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International Journal of Solids and Structures 42 (2005) 309–336
INTERNATIONAL JOURNAL OF SOLIDS and STRUCTURES
www.elsevier.com/locate/ijsolstr

On quantitative characterization of microstructures and effective properties

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Received 17 December 2003; received in revised form 21 January 2004
Available online 6 August 2004

Abstract

Proper quantitative characterization of microstructures, for the purpose of modeling the effective properties, is discussed. This is a broad subject that covers different physical properties (elastic, conductive, transport, etc.), as well as various types of microstructures. The present work focuses on microstructures that can be characterized as continuous matrices containing isolated inhomogeneities of diverse shapes, properties and orientations. We address their proper quantitative characterization in the context of elastic and conductive properties (transport and fracture-related properties are also briefly discussed).

Proper microstructural parameters must correctly represent the individual inhomogeneity contributions to the considered property. They may differ for different physical properties. The key problem is to identify the mentioned individual contributions. For the *elastic* properties, we demonstrate, on a number of microstructures, how the proper parameters are implied by the elastic potential. Relative importance of various "irregularity factors" (shape irregularities, orientation scatter) is analyzed.

We discuss similarities and differences between microstructural parameters intended for different physical properties. The possibility of *explicit cross-property connections* between two physical properties depends on whether the proper microstructural parameters for these two properties are sufficiently similar. We outline such explicit connections between the elastic and the conductive properties.

The micromechanical approach is compared with the one based on an a priori introduced "fabric" tensors and general tensor representations that contain a number of uncertain factors. Various problems arising in this context are discussed.

Keywords: Microstructure; Micromechanics; Fabric; Effective properties; Inhomogeneity; Cross-property connection

1. Introduction and overview

We discuss materials that can be described as continuous matrices containing multiple isolated inhomogeneities of diverse shapes and orientations (cracks, pores, foreign particles). The problem addressed

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doi:10.1016/j.ijsolstr.2004.06.016

here is their *proper quantitative characterization* in the context of effective properties. This means identification of the *proper microstructural parameters*, in whose terms the physical property of interest is to be expressed. The focus here is on the elastic and the conductive properties; we also briefly discuss fluid permeability for one class of microstructures, and the issue of proper parameters for brittle–elastic fracture.

The proper microstructural parameters are generally *different for different physical properties*. If they are sufficiently similar for a certain pair of physical properties, this leads to explicit *cross-property connections* between the two properties (see Section 8 of the present work).

The proper microstructural parameters should represent the individual inhomogeneities *in accordance with their contributions to the physical property considered*—otherwise, the property cannot be uniquely expressed in their terms. For example, the crack density parameters, that are proper for the effective elasticity/conductivity, take the individual contributions of crack-like pores proportionally to the crack radii *cubed* (or squared, in 2-D case); pore openings, that may be small but finite, are ignored. However, for the fluid permeability, these openings are of importance, and the crack density parameter should be revised accordingly.

Thus, identification of the proper microstructural parameters hinges on the analysis of an *individual inhomogeneity contribution to the considered property*. This is a challenging task: it involves analyses of various shape factors, since inhomogeneities in realistic microstructures may have diverse and "irregular" shapes; in anisotropic cases of non-random inhomogeneity orientations, the parameters are tensor ones; if the matrix itself is anisotropic, this further complicates the analysis. Nevertheless, a substantial progress has been made in this direction. It is overviewed in Sections 4 and 5.

The advantages of such an approach—that we call "micromechanical"—are that

- It identifies microstructural features that have a dominant effect on the given property. This leads to quantitative characterization of microstructures, in the context of this property.
- The results cover, in a unified way, *mixtures* of inhomogeneities of diverse shapes and orientations (that are typical for realistic microstructures).
- It leads to explicit cross-property connections between different physical properties, if they are expressed in terms of similar microstructural parameters (elasticity–conductivity connections, for example).

An alternative approach, that attempts to bypass difficulties of the micromechanical analyses, is based on introduction of the so-called "fabric" tensors. It is simply claimed that a tensor (or tensors) of a certain postulated rank is an appropriate characterization of microstructure. This "fabric" tensor is not explicitly linked to the microstructure (or linked in a way that is not based on micromechanical analysis and hence is not unique; it may not properly reflect "relative weights" of various microstructural elements). The effective properties (usually, the elastic ones) are given through general tensor representations that contain a substantial number of uncertain factors. The price paid for bypassing micromechanical analyses is the emergence of the mentioned factors and the fact that the effective properties are not explicitly linked to relevant microstructural features (or the linkage is not unique). This approach is discussed in Section 8.

2. The micromechanical approach. Proper microstructural parameters

A proper microstructural parameters should represent microstructural features in accordance with their actual contributions to the property. This approach—based on individual inhomogeneity contributions to the property—is called "micromechanical" in the present paper.

