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Refined polarization approximations for conductivity of isotropic composites

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ABSTRACT

The polarization approximations for the effective conductivity of isotropic multicomponent materials, constructed recently from a variational approach, are refined to include more information about the composites, if available, to improve the accuracy of the scheme. The variable reference parameter of the approximation may be determined from an asymptotic solution (in series) for the effective conductivity of a particular composite at small volume proportions of the inhomogeneities, which contains more information about the composite than the dilute solution result. Practically, the variable parameter can be calibrated through available reference numerical or experimental macroscopic conductivities of the composite at finite volume proportions of the component materials, or from a combination of those references. By construction, the approximations satisfy Hashin-Shtrikman bounds, at least, over the range of the component's volume proportions within the extreme reference points. Illustrations of applications are provided in a number of examples involving numerical and/or experimental data, which shows the flexibility and usefulness of the approach.

1. Introduction

Many natural or artificial heterogeneous materials, though having irregular microgeometries, often have relatively definite isotropic macroscopic properties, because the inhomogeneities do not have preference direction distribution in the material space and share some common specific feature. To estimate the macroscopic properties of the composites, one may use variational approach [1–4], effective medium approximation approach [5–13], computational methods [14–18]. Though a particular composite material has some specific geometric feature, it is often difficult to include it into the estimates, besides the properties and volume proportions of the components, and possibly the approximate forms of the inhomogeneities in a matrix composite or a particulate mixture. Popular effective medium approximations (EMA) such as Maxwell, self-consistent, and Mori-Tanaka, … ones may diverse from measured macroscopic properties of practical composites at substantial values of volume proportions of the included phases when the contrast between the component properties is high. Instead, in applications, various semi-empirical formulae for the macroscopic conductivities with fitting parameters are developed to approximate the properties of specific composites by practitioners in the field [7,8,19–25].

As a distinction from other EMA schemes, including the Maxwell, self-consistent, Mori-Tanaka, differential ones, which have been derived from the field equations using the inhomogeneities' dilute solution reference, recent polarization approximation of Pham and Nguyen [26] has been constructed from the minimum energy principles. The approximation contains a reference parameter that should be determined from the inhomogeneities' dilute solution result for a matrix composite, or from available numerical or experimental value of the macroscopic conductivity of the composite at certain finite-volume-proportion point of the component materials. Once the appropriate reference parameter had been chosen, the approximation should obey Hashin-Shtrikman (HS) bounds over all the ranges of volume proportions of the component materials. Still, like many other effective medium approximations, the approximation may be not very good at the components' proportions far from the reference point, when compared with numerical and experimental data.

In this work, refined polarization approximations are proposed to account for more information about a composite - if available - to make more accurate estimates of the effective property over a range of components' volume proportions of interest. In the following section,

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refined multi-point polarization approximations are proposed that contain a few dimensionless free parameters. In the next sections, the free parameters are calibrated through some available asymptotic solution results for the inhomogeneities, or from a combination of dilute solution, available numerical or experimental references, with illustrating examples, which show the usefulness of the approach.

2. One-point and multi-point polarization approximations

Transport properties of isotropic materials in the framework of linear continuum mechanics are described by a material constant (conductivity) relating solenoidal vector (flux) and irrotational vector (field intensity). Let us consider an isotropic multicomponent material in d-dimensional space ($d = 2{,}3$) that consists of n isotropic components of volume proportions v_i and conductivities c_i ($i = 1, \ldots, n$). The contacts between the component materials are assumed to be perfect. The polarization approximation (PA) for the effective conductivity c^{eff} of the composite constructed from the minimum energy principles in general d-dimensional space has the particular form [26]

$$c^{eff} = P_c(c_*) = \left(\sum_{i=1}^{n} \frac{v_i}{c_i + c_*}\right)^{-1} - c_* , \quad (1)$$

where the reference parameter c_* should be determined from a reference dilute solution result (called PA0), or reference effective conductivity of the composite at certain finite volume proportion point of the components (called PA1). The approximations (PA0 as well as PA1) obey Hashin-shtrikman (HS) bounds over all volume proportions of the material components, once the reference effective conductivity satisfies the bounds, while some other EMAs may not. In the case of matrix composite with the matrix component $v_1 = v_M$, $c_1 = c_M$, for the polarization approximation using dilute solution reference PA0, c_* is the solution of the equation

$$\sum_{\alpha=2}^{n} v_\alpha (c_\alpha - c_M)\left(\frac{c_M + c_*}{c_\alpha + c_*} - D_\alpha(c_\alpha, c_M)\right) = 0 , \quad (2)$$

presuming the respective dilute solution result for the suspension of the same-geometry inclusions with the properties c_α, volume fractions tv_α ($\alpha = 2, \ldots, n$; $t \ll 1$) in the predominant matrix of conductivity c_M is

$$c^{eff} = c_M + \sum_{\alpha=2}^{n} tv_\alpha (c_\alpha - c_M) D_\alpha(c_\alpha, c_M) , \quad t \ll 1 , \quad (3)$$

where D_α are some inclusion-functions, which are specific for every α-inclusion-component's geometry.

