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Design sensitivity analysis for the homogenized elasticity tensor of a polymer filled with rubber particles

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ABSTRACT

The main purpose of this work is the computational simulation of the sensitivity coefficients of the homogenized tensor for a polymer filled with rubber particles with respect to the material parameters of the constituents. The Representative Volume Element (RVE) of this composite contains a single spherical particle, and the composite components are treated as homogeneous isotropic media, resulting in an isotropic effective homogenized material. The sensitivity analysis presented in this paper is performed via the provided semi-analytical technique using the commercial FEM code ABAQUS and the symbolic computation package MAPLE. The analytical method applied for comparison uses the additional algebraic formulas derived for the homogenized tensor for a medium filled with spherical inclusions, while the FEM-based technique employs the polynomial response functions recovered from the Weighted Least-Squares Method. The homogenization technique consists of equating the strain energies for the real composite and the artificial isotropic material characterized by the effective elasticity tensor. The homogenization problem is solved using ABAQUS by the application of uniform deformations on specific outer surfaces of the composite RVE and the use of tetrahedral finite elements C3D4. The energy approach will allow for the future application of more realistic constitutive models of rubber-filled polymers such as that of Mullins and for RVEs of larger size that contain an agglomeration of rubber particles.
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1. Introduction

A homogenization method has been developed for the prediction of the elastic properties of polycrystals on the basis of the properties of a single crystal, and it is a relatively old idea (Kröner, 1958); some works by Voigt recalled in this study date from the end of the XIXth century. This technique has been used successfully for the prediction of the effective properties of composites consisting of reinforcing particles and fibers (Christensen, 1979) using some upper and lower bounds or direct approximations, and it has also been used for electric, thermal and magnetic fields (Milton, 2002). In the present day, we solve homogenization problems using various computational implementations of the Finite Element Method (FEM) to solve exemplary problems for the Representative Volume Element (RVE) of the entire heterogeneous structure to predict its equivalent physical properties. There are essentially two different ways, at least in the micromechanics of heterogeneous media, to accomplish this goal. The first one is based on the periodicity assumption, wherein the effective properties are calculated using some geometrical expansion procedure (Bensoussan et al., 1978; Kalamkarov and Kolpakov, 1997; Kamiński, 2005; Sanchez-Palencia, 1980), while the second approach relies on determining the strain energy caused by applying uniform strain fields to the RVE (and does not demand any periodicity conditions) (Kushnevsky et al., 1998). However, applications of the homogenization method today extend far beyond the micromechanics of composites and also address nanocrystalline structures (El-Khoury et al., 2011; Gürses and El Sayed, 2011), nonlinear constitutive relations for polycrystals (Sundararaghavan and Zabaras, 2006) and even certain contact problems (Belgith et al., 2010). Sensitivity analysis itself (Frank, 1978; Haug, 1986; Kleiber et al., 1997) and its relation to the homogenized characteristics of composites is also not a new theoretical problem (Fish and Ghouali, 2001; Kamiński, 2003). This relation is addressed in classical sensitivity analysis methods such as the Finite Difference Method (FDM) (Kamiński, 2003), the Direct Differentiation Method (DDM) and the Adjoint Variable Method (AVM). It is applied to calculate the sensitivity coefficients of effective tensors with respect to the properties of the original components (Noor and Shah, 1993; Kamiński, 2005), for certain topologies (Hassani and Hinton, 1998; de Kruijf et al., 2007) or for shape optimization (Rohan and Miara, 2006), and it is also related to the understanding of composites with uncertainties (Kamiński, 2009; Arwade and Deodatis, 2011). This particular research area is still attracting much attention, and there are plenty

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of recent results focused on computational issues (Davis and Singler, 2011; Kowalczyk, 2012), the scale-coupling effect (Unger and Könke, 2008), thermo-electro-magnetic applications (Choi and Yoo, 2008; Zhou and Li, 2008) and nanostructures (Benai and Wenig, 2009), but the well-established methods are still being applied and revisited (Neto et al., 2010; Yu et al., 2012).