The micromechanical approach is rooted in a number of classical works. Mackenzie (1950) considered effective elastic properties of a solid with spherical pores, on the basis of individual pore contributions to the overall compliance. Kröner (1958) analyzed the isotropic matrix with anisotropic inhomogeneities of

spherical shapes, and operated with a sphere contribution to the overall property. Hill (1965) considered ellipsoidal inhomogeneities and expressed their contributions to the overall elasticity using Eshelby's results (1957, 1961). Dependencies on the shapes of ellipsoids were worked out in detail by Wu (1966). In the work of Walpole (1969), results were given in a more transparent form and, in the important case of the spheroids, were derived in elementary functions. In the important case of cracks, their contributions to the overall elasticity and conductivity were given by Bristow (1960). A thorough overview of history of the basic ideas of micromechanics was given by Markov (2000).

Remark. A choice of a particular approximate scheme for the overall property—the self-consistent approximation (Hill, 1965; Budiansky, 1965) or other schemes (differential, Mori-Tanaka's)—is non-essential in this context, since they based on placing non-interacting inhomogeneities in a certain "effective environment".

To start the discussion, we overview several well known microstructural parameters and the basic underlying logic. For the ellipsoidal inhomogeneities of *identical shapes* (Hill, 1965) the simplest microstructural parameter—*volume fraction* of inhomogeneities

$$c = \frac{1}{V}\sum_i V^i \tag{1}$$

(V is a representative volume element, RVE) is, obviously, adequate, since the overall properties can be expressed in its terms (with the shape factor as a multiplier).

For *cracks*, their concentration is represented by crack density parameters. For circular randomly oriented cracks (of radii a^i), the *scalar* crack density is (Bristow, 1960):

$$\rho = \frac{1}{V}\sum_i a^{(i)3} \quad \left(\text{in 2-D case, } \rho = \frac{1}{A}\sum_i a^{(i)2}, \text{ crack lengths are } 2a^{(i)}\right) \tag{2}$$

in accordance with the fact that the individual crack contributions to the overall compliance are proportional to their sizes cubed (squared, in 2-D case).

For non-random crack orientations ($\boldsymbol{n}$ is a unit normal to a crack), the scalar crack density was generalized to second rank *crack density tensor* in the work of Kachanov (1980)

$$\boldsymbol{\alpha} = \frac{1}{V}\sum_i (a^3 \boldsymbol{nn})^i \quad \left(\text{in 2-D case, } \boldsymbol{\alpha} = \frac{1}{V}\sum_i (a^2 \boldsymbol{nn})^i\right) \tag{3}$$

($\boldsymbol{nn}$ is the dyadic product—tensor with components $n_k n_l$) where the fourth rank tensor

$$\frac{1}{V}\sum_i (a^3 \boldsymbol{nnnn})^i \tag{4}$$

was also identified as a second (in addition to $\boldsymbol{\alpha}$) crack density parameter, and was shown to play a relatively minor role (provided crack faces are traction free).

The present work focuses on materials that can be described as matrices with inhomogeneities. However, we also mention two microstructures of a different kind for which proper microstructural parameters were identified in classical works.

Continuous distribution of dislocations is described by dislocation density tensor $\boldsymbol{a}$ introduced by Nye (1953). It relates, to an area element $\boldsymbol{n}\mathrm{d}S$, the total Burgers' vector $\mathrm{d}\boldsymbol{b}$ of the dislocation lines crossing this element: $\mathrm{d}\boldsymbol{b} = \boldsymbol{a}\cdot\boldsymbol{n}\mathrm{d}S$. Tensor $\boldsymbol{a}$ is the proper micromechanical parameter because the field of microstresses generated by a continuous distribution of dislocations—the quantity for which $\boldsymbol{a}$ is intended—can be expressed in its terms (Kröner, 1960).

Microstructural characterization of a granular material for conductivity (thermal or electric). For a granular material consisting of spheres of radius R and non-conducting intergranular space, the effective conductivity (in the isotropic case) was expressed by Batchelor and O'Brien (1977) in terms of parameter $\phi NR^{-1}\sqrt{S}$ where ϕ is the volume fraction of spheres, N is the number of contacts per sphere and S is the contact area. This parameter is proper because the product $R^{-1}\sqrt{S}$ correctly represents the contribution of an individual contact to the overall conductivity.

We return now to the main focus of the present work—matrices with inhomogeneities. Microstructural parameters (1)–(3) have certain limitations. Indeed, the volume fraction parameter (1) may become inadequate in the following cases:

- Mixtures of inhomogeneities of *diverse shapes*. The proper microstructural parameters become non-trivial, even in relatively simple cases. This is illustrated by the 2-D example of randomly oriented elliptical holes (see the next section). "Irregularity" of shapes further complicates the matter.
- *Non-randomly oriented* inhomogeneities. The proper parameters are tensor, their rank being a non-trivial matter.

The crack density parameters (2) and (3) may become inadequate in the following cases:

- *Non-planar* cracks.
- Cracks that are *not traction free*, such as sliding cracks constrained against the normal opening—case relevant to the compressive stress conditions (in this case, fourth rank tensor (4) starts to play a major role) or fluid-filled cracks (for which tensor (4) has to be modified, as outlined in Section 4).

