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On the possibility to represent effective properties of a material with inhomogeneities in terms of concentration parameters

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ABSTRACT

It is argued that representation of the effective properties of heterogeneous materials in terms of a single parameter of concentration of inhomogeneities (such as volume fraction or crack density) is generally impossible for *mixtures* of inhomogeneities of diverse shapes; the exceptions – when this is possible – are identified. Application of such parameters to microstructures of "irregular" microgeometries may lead to various inconsistencies. Instead, the effective constants in such cases can be represented in terms of a "tracking" parameter for a specific process of evolution of a microstructural pattern. These issues are discussed in the context of the elastic and conductive properties.

1. Introduction

In theories of effective physical properties of materials containing inhomogeneities, the central problem is typically viewed as finding the function

$$\textit{effective property} = f\left(\underbrace{\textit{concentration parameter}}_{?}\right). \tag{1.1}$$

Much attention has been paid to specification of this function, in particular, to the way it is affected by interactions. However, the *argument* of this function is a non-trivial matter. Moreover, the very possibility of such representation is questionable, as discussed in the present work. Some of the issues discussed here may appear straightforward, but they do not seem to have been adequately addressed in literature.

A common choice of the concentration parameter is the volume fraction of inhomogeneities, ϕ. This choice implies that contribution of a given inhomogeneity to the effective property is taken as proportional to its volume. Therefore the choice of ϕ as the concentration parameter is adequate if all the inhomogeneities have identical shapes; in this case, the effective properties are expresses as a product of ϕ and shape factor (the latter is known in a closed form for the ellipsoidal shapes). However, for *mixtures* of inhomogeneities of diverse shapes, ϕ cannot be used for the reason that it distorts the actual contributions of individual inhomogeneities to the overall properties. Moreover, a mixture of diverse shapes cannot generally be replaced by inhomogeneities of identical ("average") shape (Sevostianov and Kachanov, 2012).

For cracks, limitations of using the conventional crack density parameter (scalar or tensor) are even more severe. Indeed, such parameters are defined for circular cracks only: they assume that the contribution of a crack is taken as proportional to its radius cubed, a^3 (the generalization of Budiansky and O'Connell (1976) to the elliptical cracks in the case of random orientations assumes that all ellipses have identical eccentricities). Thus, the crack density parameter is not even defined for cracks of more complex shapes. Whereas for planar cracks of random shapes one can show that an equivalent distribution of circular cracks (of generally unknown concentration) exists (Gueguen and Kachanov, 2011), such an equivalence breaks down for non-flat cracks (Mear et al., 2007).

The general requirement that the concentration parameter (such as ϕ or crack density) represents individual inhomogeneities in accordance with their actual contributions to overall property may also be violated by *interactions* between inhomogeneities (since the said parameters are insensitive for mutual positions of inhomogeneities). For example, for coplanar (or stacked) cracks, interactions make the dependence of crack contributions to the effective compliance on their radii stronger (or weaker) than a^3. Therefore using the conventional crack density parameter beyond the non-interaction approximation (NIA) – in which they are defined – is not fully logical. This difficulty is frequently by-passed by using approximate schemes that account for interactions by

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placing inhomogeneities – treated as *non-interacting* ones – into certain effective environment, either the effective matrix (as in the differential scheme, see Bruggeman (1935, 1937), Vavakin and Salganik (1975), McLaughlin (1977), Zimmerman (1991) or in the self-consistent scheme, see Kröner (1958), Skorohod (1961), Hill (1965), Budiansky (1965) and Benveniste and Milton (2010a,b) or the effective field (as in Mori–Tanaka's scheme, see Mori and Tanaka (1973) and Benveniste (1986); or the effective field method, see Levin (1975) and Kanaun (1982) and the book of Kanaun and Levin (2008).

The present work does not discuss the effect of interaction and limits of applicability of NIA (see Sevostianov and Kachanov (2013) for discussion of the mentioned limitations in detail). Instead we focus on difficulties related to *mixtures* of inhomogeneities of diverse shapes (for example, spheroids of diverse aspect ratios). Such cases are quite common in heterogeneous materials, particularly in naturally occurring ones. For them, volume fraction ϕ may be inadequate as a concentration parameter even in the NIA.

2. Cases when simple concentration parameters can be identified

The discussion of concentration parameters is best conducted in terms of *property contribution tensors* that give contributions of individual inhomogeneities to the considered effective property (see Horii and Nemat-Nasser (1983), Kachanov and Sevostianov (2005) and Eroshkin and Tsukrov (2005) for details).

In the context of linear elastic properties, we consider a reference volume V, containing an inhomogeneity, and represent, as usual, the strain $\boldsymbol{\varepsilon}$ per volume V as a sum

$$\boldsymbol{\varepsilon} = \boldsymbol{S}^0 : \boldsymbol{\sigma}^\infty + \Delta\boldsymbol{\varepsilon}, \quad \text{or, in components,}$$
$$\varepsilon_{ij} = S^0_{ijkl}\sigma^\infty_{kl} + \Delta\varepsilon_{ij}, \tag{2.1}$$

where $\boldsymbol{S}^0$ is the matrix compliance tensor and $\boldsymbol{\sigma}^\infty$ is the "remotely applied" stress (more precisely, the constant stress corresponding to homogeneous boundary conditions in tractions on the boundary of the volume, $t_i = \sigma^\infty_{ij}x_j$). The extra strain, per V, due to an inhomogeneity of volume V_1 is a linear function of the applied stress:

$$\Delta\boldsymbol{\varepsilon} = \frac{V_1}{V}\boldsymbol{H} : \boldsymbol{\sigma}^\infty, \tag{2.2}$$

where $\boldsymbol{H}$ is the fourth-rank compliance contribution tensor of the inhomogeneity, taken per unit volume of the latter. Tensor $\boldsymbol{H}$ depends on the shape of the inhomogeneity and its elastic constants, as well as constants of the matrix; it has the usual symmetries of the compliance tensor ($H_{ijkl} = H_{jikl} = H_{ijlk} = H_{klij}$).

