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# Computational homogenization of elastic–plastic composites

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ABSTRACT

This work describes a computational homogenization methodology to estimate the effective elastic–plastic response of random two-phase composite media. It is based on finite element simulations using three-dimensional cubic cells of different size but smaller than the deterministic representative volume element (DRVE) of the microstructure. We propose to extend the approach developed in the case of elastic heterogeneous media by Drugan and Willis (1996) and Kanit et al. (2003) to elastic–plastic composites. A specific polymer blend, made of two phases with highly contrasted properties, is selected to illustrate this approach; it consists of a random dispersion of elastic rubber spheres in an elastic–plastic glassy polymer matrix. It is found that the effective elastic–plastic response of this particulate composite can be accurately determined by computing a sufficient number of small subvolumes of fixed size extracted from the DRVE and containing different realizations of the random microstructure. In addition, the response of an individual subvolume is found anisotropic whereas the average of all subvolumes leads to recover the isotropic character of the DRVE. The necessary realization number to reach acceptable precision is given for two examples of particle volume fractions.



## 1. Introduction

Over the past five decades, the prediction of the effective mechanical response of random composite media has been an active research area. Many analytical works using homogenization methods have been done to bound or estimate their effective material properties (e.g. Nemat-Nasser and Hori, 1993). These methods which assume that the effective material properties can be defined as relations among the volume averages of stress and strain fields were initially developed within the linear elastic framework. The well-known Voigt–Reuss and Hashin–Shtrikman (Hashin and Shtrikman, 1963) bounds are often used to give a useful bound of the effective properties, but they are too far apart for highly contrasted properties of constituents. The direct estimation of the effective properties can be achieved using approaches based on the Eshelby equivalent inclusion theory such as the Mori–Tanaka model (Mori and Tanaka, 1973) or the self-consistent scheme (Hill, 1965). The Mori–Tanaka model considers the heterogeneities diluted in the matrix whereas in the self-consistent scheme the physical approximation is enhanced by incorporating the interaction effects between heterogeneities, see e.g. the papers of Anoukou et al. (2011a, 2011b) for a comparison of these theories. Although these analytical approaches have reached a high degree of sophistication and efficiency, and are nowadays well-established, it remains quite complex to transpose them to the plastic regime for which tangent and secant formulations were developed. In tangent formulations, the effective elastic–plastic response is computed incrementally by integrating along the loading path the effective stiffness tensor obtained from the tangent stiffness tensor of each phase (e.g. Hutchinson, 1970; Ju and Sun, 2001; Doghri and Friebel, 2005; Zaïri et al., 2011a). In secant formulations, the effective elastic–plastic response is computed from the secant stiffness tensor of each phase within the nonlinear elastic framework (Berveiller and Zaoui, 1979; Tandon and Weng, 1988; Ponte Castaneda and Suquet, 1998). Alternatively to these analytical approaches, the numerical simulations directly performed on the microstructure can be of a great help to solve non-trivial homogenization problems such as the plasticity in random composite media. The material volume used to represent the microstructure, namely the representative volume element (RVE), is therefore of prime importance. Conventionally, the RVE must be chosen sufficiently large compared to heterogeneities to contain sufficient information about the microstructure in order to be representative, but it must remain small enough, much smaller than the macroscopic body, in order to be considered as a material volume element. Drugan and Willis (1996) proposed to define this notion as follows: "*It is the smallest material volume element of the composite for which the usual spatially constant (overall modulus) macroscopic constitutive representation is a sufficiently accurate model to represent the mean constitutive response*". This definition of the

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"deterministic" representative volume element (DRVE) ought to be verified in the context of elastic–plastic composites. The effective stress–strain response, defined from spatial averages of stress and strain fields over the volume element, must be obtained with a given accuracy. For large-scale computations the computational cost is a paramount issue and it is appealing to work on volumes smaller than the DRVE. The use of smaller volumes induces fluctuations of the estimated responses which must be compensated by averaging over several realizations of the microstructure in order to get the same estimation as that obtained for the whole volume. This strategy was proposed by Huet (1990), Hazanov and Huet (1994), Drugan and Willis (1996) and Kanit et al. (2003, 2006) to estimate the linear elastic response of heterogeneous materials and it is extended in the present work to elastic–plastic composites.

The purpose of the present work is to describe a computational homogenization strategy to estimate the effective elastic–plastic response of particulate composites. The methodology is applied to a specific composite, namely a rubber-toughened thermoplastic polymer. The numerical estimates of the stress–strain response, and their scatters, obtained on volumes of fixed size but containing different realizations of a given volume of the microstructure are investigated.