For *planar non-circular* cracks, with non-circularities that are random (uncorrelated with crack sizes and orientations), second rank crack density tensor $\boldsymbol{\alpha}$ remains adequate (as indicated by experimental data on cracked rocks, Sayers and Kachanov, 1995). In particular, for the elliptical cracks, as well as for the cracks of annular geometry (containing "islands" of partial contact in the middle), radii a^i of equivalent circular cracks can be explicitly expressed in terms of crack geometries (Kachanov, 1992; Sevostianov and Kachanov, 2002b).

Broadening materials science applications increasingly address more complex microstructures—both man-made and naturally occurring. Examples are: cortical bone (several systems of pores of diverse geometries and orientations); various sprayed materials (strongly oblate, crack-like pores, mixed with pores of more or less round shapes); various reinforced composites that, in addition to embedded inhomogeneities, may develop microcracks or micropores; geological materials.

In such cases, identification of the proper microstructural parameters is a non-trivial problem. It appears unavoidable, though: in order to explicitly express the effective properties in terms of microstructural parameters, these parameters should correctly represent relevant microstructural features.

Remark. For some simple microstructures of *fixed microgeometries*, the simplest scalar microstructural parameters—porosity, crack density—may be sufficient. For example, for two families of spheroids of diverse properties, all of them strictly parallel, the effective properties can be expressed in terms of their partial volume fractions (Taya and Chou, 1981). As another example, for several families of strictly parallel circular cracks, the effective properties can be expressed in terms of the partial scalar crack densities, plus angles between the families (Piau, 1980). The limitation of such expressions is that they are restricted to the particular geometries considered. If, for instance, an orientation scatter is introduced into examples above, the concentration parameters should become tensor.

In literature, much attention has been paid to construction of various approximate schemes for the dependencies

$$\text{effective property} = f\left(\underbrace{\text{microstructural parameter}}_{?}\right) \tag{5}$$

However, the problem of identifying the *argument* of this function has received much less attention.

Identification of the proper microstructural parameters is most challenging in the context of the *elastic* properties, and this is the focus of the present work. In this context, we assume that the solid is subjected to "remotely imposed" stress $\boldsymbol{\sigma}$ that, in the absence of inhomogeneities, would have been uniform within representative volume V (homogeneous boundary conditions, Hashin, 1983).

Remark. The effective properties considered here are *linear* elastic. This may present a limitation in the case of compressive loading applied to a solid with narrow, crack-like pores: the linear elasticity results are applicable if the pores are not closed by compressive stresses, as determined by the magnitude of compressive stresses in relation to the initial pore opening (pores of the ellipsoidal shapes close at once, as the critical stress is reached; non-ellipsoidal pores close gradually as compressive stress increases, see, for example, results of Mavko and Nur (1978) for 2-D oblate non-elliptical pores).

The problem of effective elastic properties is best formulated in terms of elastic potential in stresses $f(\boldsymbol{\sigma})$, the effective compliances S_{ijkl} being obtained by differentiation: $\varepsilon_{ij} = S_{ijkl}\sigma_{kl} = \partial f/\partial\sigma_{ij}$. Representing $f(\boldsymbol{\sigma})$ as a sum

$$f = f_0 + \Delta f \tag{6}$$

where f_0 is the potential in the absence of inhomogeneities, we reduce the problem to finding the change of potential Δf due to inhomogeneities. Further, we represent Δf as a sum of terms corresponding to individual inhomogeneities

$$\Delta f = \sum \Delta f^i = \frac{1}{2}\boldsymbol{\sigma} : \sum \boldsymbol{H}^i : \boldsymbol{\sigma} \tag{7}$$

where $\boldsymbol{H}^i$ is a fourth rank *compliance contribution tensor* of i-th inhomogeneity. Treating an inhomogeneity as an *isolated* one allows one to calculate $\boldsymbol{H}$-tensors for a number of 2-D and 3-D shapes (Kachanov et al., 1994; Sevostianov and Kachanov, 2002a). These results serve as a basic building block for the non-interaction approximation, as well as for a number of approximate schemes (self-consistent, differential, Mori-Tanaka's) that place an inhomogeneity into some sort of effective homogenized environment.

Remark. Although the formulations in potentials and in compliances are equivalent, the potentials formulation has the advantage that *the structure of potential Δf identifies the proper microstructural parameters: the sum*

$$\sum \boldsymbol{H}^i \tag{8}$$

(subject to symmetrization implied by potential (7)) *is the general expression for the proper microstructural parameter*.

The advantage of the general form (8) is that it covers, in a unified way, various mixtures of inhomogeneities of diverse shapes and orientations. Various forms taken by this sum and possible simplifications (notably, the possibility to replace it by second rank tensors) are discussed in Section 4.

Remark. In the work of Johannesson and Pedersen (1998), it was suggested to average *Eshelby's tensor* (rather than $\boldsymbol{H}$-tensors) over orientations. That Eshelby's tensor is not the quantity to be averaged, is seen from the isotropic case of random orientations: in this case, the averaged Eshelby's tensor is isotropic and coincides with the one for a certain concentration of *spheres*. However, the effective elastic properties may differ substantially from those of a material with spheres: it is generally impossible to match *both* effective isotropic constants by a certain distribution of spheres (see a simple 2-D example of randomly oriented

elliptical holes, Section 4 and Kachanov et al. (1994) for a more general discussion). In other words, averaged Eshelby's tensor is not a proper microstructural parameter.

