



Effective elastic moduli of a particulate composite in terms of the dipole moments and property contribution tensors



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ABSTRACT

The paper focuses on the comparison of two approaches used for calculation of the effective elastic properties of particulate composites: the dipole moments representation and the technique based on property contribution tensors. Its specific goal is to bridge the gap between the two methods and to identify the key microstructural parameters affecting overall elastic stiffness of heterogeneous materials. The basic concepts of the homogenization theory including a consistent way of introducing the macroscopic field parameters are discussed and clarified. We provide a detailed comparison of the analytical expressions for the dipole moment tensors obtained by the multipole expansion method and for the stiffness contribution tensors and show that they coincide.

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1. Introduction

In the present paper we discuss the connection between two approaches that can be applied to calculate effective elastic properties of heterogeneous materials: (1) the multipole expansion and (2) the property contribution tensors. It can be considered as extension of the work of the present authors (Kushch and Sevostianov, 2014), where conductive properties were discussed, to the case of effective elastic properties.

Connection between the compliance contribution tensors and far-field asymptotes received some attention in literature. Jasiuk et al. (1994) and Jasiuk (1995) considering 2-D polygonal holes, made an observation that the far-field asymptotic of the hole-generated fields fully determines the compliance contribution of the hole.

Actually, sufficiency of the far-fields for proper description of the contributions of the inhomogeneities to effective properties extends to the general 3-D case as shown by Sevostianov and Kachanov (2011). The extra overall strain due to the presence of an inhomogeneity in reference volume V is given by the well-known expression in terms of an integral over the boundary ∂V (Hill, 1963):

$$\Delta \boldsymbol{\varepsilon} = \frac{1}{2V} \int_{\partial V} (\Delta \mathbf{u} \mathbf{n} + \mathbf{n} \Delta \mathbf{u}) dS, \quad (1.1)$$

where $\Delta \mathbf{u}$ are extra displacements due to the inhomogeneity and n_i is the outward unit normal to ∂V . Volume V can be arbitrarily large, hence the far-field asymptotics of $\Delta \mathbf{u}$ is sufficient for determination of the compliance contribution of an inhomogeneity. Formula (1.1) gives the compliance contribution of an inhomogeneity in terms of experimentally measurable quantities – displacements of the specimen boundaries; in this context, volume V must be large to neglect the inhomogeneity-boundary interaction thus making the far-field asymptotic necessary.

The far-field asymptotics of elastic field is *shape-dependent*, even in cases when the inhomogeneity compliance contribution is isotropic (for example, when the inhomogeneity shape has the symmetry of any equilateral polygon, except square). This is in contrast with *shape independence* of the inhomogeneity contributions to the physical properties characterized by *second-rank* tensors (see Kushch and Sevostianov, 2014), such as the conductive or dielectric ones: for them, the isotropic case is characterized by only one constant, hence any isotropic – in regard to these properties – shape (such as any equilateral polygon including square) can be replaced by a circle of appropriate radius.

The structure of the far-field and its shape dependence can be clarified using the multipole expansions (Kushch, 2013). Batchelor (1974) suggested to calculate average stress – and thus the effective stiffness of composite – in terms of the induced dipole moments of particles populating the representative volume element (RVE). The elastic dipole moment is formally defined (see, for example, Vakulenko and Kosheleva, 1980; Kosheleva, 1983) as the coefficient in the multipole series expansion of displacement

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disturbance field associated with the dipole term. Multipole expansions can be illustrated on a system of forces distributed in volume V . At distance r that is much larger than linear dimensions of V , elastic fields can be represented as a sum of terms: the first one is generated by the principal vector of forces (it decreases as r^{-2} for stresses and r^{-1} for displacements); the second one – by dipoles, i.e. pairs of equal and opposite point forces applied at closely spaced points (it decreases as r^{-3} and r^{-2}); the third one – by quadrupoles – closely spaced dipoles of opposite signs (it decreases as r^{-4} and r^{-3}), etc. The first term (generated by the principal vector) is a dominant one. Such expansions can be extended from a discrete system of forces to a distribution of stresses (or strains) in V : the role of the principal vector is played then by the integral $\int_V \sigma_{ij} dV$ and higher order moments take the form $\int_V x_k \sigma_{ij} dV$, $\int_V x_k x_l \sigma_{ij} dV$, etc. We refer to the book of Lur'e (1964) for the case of discrete system of forces and the book of Kanaun and Levin (2008) for a more general form of distributions.

The connection between the property contribution tensors and multipole expansion method is not yet well recognized and understood. This work aims at establishing the connection between two different approaches to the problem of homogenization and to identify and discuss the key microstructural parameters affecting overall elastic properties of heterogeneous materials. It follows the idea proposed by the present authors (Kushch and Sevostianov, 2014) for overall conductivity (thermal or electric) of heterogeneous materials.

2. Background material

For readers convenience, in this section we briefly outline the concepts of (1) property contribution tensors and (2) the multipole expansion. These topics, being known for several decades, are not widely used in the problems of homogenization.

2.1. Compliance and stiffness contribution tensors

Compliance contribution tensors have been first introduced by Horii and Nemat-Nasser (1983) for pores of ellipsoidal shape (explicit formulas connecting compliance contribution tensor and Eshelby tensor for an ellipsoidal pore are given in the appendix of the mentioned paper). Components of this tensor for two-dimensional pores of arbitrary shape were given by Kachanov et al. (1994) and for ellipsoidal inhomogeneities – by Sevostianov and Kachanov (1999). Connection between compliance and stiffness contribution tensors has been discussed by Sevostianov and Kachanov (2007b). The significance of these tensors for the homogenization theory is that their sum is the proper microstructural parameter in whose terms the considered effective property has to be expressed. In other words, it is *these* tensors that have to be summed up, or averaged over a RVE to calculate overall elastic properties.

