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Description of packing and size effects in particulate composites by micromechanical averaging schemes and computational homogenization

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Abstract

Different approaches to model packing and size effects are studied to model overall properties of particulate composites of different morphological features of phase distribution. The micromechanical schemes originating in the composite sphere model and its extension by morphologically-based pattern approach are taken as a basis. Analytical predictions are compared with results of computational homogenization performed on the generated representative volume elements of prescribed statistical characteristics.

Keywords: micromechanics, morphologically representative pattern, computational homogenization, size and scale effect

1. Introduction

The micromechanical approaches employed in the present study originate from the concept of composite sphere model formulated by Hashin and its further modification to the generalized self-consistent (GSC) model by Christensen, cf. [1]. In the GSC model, called the three-phase model, a single composite sphere is considered that is embedded into the equivalent homogenized medium of effective properties (see Fig. 1a). The composite sphere is composed of a particle with an associated spherical matrix region. The ratio describing the size of inner sphere with respect to the outer sphere is constant and defined by the volume fraction of particle phase in the composite. The idea was expanded in [1] to tackle multiple coatings by formulating the n-phase model and in particular the four-phase model (see Fig. 1b).

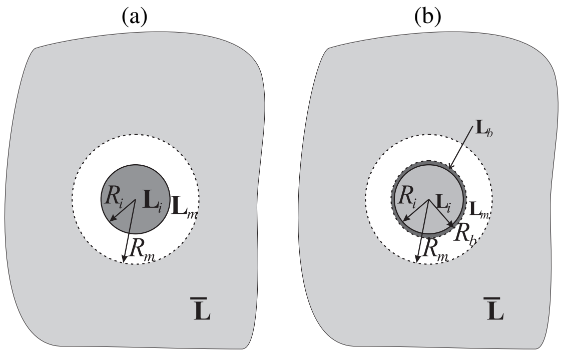

Figure 1: Schematic of (a) generalized self-consistent (GSC) model (b) four phase model (4GSC)

The concept of a coated inclusion embedded in the homogenized medium was later employed in [2], within the morphologically representative pattern-based approach (MRP-based approach), to describe the packing effects and size effects in an elastic composite composed of a continuous matrix and dispersed spherical particles. In the simplest examples of 2-pattern approach:

- to account for **a packing effect** the first pattern is a GSC pattern where the coating thickness is specified by the mean distance between nearest-neighbor particles and the second pattern is a self-consistent type problem with an inclusion made of remaining pure matrix material,
- to account for **a size effect** the first pattern is modified towards the four-phase model i.e. an interphase with a thickness independent of the particle radius and with different properties than basic two phases is introduced.

The validity of these analytical schemes as concerns the predictions of the influence of packing and size of particles on effective properties are compared with results of computational homogenization performed on the generated representative volume elements of prescribed statistical characteristics.

2. Principles of MRP-based approach

In the MRP-based approach the representative volume V with some morphological features is subdivided into the representative patterns χ with specified contributions c_χ to the overall volume V. Within each pattern one specifies the volume fraction f_i^χ of phase i such that

$$f_i^\chi = \frac{V_\chi^i}{V_\chi}\,, \quad \sum_\chi c_\chi f_i^\chi = f_i\,, \tag{1}$$

where f_i is the volume fraction of particles (inclusions) in the representative volume V.

When considering the linear problem (elasticity, viscosity) related to the subsequent patterns, the standard self-consistent procedure of micromechanics is followed. Each pattern is embedded in the infinite medium of homogenized properties to be found. For each pattern the concentration tensors $\mathbf{A}_i^\chi$ are established that relate the auxiliary far-field strain $\mathbf{E}_0$ with the average strain $\boldsymbol{\varepsilon}_i^\chi$ in inclusion phase in the pattern χ, that is

$$\boldsymbol{\varepsilon}_i^\chi = \mathbf{A}_i^\chi \cdot \mathbf{E}_0\,. \tag{2}$$

In the analyzed cases the concentration tensors $\mathbf{A}_i^\chi$ are isotropic fourth order tensors. The far field strain is not necessarily the overall average strain $\mathbf{E}$ in the representative volume. The same

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far field strain is assumed for all patterns and it is derived from the condition

$$\langle \boldsymbol{\varepsilon}_i \rangle_V = \mathbf{E}\,, \tag{3}$$

where $\boldsymbol{\varepsilon}_i$ is the average strain in phase i in the representative volume V and $\langle \cdot \rangle_V$ is a volume averaging operation defined as $1/V \int_V (\cdot) dV$, while $\boldsymbol{\varepsilon}_i$ is calculated as follows

$$\boldsymbol{\varepsilon}_i = \sum_\chi \phi_i^\chi \boldsymbol{\varepsilon}_i^\chi\,, \quad \phi_i^\chi = \frac{V_\chi^i}{V_i}\,, \quad \sum_\chi \phi_i^\chi = 1\,. \tag{4}$$

In the study there are three basic morphologies considered: the simple morphology of Eshelby problem, the morphology of the 3-phase model (Fig. 1a) and the morphology of the 4-phase model (Fig. 1b). Corresponding relations for $\mathbf{A}_i^\chi$ for the considered morphologies are to be found in [1].