Thus, identification of micromechanically based parameters involves the following two steps:

- Finding the contribution of one isolated inhomogeneity to the property considered. In cases of irregularly shaped inhomogeneities or anisotropic matrices, this is a challenging problem.
- Summation over inhomogeneities (can be replaced by integration over orientations or over shape factors, if computationally convenient).

3. Microstructural parameters are rooted in the non-interaction approximation

The individual inhomogeneity contributions to the overall property are affected by *interactions* between them. Consider, for example, an elastic solid with parallel circular cracks of radius a that are either (A) coplanar or (B) stacked. In case (A), crack contributions to the overall compliance in the normal direction depend on a stronger than a^3 (amplifying interactions); in case (B)—weaker than a^3 (shielding interactions).

Strictly speaking, interactions should be incorporated into the proper microstructural parameter, since it should correctly reflect "relative weights" of individual inhomogeneities. The effective property would then be a linear function of such a parameter. The latter would depend on mutual positions of inhomogeneities and would reflect the interaction mechanics.

Such an approach—incorporating interactions into a microstructural parameter—may not be practical in general. However, it may be realized in some cases. For illustration, we outline one such possibility for a material with interacting cracks. Assuming that the average displacement discontinuity on a crack (that determines the contribution of a crack to the overall compliance) is proportional to the average traction on it—usually, a good approximation—crack interactions can be accounted for by a simple method suggested by Kachanov (1987) and incorporated into the crack density parameter, as follows. We introduce $\boldsymbol{\Lambda}$-factors that characterize interactions between cracks in the "average" sense: second rank tensor $\boldsymbol{\Lambda}^{(ij)}$ gives the average traction vector generated along the site of jth crack (in a continuous material) by a uniform unit traction of an arbitrary direction on ith crack. Calculation of $\boldsymbol{\Lambda}$-factors reduces to integration of elementary functions—fields generated by uniformly loaded cracks—along crack surfaces (lines, in 2-D).

The $\boldsymbol{\Lambda}$-factors characterize *those features of the crack array geometry that produce a dominant effect on interactions*. The proper crack density parameter can be expressed in their terms. In the 2-D case of rectilinear cracks, this yields elastic potential in the form

$$\Delta f = (\pi/E_0)\boldsymbol{\sigma} : \boldsymbol{\omega} : \boldsymbol{\sigma} \tag{9}$$

where fourth rank tensor

$$\boldsymbol{\omega} = \frac{1}{A}\sum_{i,k} l^{(k)2}\boldsymbol{n}^k\boldsymbol{\Omega}^{(ki)}\boldsymbol{n}^i \tag{10}$$

emerges as the proper crack density parameter that accounts for interactions; it contains second rank tensor $\boldsymbol{\Omega}^{(ij)} = [\delta_{ij}\boldsymbol{I} - \boldsymbol{\Lambda}^{(ij)}]^{-1}$. This scheme can be extended to the 3-D case of circular cracks. If the interactions are neglected, $\boldsymbol{\Omega}^{(ij)} = \delta_{ij}\boldsymbol{I}$ so that $\boldsymbol{\sigma} : \boldsymbol{\omega} : \boldsymbol{\sigma} = \boldsymbol{\sigma} \cdot \boldsymbol{\sigma} : \boldsymbol{\alpha}$ and potential in terms of crack density tensor $\boldsymbol{\alpha}$, given by (3), is recovered.

Crack density parameter $\boldsymbol{\omega}$ incorporates those features of the crack array geometry that are relevant to the interaction mechanics. Note that potential Δf and, hence, the effective compliances are linear in $\boldsymbol{\omega}$. Parameter $\boldsymbol{\omega}$ is defined for a deterministic crack array; an appropriate statistical averaging would

be needed, to incorporate the statistical information of cracks. This is a non-trivial task (particularly in 3-D).

Generally, incorporating interactions into the concentration parameter may not be a practical approach—it amounts to solving the interaction problem. Therefore, microstructural parameters usually ignore the interactions, and contributions of individual inhomogeneities are taken by treating them as *isolated* ones (in particular, the parameters do not reflect the mutual positions of inhomogeneities). The effect of interactions on the effective properties is then addressed through a non-linear dependence of the property on the parameter—the one that is defined in the non-interaction approximation.

Although this approach is more practical, it has certain limitations:

- The effective property is, generally, a non-unique function of a microstructural parameter (with the exception of the non-interaction approximation). This may be acceptable if sufficiently narrow bounds can be constructed for this function—which is not always the case (cracks, or strongly oblate pores are examples).
- An attempt to incorporate the statistics of mutual positions of inhomogeneities, while retaining the microstructural parameter that does not reflect them, may or may not be realizable. Consider, for example, a periodic arrangement of diverse inhomogeneities (diverse shapes or orientations). It is not clear, a priori, whether the effective properties can be represented in terms of the product (usual microstructural parameter, rooted in the non-interaction approximation)×(periodicity parameter).