In the context of linear elastic properties, the average, over representative volume V strain can be represented as a sum

$$\langle \boldsymbol{\varepsilon} \rangle = \mathbf{S}_0 : \boldsymbol{\sigma}^\infty + \Delta \boldsymbol{\varepsilon}, \quad (2.1)$$

where \mathbf{S}_0 is the compliance tensor of the matrix and $\boldsymbol{\sigma}^\infty$ represents the homogeneous boundary conditions (tractions on ∂V have the form $\mathbf{t}_{|\partial V} = \boldsymbol{\sigma}^\infty \cdot \mathbf{n}$ where $\boldsymbol{\sigma}^\infty$ is a constant tensor); $\boldsymbol{\sigma}^\infty$ can be viewed as a far-field, or remotely applied, stress. The material is assumed to be linear elastic, hence the extra strain $\Delta \boldsymbol{\varepsilon}$ due to inhomogeneity of volume V_1 is proportional to applied stress and compliance contribution tensor is the proportionality factor in this relation:

$$\Delta \boldsymbol{\varepsilon} = (V_1/V) \mathbf{H} : \boldsymbol{\sigma}^\infty. \quad (2.2)$$

In the case of multiple inhomogeneities, $\Delta \boldsymbol{\varepsilon} = (1/V) \sum_i V_i \mathbf{H}^{(i)} : \boldsymbol{\sigma}^\infty$ so that the extra compliance due to inhomogeneities is given by

$$\Delta \mathbf{S} = (1/V) \sum_i V_i \mathbf{H}^{(i)}. \quad (2.3)$$

Alternatively, one can consider the extra average stress $\Delta \boldsymbol{\sigma}$ due to an inhomogeneity under given applied displacement homogeneous boundary conditions (displacements on ∂V have the form $\mathbf{u}_{|\partial V} = \boldsymbol{\varepsilon}^\infty \cdot \mathbf{x}$ where $\boldsymbol{\varepsilon}^\infty$ is a constant tensor). This defines the *stiffness contribution tensor* of an inhomogeneity:

$$\Delta \boldsymbol{\sigma} = (V_1/V) \mathbf{N} : \boldsymbol{\varepsilon}^\infty, \quad (2.4)$$

In the case of multiple inhomogeneities, the extra stiffness due to inhomogeneities is given by

$$\Delta \mathbf{C} = (1/V) \sum_i V_i \mathbf{N}^{(i)}. \quad (2.5)$$

The property contribution tensors, obviously, have the same rank and symmetry as the tensors characterizing the property: \mathbf{H} and \mathbf{N} are fourth-rank tensors with $ijkl$ components symmetric with respect to $i \leftrightarrow j$, $k \leftrightarrow l$ and $ij \leftrightarrow kl$.

The \mathbf{H} - and \mathbf{N} -tensors are determined by the shape of the inhomogeneity, as well as properties of the matrix and of the inhomogeneity material.

Remark. The property contribution tensors defined via Eqs. (2.2) and (2.5) do not depend on the size of inhomogeneity. This definition is different from those used, for example, by Sevostianov and Kachanov, 2002, where multiplier (V_1/V) was absorbed by the tensors. The present definition has a number of advantages. For example, the problem of distinction between infinite cylinder and a needle is irrelevant. The difference between these two shapes is in the multiplier (V_1/V) only.

The compliance and stiffness contribution tensors are also affected by elastic interactions. In the non-interaction approximation, they are taken by treating the inhomogeneities as isolated ones. These tensors for a given inhomogeneity are interrelated, as follows. The overall compliance of certain volume containing one inhomogeneity $\mathbf{S}_0 + \mathbf{H}$ is an inverse of its stiffness tensor $\mathbf{C}_0 + \mathbf{N}$, i.e. their product equals the fourth-rank unit tensor implying that $\mathbf{N} = -\mathbf{C}_0 : \mathbf{H} : \mathbf{C}_0 - \mathbf{N} : \mathbf{H} : \mathbf{C}_0$. The \mathbf{H} - and \mathbf{N} -tensors scale as the ratio l^3/V that can be made arbitrarily small by enlarging V . Hence the second term can be neglected so that

$$\mathbf{N} = -\mathbf{C}_0 : \mathbf{H} : \mathbf{C}_0 \quad (2.6)$$

or, in the case of the isotropic matrix,

$$-N_{ijkl} = \lambda_0^2 H_{mmnn} \delta_{ij} \delta_{kl} + \mu_0^2 H_{ijkl} + \lambda_0 \mu_0 (\delta_{ij} H_{mmkl} + \delta_{kl} H_{mmij}), \quad (2.7)$$

where λ_0 and μ_0 are Lamé constants of the matrix.

For an *ellipsoidal inhomogeneity*, compliance and stiffness contribution tensors can be explicitly expressed in terms of Hill's tensors \mathbf{Q} and \mathbf{P} (Walpole, 1966) or in terms of Eshelby's tensor \mathbf{s} (given for example in book of Mura, 1987) and, therefore, in terms of ellipsoid geometry. For compliance contribution tensor, one can write (Sevostianov and Kachanov, 1999):

$$\mathbf{H} = [(\mathbf{S}_1 - \mathbf{S}_0)^{-1} + \mathbf{Q}]^{-1}. \quad (2.8)$$

where \mathbf{S}_1 is compliance of the inhomogeneity material. In the case of a pore, $\mathbf{H} = \mathbf{Q}^{-1}$. Similarly, the stiffness contribution tensor is obtained as

$$\mathbf{N} = [(\mathbf{C}_1 - \mathbf{C}_0)^{-1} + \mathbf{P}]^{-1}. \quad (2.9)$$

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