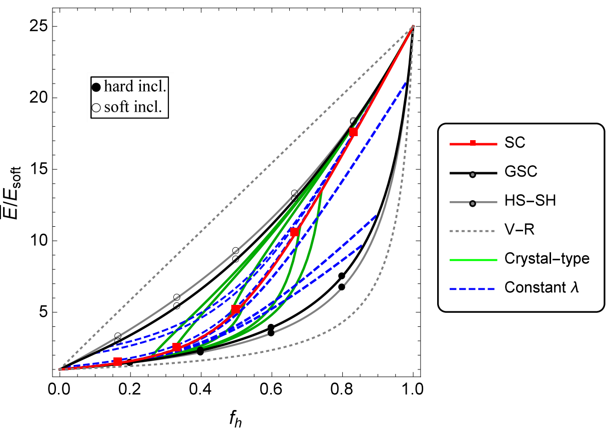

Figure 2: Basic micromechanical estimates of overall Young modulus $\bar{E}$ of a two-phase composite for the phase properties: E_{soft}/E_{hard}=25, ν_{soft}=0.33, ν_{hard}=0.17 and $f_h = V_{hard}/V$ - a volume content of a hard phase in RVE. Notation for models: V - Voigt, R - Reuss, HS/SH - Hashin-Shtrikman bounds equivalent here to the Mori-Tanaka scheme with soft/hard matrix phase, GSC - generalized self-consistent, SC - self-consistent

Let us demonstrate the predicted influence of packing on effective properties for elastic metal-ceramic composites. Results for two possible opposite cases are presented: ceramic inclusions dispersed in the metal matrix and reversely. Let us denote by λ the mean distance between nearest neighbor particles scaled by the particle diameter. Then in a 2-pattern approach the volume fraction of the GSC-type pattern can be calculated as

$$c = f_i \left(1 + \lambda\right)^3\,, \tag{5}$$

where f_i is the volume fraction of the inclusion phase. For specified volume fraction f_i, the parameter λ may vary from 0 (nearest particles are in contact) to the value specified by the matrix phase fraction λ_{max}. In the first limit case the MRP-based approach reduces to the classical self-consistent scheme and in the second case, since $1 - c = 0$, only one pattern is considered, so the result of the generalized self-consistent scheme is recovered. In Fig. 2 the estimates of the overall Young modulus $\bar{E}$ obtained for these two limit cases are presented as a function of ceramic (hard) phase content f_h, being either inclusion (*hard* inclusion case) or matrix material (*soft* inclusion case). Obviously, following the known result for SC scheme, when $\lambda = 0$ specification of the inclusion phase does not alter the result. Note that in both dilute limits, when the content of the inclusion phase tends to zero, both curves (SC and GSC) are tangent to each other. For completeness the other classical bounds and estimates specified for the two-phase isotropic composite are also included in the figure.

Moreover, in Fig. 2 the MRP-based estimates of $\bar{E}$ under assumption of constant value of λ are shown. Note that under such assumption there exists maximal volume fraction of an inclusion phase in a composite to be achieved (see Eqn (5)). For this value the corresponding curve sticks to the respective GSC limit curve. The smaller λ the closer MRP-based estimate is to the SC scheme prediction. Additionally, in Fig. 2 the MRP-based estimates of $\bar{E}$ are shown for the regular cubic, bcc and fcc distributions of particles, or more precisely, for λ varying in the same way with inclusion volume fraction as for these ordered ways of particle distribution. It results with a constant c value, independent of f_i, namely $c^{reg} = \pi/6 \sim 0.52$, $c^{bcc} = \sqrt{3}\pi/8 \sim 0.68$, $c^{fcc} = \sqrt{2}\pi/6 \sim 0.74$. The maximum volume fractions of inclusion phase possible to obtain for such packing patterns are specified by conditions $\lambda \to 0$ and are equal to c. Thus, for this limit values the MRP-based estimates stick to the SC curve. On the basis of the above analysis it can be concluded that other constant values of c_1 assumed in MRP-based pattern would correspond to some isotropic distribution of particles within the representative volume with a radius specified by f_i.

3. Computational homogenization

In order to verify micromechanical estimates presented in the previous section computational homogenization will be performed on representative volume elements with randomly distributed non-overlapping spherical inclusions [3]. Successive spheres are placed in the volume by random sequential addition, until a prescribed volume fraction of inclusions c is reached. To provide more control over the morphology, the spheres are positioned according to either a uniform or a cluster probability distribution over the volume. The width of clusters is adjustable and their spatial arrangement is itself random. The use of clusters allows to change the mean nearest-neighbour distance between inclusions while keeping c constant, as shown in Fig. 3.

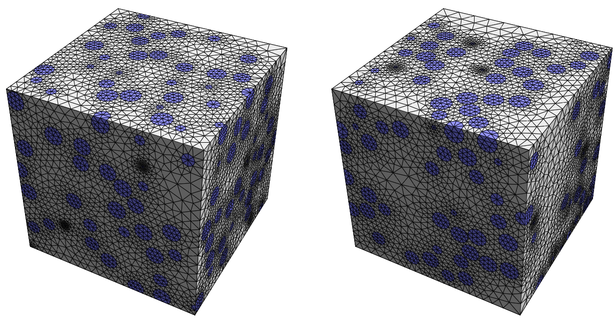

Figure 3: Cubes with a volume fraction $c = 0.22$ of randomly distributed inclusions: a) uniform distribution with $\lambda = 0.112$ and b) cluster distribution with $\lambda = 0.071$

References

[1] Herve, E., Zaoui, A., n-Layered inclusion-based micromechanical modelling, *Int. J. Engng Sci.*, 31, pp. 1-10, 1993.

[2] Marcadon, V., Herve, E., Zaoui, A., Micromechanical modeling of packing and size effects in particulate composites, *Int. J. Solids Struct.*, 44, pp. 8213-8228, 2007.

[3] Torquato, S., *Random Heterogeneous Materials. Microstructure and Macroscopic Properties*, first ed., Springer, 2002.