The present paper is organized as follows. In Section 2, we present the investigated microstructure and the computational method. The results are presented and discussed in Section 3. Some concluding remarks are given in Section 4.

## 2. Computational homogenization

### *2.1. Microstructure and mechanical properties of the studied polymer blend*

The example of microstructure chosen in the present investigation to illustrate the methodology is a rubber-toughened poly(-methyl methacrylate). It is constituted by a disordered distribution of soft rubbery inclusions in a stiff polymer matrix. The mechanical properties are known for the two individual constituents and were thoroughly investigated by Zaïri et al. (2011b) under uniaxial tensile loading. The rubbery inclusions are assumed linear elastic while the matrix is elastic–plastic. A very large contrast exists in the mechanical properties of the constituents. The Young's moduli are 1550 MPa and 1 MPa for the matrix and the inclusions, respectively. The Poisson's ratios are 0.4 and 0.49, respectively. The inelastic properties of the matrix were taken from the experimental data employed by Zaïri et al. (2011b). The choice of a microstructure with such a contrast in properties allows enhancing the variability of apparent mechanical responses obtained from small material volume elements. The elastic–plastic response of rubber-toughened thermoplastic polymers have been investigated in the past by several authors (Steenbrink et al., 1997; Socrate and Boyce, 2000; Riku et al., 2008) via numerical simulations of either a unit cell or a representative microstructure but never related to the issue of representativity of the volume element. By contrast, the representativity of the elastic–plastic responses obtained from limited domains of the random composite material is investigated in this work.

### *2.2. Mesh generation*

The finite element (FE) method was chosen for the computations presented in this work. The FE calculations were carried out with Zebulon FE software. The 3D microstructure was reconstructed from 2D images by means of a serial sectioning process. A numerical procedure was used to randomly generate the 2D microstructure section by section. These images have being assembled to generate the wanted 3D cubic microstructure. The procedure is illustrated in Fig. 1. The obtained microstructure consists in randomly distributed non-overlapping identical spherical particles embedded in the matrix. The volume is considered large enough to represent the investigated microstructure. A FE mesh was then superimposed on the 3D image using quadratic brick elements.

### *2.3. Boundary conditions*

The second important issue for the numerical tests after generating microstructures concerns the boundary conditions (see e.g. Kanit et al., 2003; Li and Ostoja-Starzewski, 2006) which for a uni-

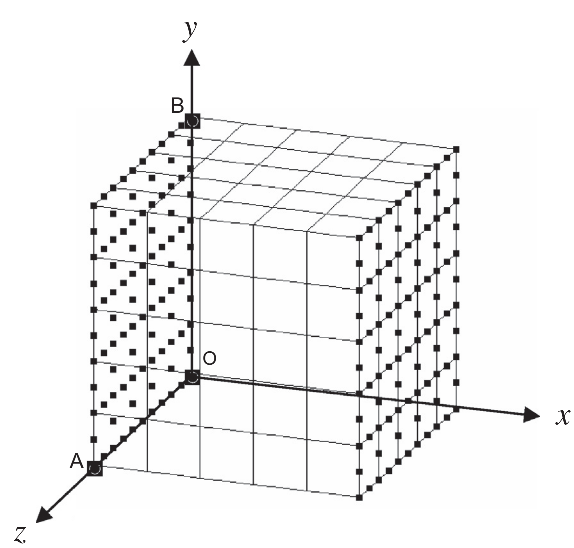


**Fig. 2.** Description of the boundary conditions.

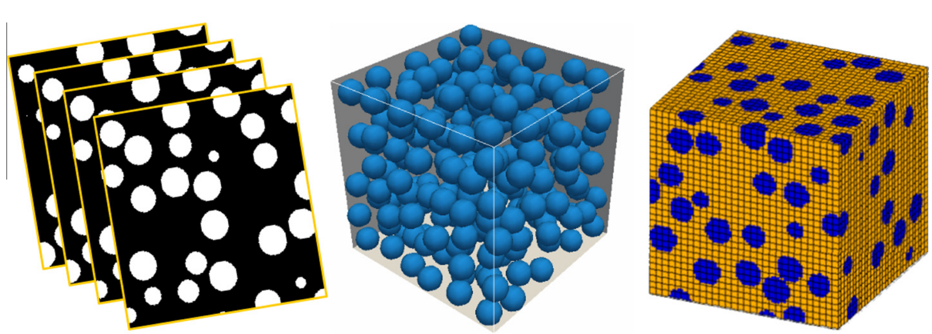

**Fig. 1.** 3D image reconstruction from 2D images and finite element mesh.