EQUIVALENT-INCLUSION APPROACH FOR THE CONDUCTIVITY OF ISOTROPIC MATRIX COMPOSITES WITH ANISOTROPIC INCLUSIONS

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Abstract. Many effective medium approximations for effective conductivity are elaborated for matrix composites made from isotropic continuous matrix and isotropic inclusions associated with simple shapes such as circles or spheres, . . . In this paper, we focus specially on the effective conductivity of the isotropic composites containing the disorderly oriented anisotropic inclusions. We aim to replace those inhomogeneities by simple equivalent circular (spherical) isotropic inclusions with modified conductivities. Available simple approximations for the equivalent circular (spherical)-inclusion media then can be used to estimate the effective conductivity of the original composite. The equivalent-inclusion approach agrees well with numerical extended finite elements results.

Keywords: Isotropic multicomponent material, disorderly oriented anisotropic inclusions, effective conductivity, matrix composite, equivalent inclusion.

1. INTRODUCTION

Theoretical determination of effective properties of multicomponent materials generally is difficult because of their complex microstructure and the random distribution of inclusions. The most rigorous approach is to to construct upper and lower bounds on the possible values of the effective properties, [1–3]. The bounds containing the properties and volume fractions of the component materials are not very useful in the case of high contrast of matrix-inclusion properties. The numerical methods [4–9], such as finite element one, fast Fourier transformation may give better results. However, they require much computer resources and computational time when the microstructure is complex and the inclusions are close to each other.

Engineers would prefer more simple effective medium approximations developed over years from the most simple arithmetic and harmonic volume-weighted averages to

more advanced self-consistent, differential, Mori-Tanaka approximation, correlation approximation... [10–17], which often account just for the shapes of the inhomogeneities and the matrix-inclusion interactions. Many approximations are actually applicable for only the composites with isotropic inclusions of simple shapes. The main objective here is to construct a novel approach for macroscopically isotropic composites containing the disorderly oriented anisotropic inclusions, which substitutes those inhomogeneities by circular (spherical) isotropic inclusions with equivalent conductivity. Above approximations then can be used to estimate the conductivity of original media. The layout of this paper is as follows.

First, we present the details of the proposed approach in section 2. In section 3, the effective medium approximation for effective conductivity of macroscopically isotropic composites containing the disorderly oriented anisotropic inclusions are compared with extended finite element results for some composites with complex microstructure, including that associated with random geometry. The conclusion completes the paper.

2. THE EQUIVALENT-INCLUSION APPROACH

Let us consider a d-dimensional macroscopically isotropic medium associated with anisotropic particles of certain shapes. The effective conductivity of a dilute suspension of those randomly-oriented particles having principal conductivities $c_{I1}, c_{I2}, \ldots, c_{Id}$ and volume proportion v_I in a matrix of conductivity c_M has the form

$$c^{eff} = c_M \left[1 + v_I D \left(c_{I1}, \ldots, c_{Id}, c_M \right) + O \left(v_I{}^2 \right) \right]. \tag{1}$$

In the meantime, the dilute suspension of circular (spherical) particles having conductivity $\bar{c}_I$ and volume proportion v_I in the matrix of the same conductivity c_M has the particular expression

$$c^{eff} = c_M \left[1 + v_I \frac{2(\bar{c}_I - c_M)}{[\bar{c}_I + (d-1)c_M]} \right]. \tag{2}$$

Equalizing (1) and (2), one finds

$$\bar{c}_I = c_M \frac{D \left(c_{I1}, \ldots, c_{Id}, c_M \right) (d-1) + 2}{2 - D \left(c_{I1}, \ldots, c_{Id}, c_M \right)}. \tag{3}$$

In the special case the anisotropic inclusions have the circular (spherical) shape, (1) has the particular expression [18]

$$c^{eff} = c_M \left[1 + v_I \sum_{i=1}^{d} \left(\frac{c_{Ii} - c_M}{c_{Ii} + (d-1)c_M} \right) \right], \quad v_I \ll 1. \tag{4}$$

In that case

$$D \left(c_{I1}, \ldots, c_{Id}, c_M \right) = \sum_{i=1}^{d} \left(\frac{c_{Ii} - c_M}{c_{Ii} + (d-1)c_M} \right). \tag{5}$$

$\bar{c}_I$ is referred to as the conductivity of the equivalent circular (spherical) inclusion for the original inclusions of conductivity c_I.

The simplest approximation for the conductivity of matrix circular (spherical)-inclusion composites is the Maxwell one [17,19], which will be used in applications with $\bar{c}_I$ taking the place of c_I.

