mathbf{v}) = \int_{\Omega} C_{ijkl}(\mathbf{y}) \varepsilon_{ij}(\mathbf{u}) \varepsilon_{kl}(\mathbf{v}) d\Omega, \tag{8}$$

and the homogenization function $\chi_{(ij)k} \in P(\Omega)$ (also of the displacement type) as a solution for the so-called local problem on a periodicity cell

$$a_y\left(\left(\chi_{(ij)k} + y_j \delta_{ki}\right) \mathbf{n}_k, \mathbf{w}\right) = 0, \tag{9}$$

for any $\mathbf{w} \in P(\Omega)$, where $\mathbf{n}_k$ is the unit coordinate vector. The existence and uniqueness of the solution of this problem was studies in the literature concerning the homogenization method in its original deterministic formulation [15]. The kinematic boundary conditions consisting of zeroing of the vertical displacements on the outer faces of the RVE preserve against the rigid body motion in this boundary value problem. Assuming further boundedness, ellipticity and symmetry of the fourth order elasticity tensor one may