Homogenization of triply periodic elastic media with random imperfections

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Summary. Triply periodic particulate matrix composites with imperfect unit cells are analyzed by three new different versions of the multiparticle effective field method (MEFM) proposed previously for the analysis of both the perfect periodic and random media. The general scheme and particular cases are presented which are based on the choice of a comparison medium coinciding with either the matrix or perfect periodic structure.

Micromechanical modeling and simulation of random structures are becoming more and more ambitious due to an advantage of modern computer software and hardware (see e.g. [1]). Triply periodic particulate matrix composites with random imperfect unit cells are analyzed in this paper by the multiparticle effective field method (MEFM). The MEFM is originally based on the homogeneity hypothesis **H1)** (see for details [2]) of effective field acting on the inclusions. In this way the pair interaction of different inclusions is taken directly into account by the use of analytical approximate solution. For the perfect periodic structures, the hypothesis **H1)** is enough for estimation of effective properties (see [3]). Imperfection of packing necessitates exploring an additional assumption called a closing hypothesis. The next imperfections were analyzed. A) The probability $\lambda^{(1)}$ of location of an inclusion in the center of a unit cell below one (missing inclusion). B) Some hard inclusions are randomly replaced by the porous (modeling the complete debonding) with the probability $\lambda^{(2)}$. The mentioned problems are solved by three methods. The first one is a generalization of the version of the MEFM proposed for the analysis of the perfect periodic particulate composites ($\boldsymbol{L}(\boldsymbol{x})=\boldsymbol{L}^{\rm per}(\boldsymbol{x})$) and based on the choice of a comparison medium coinciding with the matrix $\boldsymbol{L}^{\rm c}=\boldsymbol{L}^{(0)}$. The second one is a Monte Carlo simulation exploring an analytical approximate solution for the binary interacting inclusions obtained in the framework of the hypothesis H1). The third method uses a decomposition of the desired solution on the solution for the perfect periodic structure and on the perturbation produced by the imperfections in the perfect periodic structure.

In Fig. 1 the results of the first method obtained by the two-particle approximation are presented for the initially perfect packing of hard spheres $v^{(1)}$ ($\lambda^{(1)}=1$, $\lambda^{(2)}=0$) disordering by the random replacement of some hard spheres by the holes $v^{(2)}$. At the variation of the concentration of the hard inclusions $c^{(1)}(\lambda^{(1)})$ and the holes $c^{(2)}(\lambda^{(2)})$, their complete concentration is fixed $c^{(1)}(\lambda^{(1)}) + c^{(2)}(\lambda^{(2)})=0.3$. Effective elastic moduli presented in Fig. 1 are consistent with a continuous transition from the perfect packing of hard spheres ($\lambda^{(1)}=1$, $\lambda^{(2)}=0$) to the perfect packing of holes ($\lambda^{(1)}=0$, $\lambda^{(2)}=1$). The example in Fig. 1 can be considered as a simplified damage model where the broken inclusions are replaced by some microdiscontinuities, that is, the stiffness tensor of one broken inclusion is reduced to zero. More detailed analysis of damage models is beyond the scope of the present paper. It should be mentioned that the representation of effective properties in the second method was obtained by the average over the realization number $n^{\rm MC}$ of periodic structure with mesocell $\boldsymbol{\Omega}^{\rm meso}$ containing the random set of inclusions $X^{\rm meso}$. In the theory of periodic structures (see e.g. [4], [5]) this problem is usually solved on the mesocell $X^{\rm meso}$ with periodic boundary conditions. In the current approach, we analyzed all the inclusions from the whole space R^3 with the boundary conditions at infinity. However, due to the absolute convergence of the right-hand side of the obtained equation for the average strains in the inclusions, the real number of analyzed inclusions is limited by the inclusions belonging to the ellipsoidal domain $w^{\rm el}$ with linear size exceeding in a few times the linear size of $\boldsymbol{\Omega}^{\rm meso}$ (see for details [2]). Thus, although the periodic boundary conditions were not used in the obtained equation, nevertheless, the periodicity condition was explored for the solution $\boldsymbol{\varepsilon}(\boldsymbol{x})$, and, because of this, this equation contains only $N^{\rm meso}$ unknown strains associated with the inclusions contained in the mesocell $\boldsymbol{\Omega}^{\rm meso}$. As an example, we will considered an imperfect SC packing of identical hard spherical inclusions (the phase $v^{(1)}$) randomly replaced by the spherical voids of the same radius (the phase $v^{(2)}$). The statistical descriptors of the imperfect packing are fixed: $c^{(1)}(\lambda^{(1)}) + c^{(2)}(\lambda^{(2)})=0.4$, $\lambda^{(1)}=0.9$, $\lambda^{(2)}=0.1$. For instance, the values $\mu^{*}/\mu^{(0)}$ estimated for $400<n^{\rm MC}<500$ distinguish from their estimations for $n^{\rm MC}=2000$ and $n^{\rm MC}=600$ no more than 1.0% and 0.05% for $N^{\rm meso}=27$ and $N^{\rm meso}=343$, respectively. In so doing, the values $\mu^{*}/\mu^{(0)}$ estimated for $N^{\rm meso}=27$ and $N^{\rm meso}=343$ at $n^{\rm MC}=2000$ and $n^{\rm MC}=600$, respectively, can be distinguished by 0.35% (CPU times exploited for $n^{\rm MC}=1$ equal 5 sec. and 310 sec. for $N^{\rm meso}=27$ and $N^{\rm meso}=343$, respectively). The main idea of the fundamentally new third method is a decomposition of the desired solution on the known solution for the perfect periodic structure ($\boldsymbol{L}(\boldsymbol{x})=\boldsymbol{L}^{\rm per}(\boldsymbol{x})$), and on the perturbation produced by the imperfections in the perfect periodic structure. Analogously to the random structure matrix composites (RSMC), the effective moduli depend on three particular solutions: strain concentration factor $\boldsymbol{A}^{\rm per}(\boldsymbol{x})$ in the perfect periodic structure (analog of homogeneous strains in the RSMC without defects), strain concentration factor $\mathbf{A}_i^{imp}(\mathbf{x})$ in the infinite periodic medium with one imperfection (analog of Eshelby solution in the RSMC), strain concentration factor