Considering the above discussion, the main issue in this paper is the computational investigation of the sensitivity coefficients of the energy under uniform strain of the RVE and the investigation of the resulting homogenized tensor with respect to the elastic parameters of its components. Although the 3D FEM analysis is demonstrated for a composite filled with a certain type of particle, the methodology is also valid for composites reinforced with short or long fibers. Similar studies have been conducted previously (Yanase and Ju, 2012) but only for composites reinforced, rather than filled, with particles (Burr and Monnerie, 2000); in this case, of course, the matrix has a smaller Young modulus and usually a larger Poisson ratio. The method of determining the sensitivity coefficients remains the same as for particle-reinforced composites, but it may yield quite different qualitative results. The sensitivity analysis, however, is performed in a non-traditional way, using the so-called response polynomial functions that relate all the components of the effective elasticity tensor to the base material parameters of the composite components, which are all determined in a semi-analytical manner (the so-called Response Function Method, or RFM). First, these response functions are created using several solutions of the RVE problem with the design parameters fluctuating around their average values and using the classical Weighted version of the Least-Squares Method (WLSM) (Kamiński, 2013). This method is implemented in the symbolic computer program MAPLE, v. 14, to recover the unknown coefficients of such a polynomial form. Then, we use analytical differentiation to calculate the sensitivity coefficients of the homogenized tensor, and furthermore, these coefficients are derived as functions of the input design parameters in the close neighborhood of their mean values and also with respect to the order of the approximating polynomial. This approach provides an effective means for the engineering optimization of such a composition of matrix and filler, where there is still some opportunity to modify the elastic properties of the components within certain intervals during the manufacturing process. Numerical experiments are performed on a very dense mesh to eliminate the mesh sensitivity of the coefficients being determined and also using tetrahedral finite elements in the commercial program ABAQUS, wherein a detailed verification of the interface continuity was performed to include some 3D discontinuities in future extensions of this model (Yanase and Ju, 2012). Such a detailed FEM discretization eliminates the necessity for any mesh adaptation procedures, but for future applications, some adaptation to optimize the mesh would be advised. The benefit of this fine mesh and, at the same time, the positive verification of the method is the perfect agreement of the resulting homogenized characteristics with these that are analytically obtained by following the Eshelby model (Christensen, 1979) and based only on the volume fractions; this situation might change if the spherical particle shape were to be replaced with an ellipsoidal one, for example. It should be emphasized that the overall computational effort requires n times the effort of the deterministic solution to the RVE problem, where n is the total number of trial points necessary to build up the response functions $C_{ijkl}^{(eff)} = C_{ijkl}^{(eff)}(h)$ (four different sets of responses associated with all the input design parameters and three responses for each of these components individually). The first part is performed entirely using the FEA system ABAQUS, while the approximation is performed using the MAPLE system. Further numerical processing of these response functions during the analytical computation of both first- and second-order coefficients is very rapid, while the use of Central Finite Difference algorithms usually doubles the time consumption of the entire solution.

2. Homogenization method

Let us consider a heterogeneous and bounded continuum $\Omega \subset \Re^3$, where elastic properties of the constituents included in this region are treated as design parameters, and they result in the displacement field $u_i(\mathbf{x})$ and the stress tensor $\sigma_{ij}(\mathbf{x})$, which satisfy the linear elasticity elliptic boundary value problem; vector $\mathbf{x} = (x_1, x_2, x_3)$ denotes local Cartesian coordinates (see Fig. 1). The Representative Volume Element (RVE) Ω of this composite has dimensions of $2l_1 \times 2l_2 \times 2l_3$ in these coordinates, respectively, and contains a centrally located spherical particle that is perfectly connected to a continuous matrix. Let us assume further that there are non-empty subsets of the external boundaries of the region Ω, namely, $\partial\Omega_\sigma$ and $\partial\Omega_u$, where the Dirichlet and von Neumann boundary conditions are imposed, respectively. It should be emphasized that the proposed homogenization method does not require any Dirichlet boundary conditions, in contrast to the homogenization approach presented in Kamiński (2005, 2013), where both boundary conditions were used.

Considering the proposed numerical technique, the entire set of boundary-value problems with the same boundary conditions and with additionally modified input design variables $h^{(\alpha)}$, $\alpha = 1, \ldots, n$ (Kleiber et al., 1997; Kamiński, 2005), is to be solved. Henceforth, we denote the total number of different values of our design parameter (chosen near its average value) by n. Thus, the upper index α indicates the different structural responses associated with these input values. The solution to the particular boundary differential-equation systems that describe the static equilibrium near the average value of this parameter is sought:

$$\sigma_{ij}^{(\alpha)}(\mathbf{x}) = C_{ijkl}^{(\alpha)}(\mathbf{x})\varepsilon_{kl}^{(\alpha)}(\mathbf{x}), \tag{1}$$

$$\varepsilon_{ij}^{(\alpha)}(\mathbf{x}) = \frac{1}{2}\left(\frac{\partial u_i^{(\alpha)}(\mathbf{x})}{\partial x_j} + \frac{\partial u_j^{(\alpha)}(\mathbf{x})}{\partial x_i}\right), \tag{2}$$

$$\sigma_{ij,j}^{(\alpha)}(\mathbf{x}) = 0, \tag{3}$$

$$u_i^{(\alpha)}(\mathbf{x}) = \hat{u}_i(\mathbf{x}); \quad \mathbf{x} \in \partial\Omega_u, \tag{4}$$

$$\sigma_{ij}^{(\alpha)}(\mathbf{x})n_j = \hat{t}_i(\mathbf{x}); \quad \mathbf{x} \in \partial\Omega_\sigma. \tag{5}$$

The elasticity tensor that satisfies the symmetry, boundedness and ellipticity conditions is defined as

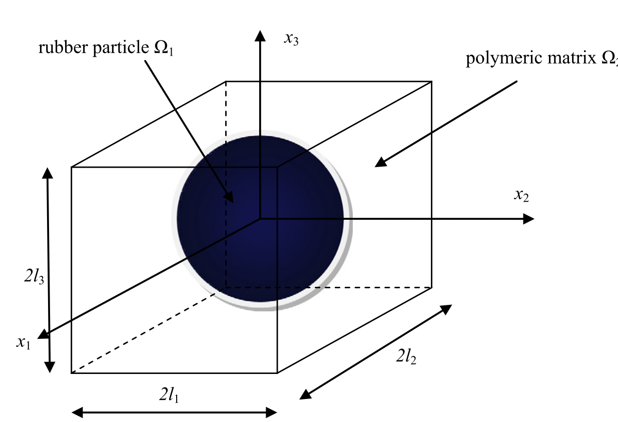

Fig. 1. Spatial idealization of periodic two-component composite.

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