The present work focuses on the microstructural parameters rooted in the non-interaction approximation (obtained by summing the contributions of individual inhomogeneities—treated as isolated ones—to overall property). They are rigorously proper for the non-interaction approximation, as well as for a number of approximate schemes (self-consistent, differential, Mori-Tanaka's) that place an inhomogeneity into an effective homogenized environment.

In this framework, the main challenge is to properly incorporate shapes and orientations of the inhomogeneities. This will produce microstructural parameters that cover, in a unified way, mixtures of diverse inhomogeneities.

4. Elastic solids with various inhomogeneities: proper microstructural parameters and effective properties

The proper microstructural parameters will be identified, in a systematic way, through the structure of the elastic potential Δf. (As discussed above, the parameters are rooted in the non-interaction approximation, hence, Δf will be given in this approximation.) The proper parameters may be non-trivial, even in the cases of overall isotropy. This is best illustrated by a 2-D case of randomly oriented elliptical holes. We demonstrate the benefits gained by identifying the proper parameters—in particular, clarification of the overall anisotropy and of the importance of various microstructural features.

Representative volume is denoted by V and representative area (in 2-D case)—by A.

4.1. Two-dimensional solid with rectilinear cracks

Denoting crack lengths by $2a^i$ and unit normals to cracks by $\boldsymbol{n}^i$ the strain per representative area A has the form

$$\boldsymbol{\varepsilon} = \boldsymbol{S}^0 : \boldsymbol{\sigma} + \underbrace{\frac{1}{A}\sum_i \frac{1}{2}(\boldsymbol{bn} + \boldsymbol{nb})^i 2a^i}_{\Delta\boldsymbol{\varepsilon}} \tag{11}$$

where the sum (over all cracks in A) is the extra strain $\Delta\boldsymbol{\varepsilon}$ due to cracks; this sum may be replaced by integration over orientations, if computationally convenient; $\boldsymbol{S}^0$ is the compliance tensor of the bulk material. Vector $\boldsymbol{b} = \langle \boldsymbol{u}^+ - \boldsymbol{u}^- \rangle$ is the average displacement discontinuity on a crack. Representation (11), as well as its extension to pores, in terms of surface integrals over the pore boundaries $\int(un + nu)\,\mathrm{d}S$, is an immediate consequence of a footnote remark of Hill (1963); in the explicit form, it was given, for example, by Vavakin and Salganik (1975).

The following fact is of a key importance: for each crack, vector $\boldsymbol{b}$ is parallel to $\boldsymbol{n}\cdot\boldsymbol{\sigma}$

$$\boldsymbol{b} = \frac{\pi a}{E_0}\boldsymbol{n}\cdot\boldsymbol{\sigma} \tag{12}$$

where E_0 is 2-D Young's modulus (that coincide with 3-D one for plane stress and, for plane strain, can be obtained from 3-D one by dividing it over $(1-\nu^2)$ where ν is 3-D Poisson's ratio). This follows from equality of crack compliances in the normal and shear modes: if p and τ are uniform normal and shear tractions applied to crack faces, then the corresponding average displacement discontinuities are

$$\left.\begin{matrix} b_n \\ b_\tau \end{matrix}\right\} = \frac{\pi a}{E_0}\left\{\begin{matrix} p \\ \tau \end{matrix}\right. \tag{13}$$

with the *same* proportionality coefficient $\pi a/E_0$.

The proportionality (12) implies that the change of elastic potential Δf due to multiple cracks of diverse orientations and sizes is

$$\Delta f = \frac{1}{2}\boldsymbol{\sigma} : \Delta\boldsymbol{\varepsilon} = \frac{1}{A}\sum_i \boldsymbol{n}^i\cdot\boldsymbol{\sigma}\cdot\boldsymbol{b}^i a^i = \frac{\pi}{E_0}(\boldsymbol{\sigma}\cdot\boldsymbol{\sigma}) : \frac{1}{A}\sum_i (a^2\boldsymbol{nn})^i = \frac{\pi}{E_0}(\boldsymbol{\sigma}\cdot\boldsymbol{\sigma}) : \boldsymbol{\alpha} \tag{14}$$

thus identifying the crack density tensor (3) as the proper parameter of crack density. We emphasize that tensor $\boldsymbol{\alpha}$ is not introduced a priori, but is *implied by the structure of* Δf.

Tensor $\boldsymbol{\alpha}$ is a natural generalization of the scalar crack density ρ. Its linear invariant $\mathrm{tr}\,\boldsymbol{\alpha} = \rho$; for randomly oriented cracks $\boldsymbol{\alpha} = (1/2)\rho\boldsymbol{I}$, where $\boldsymbol{I}$ is the unit tensor.

For any particular fixed orientation distribution of cracks, the effective compliances can be found, of course, without using $\boldsymbol{\alpha}$—in terms of the overall scalar crack density ρ plus parameters of this specific distribution. The advantage of using tensor $\boldsymbol{\alpha}$ is that it yields a *unified* result with respect to all orientation distributions. For example, in the case of a preferential orientation with some scatter, the latter is incorporated in $\boldsymbol{\alpha}$.