For instance, in the case of two-component matrix composite, with the volume proportions and conductivities of the matrix and inclusion components being $v_1 = v_M$, $c_1 = c_M$ and $v_2 = v_I$, $c_2 = c_I$, respectively, equation (2) is solved explicitly

$$c_* = \frac{D(c_I, c_M)c_I - c_M}{1 - D(c_I, c_M)} , \quad (4)$$

where $D(c_I, c_M)$ is the respective inclusion-function. The approximation

$$c^{eff} = \left(\frac{v_I}{c_I + c_*} + \frac{v_M}{c_M + c_*}\right)^{-1} - c_* , \quad (5)$$

with c_* from (4) is PA0 for the two-component d-dimensional matrix composite. In the case of sphere-like (circular-like) inclusion, we have

$$D(c_I, c_M) = \frac{dc_M}{c_I + (d-1)c_M} , \quad (6)$$

and

$$c^{eff} = \left(\frac{v_I}{c_I + c_{*M}} + \frac{v_M}{c_M + c_{*M}}\right)^{-1} - c_{*M} , \quad c_{*M} = (d-1)c_M . \quad (7)$$

In the 2-dimensional case of elliptic inclusions with the aspect ratio

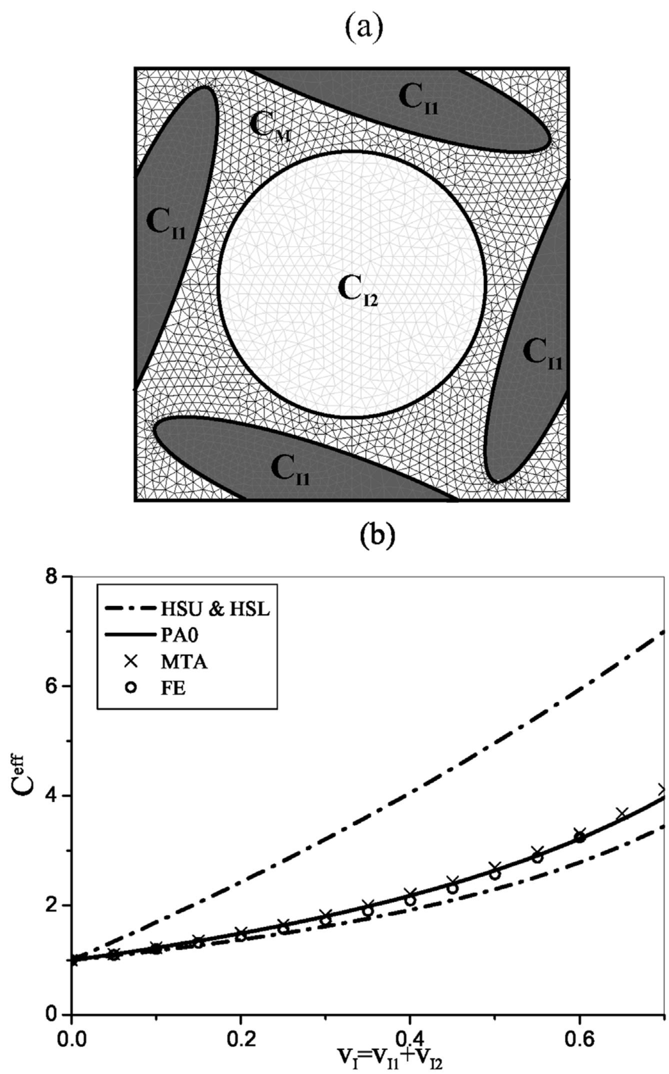

Fig. 1. Approximations PA0 and MTA versus the finite element result FE, and HS bounds for the conductivity of a 2D periodic three-component matrix composite: (a)- a periodic cell; (b) The results in the case $C_M = 1$, $C_{I1} = 5$ (circular inclusion), $C_{I2} = 20$ (elliptic inclusion - aspect ratio 1: 5), $v_{I1}/v_{I2} = 1$.

$r = a_1 : a_2$ (a_1 and a_2 are the axes of the ellipse) one has

$$D(c_I, c_M) = \frac{c_M(c_I + c_M)(1 + r)^2}{2(c_I + rc_M)(rc_I + c_M)} . \quad (8)$$

It can be verified that PA0 for isotropic two-component matrix composites with 3D ellipsoidal (or 2D elliptic) inclusions happens to coincide with Mori-Tanaka approximation (MTA). Generally for multi-component materials they differ. As an example we consider a 2D periodic three-component configuration having isotropic macroscopic conductivity, a periodic cell of which is presented in Fig. 1a. The conductivity of the matrix phase is normalized to be unity $c_M = 1$; the circular inclusions have conductivity $c_{I1} = 5$; the elliptic inclusions (aspect ratio 1: 5) - $c_{I2} = 10$; the relative volume proportion of the inclusion components $v_{I1}/v_{I2} = 1$. The finite element numerical results (FE) for the effective conductivity, over a volume proportion range of the included phases $v_I = v_{I1} + v_{I2}$, are compared with the approximations PA0 from (1)–(2) and MTA in Fig. 1b. The results are close to each other, but differ; all lie within Hashin-Shtrikman bounds (HSU & HSL).

PA0 always satisfies HS bounds, while MTA may not. Norris [27] has found a 3D three-component matrix composite with circular disk inclusions, the MTA for the effective conductivity of which violates the HS upper bound at certain components' conductivity and volume