$\mathbf{A}_{i,j}^{\mathrm{imp}}(\mathbf{x})$ in the infinite periodic medium with two arbitrary located imperfections (analog of the solution for two inclusions inside an infinite matrix, see [1]):

$$\mathbf{L}^{*} = \mathbf{L}^{(0)} + \sum_{i,j=2}^{N} \lambda^{(i)} \mathbf{R}^{(i)} \mathbf{D}_{ij} + \lambda^{(1)} \left\langle \mathbf{L}_2(\mathbf{x}) \mathbf{A}^{\mathrm{per}}(\mathbf{x}) \mathbf{D}_0(\mathbf{x}) \right\rangle_{(i)}^{\Omega} \qquad (1)$$

from which the effective elastic modulus for the perfect periodic structures $\mathbf{L}^{\mathrm{per}}$* can be extracted. Here $\mathbf{L}_2(\boldsymbol{x})=\mathbf{L}^{\mathrm{per}}(\boldsymbol{x})-\mathbf{L}^{(0)}$, $\mathbf{L}_3(\boldsymbol{x})=\mathbf{L}^{\mathrm{imp}}(\boldsymbol{x})-\mathbf{L}^{\mathrm{per}}(\boldsymbol{x})$, $\mathbf{R}^{(i)}$ is obtained by the volume average over the unite cell $\langle(.)\rangle_{(i)}^{\Omega}$ with one imperfection: $\mathbf{R}^{(i)} = \left\langle \mathbf{L}_3(\mathbf{x})[\mathbf{A}_i^{\mathrm{imp}}(\mathbf{x}) + \mathbf{A}^{\mathrm{per}}(\mathbf{x})] \right\rangle_{(i)}^{\Omega}$, and the tensors $\mathbf{D}_{ij}$ and $\mathbf{D}_0(\boldsymbol{x})$ depend on all three solutions $\mathbf{A}^{\mathrm{per}}(\mathbf{x})$, $\mathbf{A}_i^{\mathrm{imp}}(\mathbf{x})$ and $\mathbf{A}_{i,j}^{\mathrm{imp}}(\mathbf{x})$. The method proposed is general, it is not limited by concrete numerical scheme, and can use particular known solutions for particular problems mentioned above (for example, the solutions for the perfect periodic structure $\mathbf{A}^{\mathrm{per}}(\mathbf{x})$ as well as the solution for one crack in doubly-periodic structure $\mathbf{A}_i^{\mathrm{imp}}(\mathbf{x})$, see [5]). The numerical results are obtained in the framework of the hypothesis **H1)**. All three methods proposed lead to close results in the considered example ($c^{(1)}(\lambda^{(1)}) + c^{(2)}(\lambda^{(2)})=0.4$, see Fig.3), however, the CPU time expended for the solution estimation by Monte Carlo simulation differ by a factor of 1000. Thus, we proposed general explicit analytical representation of effective moduli of periodic structures with the random field of imperfections (see for details [6]) depending on three tensors $\boldsymbol{A}^{\mathrm{per}}(\boldsymbol{x})$, $\mathbf{A}_i^{\mathrm{imp}}(\mathbf{x})$, $\mathbf{A}_{i,j}^{\mathrm{imp}}(\mathbf{x})$. No restrictions were assumed on both the concrete microstructure and method used for obtaining these solutions. It should be mentioned that the known numerical methods (such as e.g. finite element analysis and boundary element method) have a series of advantages and disadvantages (see for references [7]). However, their analysis is beyond the scope of the current paper where we considered the application of proposed scheme in the framework of the hypothesis **H1)** significantly simplifying the analytical representations of the tensors.