Another advantage of using $\boldsymbol{\alpha}$ is that it identifies the *overall anisotropy* due to cracks: it is orthotropy (its principal axes being coaxial to the ones of $\boldsymbol{\alpha}$), since $\boldsymbol{\alpha}$ is a symmetric second rank tensor. This result is not trivial and may even seem counterintuitive, since it applies to *any* orientation distribution of cracks (for example, to two families of parallel cracks inclined at an arbitrary angle to each other). Moreover, the orthotropy is of a rather special type—the number of independent elastic constants is reduced and their orientation dependence is simplified (Kachanov, 1980).

The possibility to characterize an arbitrary field of cracks by a symmetric second rank tensor $\boldsymbol{\alpha}$, without involving tensors of higher ranks, is due to equality of the normal and shear crack compliances (13). Therefore, the possibility to retain $\boldsymbol{\alpha}$ as the *sole* crack density parameter in more complex situations (3-D cracks, sliding closed cracks, fluid-filled cracks) depends on *whether this equality continues to hold.* If it is violated, a fourth rank tensor may emerge as a second (in addition to $\boldsymbol{\alpha}$) crack density parameter. Its importance (more precisely, the value of a factor at the term containing this tensor) depends on the extent of the violation. This is illustrated by the examples to follow.

4.2. Three-dimensional solid with cracks

For a circular (penny shaped) crack, of radius a, the normal and the shear compliances are not equal. However, they are relatively close, differing by a factor of $1 - \nu_0/2$ (ν_0 is Poisson's ratio of the matrix). This yield the following expression for Δf (Kachanov, 1980):

$$\Delta f = \frac{16(1-\nu_0^2)}{3(2-\nu_0)E_0}\left[(\boldsymbol{\sigma}\cdot\boldsymbol{\sigma}):\boldsymbol{\alpha} - \frac{\nu_0}{2}\boldsymbol{\sigma}:\frac{1}{V}\sum_i (a^3\mathbf{nnnn})^i:\boldsymbol{\sigma}\right] \tag{15}$$

thus identifying the fourth rank tensor $(1/V)\sum(a^3\mathbf{nnnn})^i$ as a second (in addition to $\boldsymbol{\alpha}$) crack density parameter. However, its overall impact is, typically, relatively small, due to a relatively small multiplier $\nu_0/2$ at the second term. It can be made even smaller by assigning the same (average) value to both the normal and the shear crack compliances. Thus, retaining $\boldsymbol{\alpha}$ as the *sole* crack density parameter constitutes a good approximation.

Cracks of the *elliptical* shape can be well approximated, in their impact on Δf, by certain equivalent circular cracks, provided the deviations from circularity are random, i.e. not correlated with crack sizes and orientations (see results of Kachanov, 1992 based on calculations of Budiansky and O'Connell, 1976). For cracks of *general irregular shapes* (with random irregularities), experimental data on anisotropic wave patterns in cracked rocks indicates that the normal and the shear crack compliances are, on average, quite close (Sayers and Kachanov, 1995). Therefore, characterization of such crack arrays solely by the second rank tensor $\boldsymbol{\alpha}$ constitutes a good approximation.

4.3. Three-dimensional solid with sliding cracks constrained against the normal opening (''closed'' cracks)

In this case (relevant for the compressive loading conditions), the equality of normal/shear compliances (13) is, obviously violated—the normal compliance is zero. Here, we consider frictionless (''lubricated'') cracks, so that potential Δf exists (results for a more general case of *frictional* sliding, involving stress induced anisotropy and loading path-dependence, were given by Kachanov (1982a,b)). Then potential

$$\Delta f = \frac{16(1-\nu^2)}{3(2-\nu)E}\left[(\boldsymbol{\sigma}\cdot\boldsymbol{\sigma}):\boldsymbol{\alpha} - \boldsymbol{\sigma}:\frac{1}{V}\sum_i (a^3\mathbf{nnnn}^i:\boldsymbol{\sigma})\right] \tag{16}$$

has the same form as (15), but *without* the small factor of $\nu_0/2$ at the second term. Hence, contributions of $\boldsymbol{\alpha}$ and fourth rank tensor (4) are comparable and *both* tensors should be retained as crack density parameters. This, obviously, violates the overall orthotropy.

4.4. Fluid-filled crack-like pores (strongly oblate spheroids)

We consider the ''undrained'' case (fluid mass in each pore remains constant during deformation). The presence of fluid does not affect the shear crack compliances (assuming no viscosity), whereas the normal crack compliances are reduced.

For a crack with the initial (prior to loading) average aspect ratio ξ, the impact of the fluid on the effective elastic response depends on the dimensionless parameter $\delta = \kappa E_0 \xi$ (it is similar to the one introduced by Budiansky and O'Connell (1976)), where κ is the fluid compressibility. The impact of the fluid increases as δ decreases. For different cracks, ξ's and, therefore, δ's may be different.