3. NUMERICAL EXAMPLES FOR EFFECTIVE CONDUCTIVITY

3.1. Basic of XFEM/Level-set method

In this section, we use the Maxwell Approximation (MA) and eXtended Finite Elements method (XFEM) to estimate the conductivity of the isotropic composite containing the disorderly oriented anisotropic inclusions. Introducing equivalent inclusion with conductivity $\bar{c}_I$ defined in (3) instead of c_I in the polarization formula [16], which is similar to Maxwell one, one finds

$$c^{eff} = P(c_M),\tag{6}$$

where

$$P(c_0) = \left[\frac{v_M}{c_M + c_0} + \frac{v_I}{2}\left(\frac{1}{c_{I1} + c_0} + \frac{1}{c_{I2} + c_0}\right)\right]^{-1} - c_0 .\tag{7}$$

For numerical computations, the extended finite elements method [20–24] will be used. In this framework, the level-set function is involved to describe the interface of inclusions. The essence of this method is to enrich the finite element approximation with additional functions to model interfaces or singularities independently of the background mesh. So the XFEM does not require a mesh conforming with all internal surfaces of inclusions as the finite element mesh.

Consider a domain $\Omega \subset \mathbf{R}^D$ with boundary $\partial\Omega$ (D being the dimension of the domain) which is partitioned into finite elements, and $\mathcal{S} \subset \mathbf{N}^*$ ($\mathbf{N}^*$ being the set of positive natural numbers) be a set of N nodes indices in the mesh. The XFEM temperature field approximation can be expressed by

$$T^h(\mathbf{x}) = \sum_{i \in \mathcal{S}} N_i(\mathbf{x})T_i + \sum_{j \in \mathcal{S}^e} N_j^*(\mathbf{x})\psi(\mathbf{x})a_j .\tag{8}$$

In the above equation, T_i and a_j are nodal unknowns, $N_i(\mathbf{x})$ and $N_j^*(\mathbf{x})$ are finite element shape functions, not necessarily the same. The nodal set $\mathcal{S}^e$ is defined as:

$$\mathcal{S}^e = \left\{j | j \in \mathcal{S}, \omega_j \cap \Gamma \neq \varnothing\right\},\tag{9}$$

where Γ is an interface, that does not necessarily coincide with the mesh. $\omega_i = supp(n_i)$ is the support of the nodal shape function N_i, which consists of the union of all elements connected to the node n_i. The function $\psi(\mathbf{x})$ is an enrichment function with the desirable discontinuous properties. In this work, the enrichment function $\psi(\mathbf{x})$ can be chosen in the form proposed by Moës et al. [20]

$$\psi(\mathbf{x}) = \sum_i |\phi_i| N_i(\mathbf{x}) - \left|\sum_i \phi_i N_i(\mathbf{x})\right| .\tag{10}$$

where $\phi(\mathbf{x})$ is level-set function [20,23].

The field equations of thermo-static problem are given by

$$\nabla \cdot \mathbf{q}(\mathbf{x}) - r(\mathbf{x}) = 0 \text{ in } \Omega, \tag{11}$$

$$\mathbf{q}(\mathbf{x}) = -\mathbf{C}(\mathbf{x})\nabla T(\mathbf{x}). \tag{12}$$

Above, $\mathbf{q}(\mathbf{x})$ denotes the heat flux, $r(\mathbf{x})$ is a heat source term and $c(\mathbf{x})$ the conductivity tensor. The periodic boundary conditions are: $\mathbf{q}.\mathbf{n}$ is antiperiodic on $\partial\Omega$, and T is periodic on $\partial\Omega$. ($\mathbf{C}$) is the conductivity matrix. More precisely, $\mathbf{C}(\mathbf{x}) = \mathbf{C_I}$ for anisotropic inclusions is defined as

$$\mathbf{C_I} = -\mathbf{R^T}\mathbf{C^*}\mathbf{R}, \tag{13}$$

where $\mathbf{C^*}$ is conductivity matrix in local coordinate system (1,2), which reads as

$$\mathbf{C_I^*} = \begin{bmatrix} c_{I1} & 0 \\ 0 & c_{I2} \end{bmatrix}, \tag{14}$$

and $\mathbf{R}$ is rotation matrix expressed by

$$\mathbf{R} = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \tag{15}$$

The weak form associated with Eqs. (11)-(12) is given by finding $T \in \mathcal{D} = \{T | T = \bar{T} \text{ on } \partial\Omega_T, T \text{ in } H^1(\Omega)\}$ such that

$$\int_\Omega \mathbf{q}\nabla\left(\delta T\right) d\Omega + \int_\Omega r\delta T d\Omega = 0, \tag{16}$$

where $H_0^1(\Omega) = \{\delta T | \delta T \in H^1(\Omega), \delta T = 0 \text{ on } \partial\Omega_T\}$.