The extra strain due to *multiple* inhomogeneities – with interactions between them neglected – is a sum

$$\Delta\boldsymbol{\varepsilon} = \frac{1}{V}\sum V_k\boldsymbol{H}^{(k)} : \boldsymbol{\sigma}^\infty, \tag{2.3}$$

so that the extra compliance is given by

$$\Delta\boldsymbol{S} = \frac{1}{V}\sum V_k\boldsymbol{H}^{(k)}. \tag{2.4}$$

Relation (2.4) solves the problem in the NIA provided the $\boldsymbol{H}$-tensors of inhomogeneities – treated as isolated ones – are known. It also shows the key role of $\boldsymbol{H}$-tensors in the problem of effective properties: it is *them* that have to be summed up.

The problem addressed in the present work can be formulated as follows: can the sum (2.4) be expressed in terms of certain concentration parameter (scalar, in the isotropic case of random orientations, or tensor, in anisotropic cases)?

We start with the general requirement to proper concentration parameters: *They must represent individual inhomogeneities in accordance with their actual contributions to the considered property*. Violation of this requirement may lead to non-uniqueness of the function (1.1), even in the NIA.

It appears unlikely that, in the general case, the expression $(1/V)\sum V_k\boldsymbol{H}^{(k)}$ for the extra compliance due to inhomogeneities can be represented in terms of certain simple concentration parameter, such as volume fraction or crack density. Table 1 summarizes the cases for which such a representation is possible.

The following comments on Table 1 should be made:

- Coefficients s_1, s_2 entering the representation for the isotropic fourth-rank tensor of elastic constants are expressed in terms of traces of the $\boldsymbol{H}$-tensors, namely, $s_1 = (1/15)(2H_{ijij} - H_{iikk})$; $s_2 = (1/30)(3H_{ijij} - H_{iikk})$. Constants a_1 and a_2 can be specified using the results of Bristow (1960). Constant $C = 32(1-\nu^2)/(3(2-\nu)E)$. For flat non-circular cracks, constants C_1, C_2 cannot generally be related to crack geometries by closed-form expressions (see Gueguen and Kachanov, 2011);
- Scalar crack density (for the isotropic case of random orientations) and its second- and fourth-rank tensor generalizations are defined by $\rho = (1/V)\sum a_k^3$ and $\boldsymbol{\alpha} = (1/V)\sum(a^3\boldsymbol{nn})^{(k)}$, $\boldsymbol{\beta} = (1/V)\sum(a^3\boldsymbol{nnnn})^{(k)}$, where a_k are crack radii;
- The scalar crack density parameter can also be applied to the isotropic case of randomly oriented *elliptical* cracks, provided all the ellipses have the same eccentricity (Budiansky and O'Connell, 1976);

Table 1
Effective elastic properties: cases when simple concentration parameters can be identified.

Microstructure	Formula for $(1/V)\sum V_k H^{(k)}$	Parameter
Distributions over shapes and orientations are statistically independent		
Arbitrary	$(1/V)\sum V_k\boldsymbol{H}^{(k)} = \phi\langle\boldsymbol{H}\rangle$	ϕ
Inhomogeneities of arbitrary identical shape or inhomogeneities of diverse shapes for which equivalent shape can be identified		
Inhomogeneities of arbitrary shapes and of arbitrary orientation distribution	$(1/V)\sum_n V_n H^{(n)}_{ijkl} = \phi\sum_n Q^{(n)}_{ip}Q^{(n)}_{jq}Q^{(n)}_{kr}Q^{(n)}_{lt}H^0_{pqrt}$ ($Q^{(n)}_{ij}$ are directional cosines of $\boldsymbol{H}^{(n)}$)	ϕ
Parallel inhomogeneities	$(1/V)\sum V_n\boldsymbol{H}^{(n)} = \phi\boldsymbol{H}$	ϕ
Isotropic mixture of inhomogeneities	$(1/V)\sum V_n H^{(n)}_{ijkl} = \phi[s_1\delta_{ij}\delta_{kl} + s_2(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})]$	ϕ
Cracks		
Arbitrary orientation distribution of circular cracks	$(1/V)\sum V_n H^{(n)}_{ijkl} = C[(\delta_{ik}\alpha_{jl} + \delta_{il}\alpha_{jk} + \delta_{jk}\alpha_{il} + \delta_{jl}\alpha_{ik})/4 + \nu_0\beta_{ijkl}/2]$	α_{ij}, β_{ijkl}
Randomly oriented circular cracks	$(1/V)\sum V_n H^{(n)}_{ijkl} = \rho[a_1\delta_{ij}\delta_{kl} + a_2(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})]$	ρ
Strongly oblate spheroidal pores of small diverse aspect ratios	$(1/V)\sum V_n H^{(n)}_{ijkl} = C[(\delta_{ik}\alpha_{jl} + \delta_{il}\alpha_{jk} + \delta_{jk}\alpha_{il} + \delta_{jl}\alpha_{ik})/4 + \nu_0\beta_{ijkl}/2]$	α_{ij}, β_{ijkl}
Multiple flat cracks of non-circular shapes with random deviations from circles	$(1/V)\sum V_n H^{(n)}_{ijkl} = C_1(\delta_{ik}\alpha^*_{jl} + \delta_{il}\alpha^*_{jk} + \delta_{jk}\alpha^*_{il} + \delta_{jl}\alpha^*_{ik})/4 + C_2\beta^*_{ijkl}$	α^*_{ij}, β^*_{ijkl}