Potential Δf has the form (Kachanov, 1994):

$$\Delta f = \frac{16(1-\nu_0^2)}{3(2-\nu_0)E_0}\left[(\boldsymbol{\sigma}\cdot\boldsymbol{\sigma}):\boldsymbol{\alpha} - \boldsymbol{\sigma}:\frac{1}{V}\sum_i\left(\frac{2+\nu_0\delta}{2(1+\delta)}a^3\boldsymbol{nnnn}\right)^i:\boldsymbol{\sigma}\right] \tag{17}$$

It covers, in a unified way, various mixtures of crack-like pores of diverse aspect ratios and orientations. The limit of $\delta^i \to 0$ corresponds to closed sliding (frictionless) cracks (17); the opposite limit of $\delta^i \to \infty$ corresponds to "dry" freely opening cracks (15).

Thus, the structure of the elastic potential identifies fourth rank tensor

$$\frac{1}{V}\sum_i\left(\frac{2+\nu_0\delta}{2(1+\delta)}a^3\boldsymbol{nnnn}\right)^i \tag{18}$$

as a second (in addition to $\boldsymbol{\alpha}$) crack density parameter. This parameter—that is not easily identifiable without the micromechanical analysis—reflects the fact that the individual contributions of crack-like pores depend on their aspect ratios. This is in contrast with "dry" cracks, where, for strongly oblate shapes there is no such dependence.

Only in the case when *aspect ratios are identical* for all cracks, a common multiplier $(1+\nu_0\delta/2)/(1+\delta)$ can be taken out of the sum as a parameter. This case (considered by Budiansky and O'Connell, 1976; Piau, 1980) seems to be of a limited applicability, though—crack aspect ratios (small but finite) may be as diverse as the crack radii.

Remark. The above results can be further extended to general ellipsoidal pores filled with compressible fluid (Shafiro and Kachanov, 1997).

4.5. Anisotropic two-dimensional solid with cracks of arbitrary orientations

Analyses of Mauge and Kachanov (1994b) and Tsukrov and Kachanov (2000) show that, for a 2-D orthotropic material with arbitrarily oriented cracks,

$$\Delta f = \boldsymbol{\sigma}:\frac{1}{A}\sum_i(a^2\boldsymbol{nBn})^i:\boldsymbol{\sigma} \tag{19}$$

where $\boldsymbol{B}$ is a symmetric second rank *crack opening displacement tensor* (or COD tensor of a crack), that relates (normalized) vector $\overline{\boldsymbol{b}} = \boldsymbol{b}/a$ of the average displacement discontinuity to the vector of uniform traction $\boldsymbol{t}$ of an arbitrary direction applied on the crack:

$$\overline{\boldsymbol{b}} = \boldsymbol{B}\cdot\boldsymbol{t} \tag{20}$$

For the *isotropic* matrix, $\boldsymbol{B} = (\pi/E_0)\boldsymbol{I}$ recovering collinearity (12) of $\boldsymbol{b}$ and $\boldsymbol{t}$. For the *orthotropic* matrix,

$$\boldsymbol{B} = \frac{\pi C}{2}(1+D)\boldsymbol{e}_1\boldsymbol{e}_1 + \frac{\pi C}{2}(1-D)\boldsymbol{e}_2\boldsymbol{e}_2 \tag{21}$$

where

$$D = (\sqrt{E_1}-\sqrt{E_2})/(\sqrt{E_1}+\sqrt{E_2}); \qquad C = \frac{1}{2}\frac{\sqrt{E_1}+\sqrt{E_2}}{\sqrt{E_1E_2}}\sqrt{\frac{1}{G_{12}} - \frac{2\nu_{12}}{E_1} + \frac{2}{\sqrt{E_1E_2}}}$$

and E_1, E_2, G_{12}, ν_{12} are Young's and shear moduli and Poisson's ratio of the matrix in the principal axes of orthotropy x_1x_2. Thus, $\boldsymbol{B}$ is independent of a crack orientation $\boldsymbol{n}$ (the deviation from collinearity of vectors $\boldsymbol{t}$ and $\boldsymbol{b}$ is the same for cracks of all orientations). This, somewhat unexpected, constancy of $\boldsymbol{B}$ allows one to transform the potential (19) to the form

$$\Delta f = (\boldsymbol{\sigma}\cdot\boldsymbol{B}\cdot\boldsymbol{\sigma}) : \frac{1}{A}\sum (a^2\boldsymbol{nn})^i = (\boldsymbol{\sigma}\cdot\boldsymbol{B}\cdot\boldsymbol{\sigma}) : \boldsymbol{\alpha} \tag{22}$$

identifying, again, second rank crack density tensor $\boldsymbol{\alpha}$ as the *sole* crack density parameter.

Without the micromechanical analysis, it would be difficult to foresee the result (22) and sufficiency of $\boldsymbol{\alpha}$: they follow from a (somewhat unexpected) independence of $\boldsymbol{B}$ on crack orientation $\boldsymbol{n}$. Whether this independence holds for the 3-D anisotropic material with cracks, or for a 2-D material with anisotropy more complex than orthotropy, remains an open question. If it does not hold, reduction to $\boldsymbol{\alpha}$ is not possible, and one would have to revert to fourth rank tensor $(1/V)\sum (a^3\boldsymbol{nBn})^i$ as the proper crack density parameter.