By substituting the temperature field defined in (8) into the weak form (16) we obtain the discrete system of linear ordinary equations

$$\mathbf{Kd} = \mathbf{Q}, \quad \mathbf{d} = \{\mathbf{T} \quad \mathbf{a}\}^T, \tag{17}$$

where $\mathbf{d}$ are nodal unknowns and $\mathbf{K}$ and $\mathbf{Q}$ are the global stiffness matrix and external flux, respectively. More precisely, the matrix $\mathbf{K}$ and vector $\mathbf{Q}$ are defined by

$$\mathbf{K} = \int_\Omega \mathbf{B}^T\mathbf{C}(\mathbf{x})\mathbf{B}d\Omega, \mathbf{Q} = \int_\Omega \mathbf{N}^T r d\Omega, \tag{18}$$

where $\mathbf{B}$ and $\mathbf{N}$ are the matrices of shape function derivatives and shape functions associated with the approximation scheme (8).

The periodic boundary condition is finally introduced to (17) by mean of multiplicator Lagrange.

3.2. Numerical example

As a numerical example we consider the two-component 2D square-periodic suspension of anisotropic inclusions having conductivity c_{I1} and c_{I2} in a matrix of conductivity c_M (Fig. 1(a)) (the principal axis is shown in the figure, secondary axis is perpendicular to the principal one), which have macroscopically isotropic conductivity c^{eff}. For the next model, we consider the hexagonal-periodic suspension with position of inclusions being located same as in Fig. 1(b). The local coordinate system (1,2) makes an angle θ with

the global coordinate system (x, y) of the square cell. In the random model (Fig. 1(c)), the position of inclusions is generated with non-penetration algorithm; The radii of the inclusions vary from $0.035L$ to $0.08L$, L being the dimension of the square cell. The equivalent configuration is that with circular (spherical) inclusions of the same centers and same volumes as the original one, but with different isotropic conductivity $\bar{c}_I$. The regular mesh
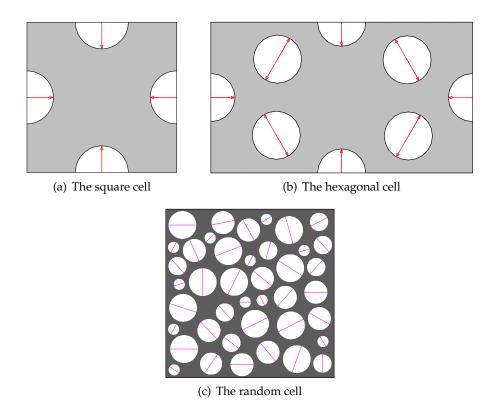

(a) The square cell   (b) The hexagonal cell

(c) The random cell

Fig. 1. The periodic cells of disorderly anisotropic inclusions having circular shape

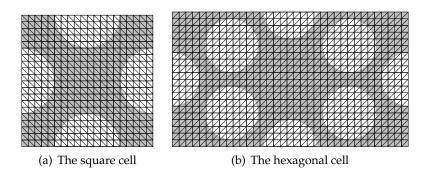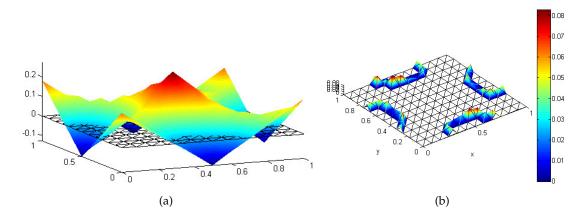(a) The square cell   (b) The hexagonal cell

Fig. 2. The regular mesh of the configuration

of the configuration is illustrated in Fig. 2. The level-set function for elliptic inclusions is defined by

$$\phi\left(\mathbf{x}\right) = \min_{k=1,\dots,n_c} \left(\sqrt{(x - x_{ck})^2 + (y - y_{ck})^2} - r_k \right), \tag{19}$$

where (x_{ck}, y_{ck}) being the centers of inclusions, r_k are radius of circular (spherical) inclusions; n_c being number of inclusions. The level set function $\phi\left(\mathbf{x}\right)$ and the enrichment function $\psi(\mathbf{x})$ defined in Eq. (10) are illustrated in Fig. 3.
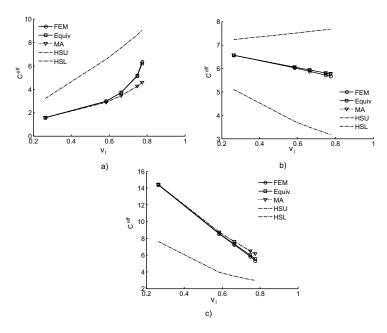