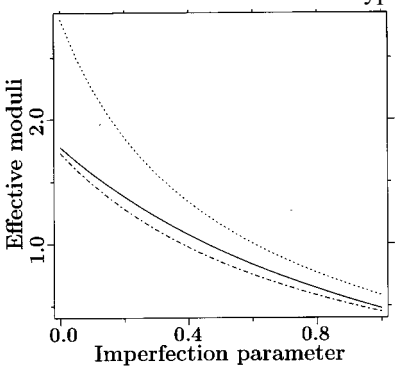

Fig. 1. Normalized effective moduli as the functions of $\lambda^{(2)}$: $\tilde{\mu}^{*}/\mu^{(0)}$ (dotted line), $\mu^{*}/\mu^{(0)}$ (solid line), $k^{*}/k^{(0)}$ (dashed line).

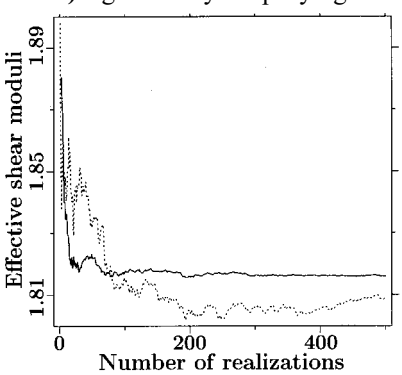

Fig. 2. Normalized effective elastic moduli $\mu^{*}/\mu^{(0)}$ as the functions of the number of Monte Carlo realizations n^{MC} for $\mathrm{N}^{\mathrm{meso}}$=343 (solid line), $\mathrm{N}^{\mathrm{meso}}$=27 (dotted line).

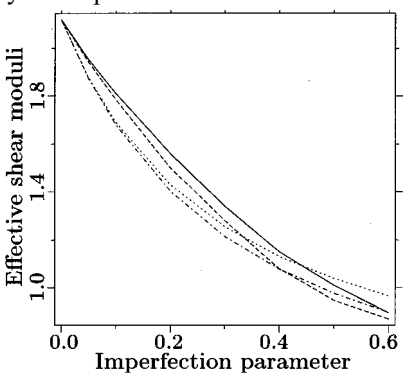

Fig. 3. $\mu^{*}/\mu^{(0)}$ vs $\lambda^{(2)}$: MC simulation (solid line), one point approximation ($\boldsymbol{L}^{\mathrm{c}}=\boldsymbol{L}^{(0)}$,dashed line), one-point approx. ($\boldsymbol{L}^{\mathrm{c}}(\boldsymbol{x})=\boldsymbol{L}^{\mathrm{per}}(\boldsymbol{x})$, dotted line), two-point approx. ($\boldsymbol{L}^{\mathrm{c}}(\boldsymbol{x})=\boldsymbol{L}^{\mathrm{per}}(\boldsymbol{x})$,dot-dashed line).

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