Fig. 3. (a) Level-Set functions of elliptic inclusions; (b) Enrichment function corresponding to above level-set functions

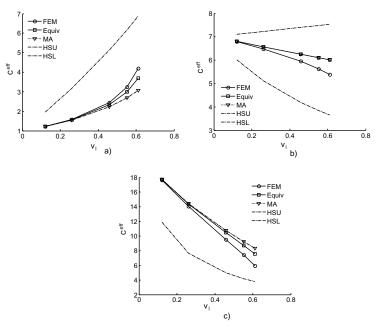For numerical calculations, we take the material parameters given in Tab. 1.

Table 1. Material parameters for numerical calculations

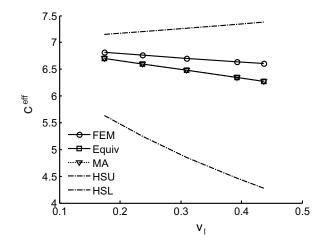| (a)	$c_M = 7$	$c_{I1} = 1$	$c_{I2} = 21$	$\bar{c}_I = 5.44$
(b)	$c_M = 1$	$c_{I1} = 7$	$c_{I2} = 21$	$\bar{c}_I = 10.73$
(c)	$c_M = 21$	$c_{I1} = 1$	$c_{I2} = 7$	$\bar{c}_I = 3.64$

The equivalent circular (spherical) inclusion has the conductivity $\bar{c}_I$ according to (3). The obtained effective conductivity is shown in the Fig. 4, FEM and Equiv, corresponding to the finite element results for original and equivalent configuration, are compared with Maxwell approximation using equivalent inclusion (MA), Hashin-Shtrikman bounds (HSU-Upper bound; HSL-Lower bound). The numerical results lie between the bounds. Both Equiv and MA are close to exact FEM, but MA is less close, as expected (because MAE is a double approximation). The approximations become less accurate at higher volume fractions of the inclusion phases, as expected, because of interactions between the inclusions that no simple approximations can cover. Still, the approximation appears relatively at small to intermediate values of volume proportions of the inclusions. For the hexagonal microstructure, we also take the material parameters given in the table , and

Fig. 4. The graphics of the effective conductivity for square cell. (a) $C_M = 1$; $C_{I1} = 7$; $C_{I2} = 21$; (b) $C_M = 7$; $C_{I1} = 1$; $C_{I2} = 21$; (c) $C_M = 21$; $C_{I1} = 1$; $C_{I2} = 7$

Fig. 5. The graphics of the effective conductivity for hexagonal cell. (a) $C_M = 1$; $C_{I1} = 7$; $C_{I2} = 21$; (b) $C_M = 7$; $C_{I1} = 1$; $C_{I2} = 21$; (c) $C_M = 21$; $C_{I1} = 1$; $C_{I2} = 7$

Fig. 6. Graphics of the effective conductivity with random cell. $C_M = 7$; $C_{I1} = 1$; $C_{I2} = 21$

get the results presented in Fig. 5. The differences seem to be larger because of agglomeration of the inclusion particles. For the random model with high complexity, the results presented in the Fig. 6 indicate that the numerical equivalent-inclusions result (Equiv) and Maxwell approximation (MA) almost coincide, and both are close to FEM results for original composites.

4. CONCLUSION

The main idea here is to replace the original composite with disorderly-oriented-anisotropic circular (or spherical) inclusion by the equivalent isotropic circular (or spherical) inclusions composite, to which much more simple approximations can be applied to estimate the effective conductivity. The proposed approach is based on equalizing the dilute solution results for the original anisotropic inclusions and that for the circular isotropic inclusions of the same volume fractions, but with some equivalent conductivity. It permits to substitute the original composite by an equivalent composite containing only circular (or spherical) inclusions. Then available effective medium schemas for circular (or spherical) inclusion composites, such as the Maxwell one can be applied to the equivalent medium. The numerical example have demonstrated the robustness, efficiency and accuracy of the approach. Clearly the approach can be extended also for macroscopically isotropic composites with anisotropic inclusions of non-circular (non-spherical) forms.

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