Additional insights implied by (22) are as follows:

- Stress $\boldsymbol{\sigma}$ enters (22) through $\boldsymbol{\sigma}\cdot\boldsymbol{B}\cdot\boldsymbol{\sigma}$ (rather than through $\boldsymbol{\sigma}\cdot\boldsymbol{\sigma}$, as in the case of the isotropic matrix). Hence, not only the crack orientations $\boldsymbol{n}$ with respect to $\boldsymbol{\sigma}$ matter (they enter through crack density tensor $\boldsymbol{\alpha}$), but, also, their orientations with respect to the matrix orthotropy axes. For example, a crack normal to the "stiffer" direction of the matrix produces a larger contribution to the overall compliance than a crack of the same size normal to the "softer" direction.
- Of the four independent elastic constants of a 2-D orthotropic matrix, only two combinations of them, C and D, enter potential Δf.
- Since D is independent of the shear modulus G_{12}, for a matrix of *cubic symmetry* ($E_1 = E_2$, but G_{12} is an independent constant), $\boldsymbol{B}$-tensor is proportional to $\boldsymbol{I}$, i.e. the normal and the shear crack compliances are equal—as for the *isotropic* matrix.

4.6. Two-dimensional isotropic matrix with elliptical holes

This is an important example: it demonstrates that, even in a relatively simple special case of isotropy (randomly oriented ellipses), the proper microstructural parameters are non-trivial.

We consider a mixture of elliptical holes of diverse eccentricities and orientations; $2a$ and $2b$ are ellipses' axes and $\boldsymbol{m}$, $\boldsymbol{n}$—unit vectors along them, correspondingly. In the general anisotropic case (arbitrary orientation distribution), potential Δf, given by Tsukrov and Kachanov (2000) and Kachanov et al. (1994), has the form

$$\Delta f = \frac{1}{2E}\{[2\boldsymbol{\sigma}:\boldsymbol{\sigma} - (\operatorname{tr}\boldsymbol{\sigma})^2]p + 2(\boldsymbol{\sigma}\cdot\boldsymbol{\sigma}) : \boldsymbol{\beta}\} \tag{23}$$

where

$$\left.\begin{aligned} p &= \frac{1}{A}\pi\sum_i (ab)^i \qquad \text{(2-D porosity)} \\ \boldsymbol{\beta} &= \frac{1}{A}\pi\sum_i (a^2\boldsymbol{nn} + b^2\boldsymbol{mm})^i \quad \text{(second rank hole density tensor)} \end{aligned}\right\} \tag{24}$$

thus identifying $(p, \boldsymbol{\beta})$ as the proper microstructural parameters. In the limit of *cracks* (all $b^i = 0$), $p = 0$ and tensor $\boldsymbol{\beta}/\pi$ reduces to the crack density tensor $\boldsymbol{\alpha}$. Note that no degeneracies or indeterminate ratios emerge in this limit. In the case of *circles* ($a^i = b^i$), $\boldsymbol{\beta} = p\boldsymbol{I}$ ($\boldsymbol{I}$ is 2-D unit tensor) thus identifying porosity p as the sole microstructural parameter. The general representation (23) covers all mixtures of diverse ellipses in a unified way (for example, a mixture of circular holes and cracks).

Proper concentration parameters are non-trivial even in the *isotropic case of randomly oriented ellipses*. In this case, $\boldsymbol{\beta} = (1/A)(\pi/2)\sum (a^2 + b^2)^i\boldsymbol{I}$ and the structure of Δf implies that parameters $(p, \boldsymbol{\beta})$ can be replaced by two scalars: p and the *average eccentricity*

$$q = \frac{1}{A}\pi \sum (a^i - b^i)^2 \tag{25}$$

In the limit of cracks, q/π reduces to the conventional crack density (2).

A further non-trivial result pertaining to this case is that two effective elastic moduli—for example, Young's modulus and bulk modulus—are expressed in terms of *different combinations* of (p, q):

$$E_{\text{eff}} = \frac{E_0}{1 + 3p + q}; \qquad K_{\text{eff}} = \frac{K_0(1 - v_0)}{1 - v_0 + 2p + q} \tag{26}$$

where 2-D elastic moduli E_0 and v_0 coincide with 3-D ones for plane stress; in the case of plane strain, E_0 and v_0 are obtained from 3-D ones by dividing them over $(1 - v^2)$ and $(1 - v)$, respectively, where v is 3-D Poisson's ratio. Two-dimensional bulk modulus K_0 is related to 2-D E_0 and v_0 by $K_0 = E_0/(2 - 2v_0)$. This has an interesting implication: if one wants to plot E_{eff} and K_{eff} in terms of a single microstructural parameter, this parameter will be *different* for the two moduli ($3p + q$ and $2p + q$, correspondingly).

4.7. Two-dimensional orthotropic matrix with elliptical holes of arbitrary orientations

This problem unifies the two cases considered above—the *isotropic* matrix with elliptical holes and the orthotropic matrix with cracks. In this case (Tsukrov and Kachanov, 2000), the proper concentration parameter $\sum \boldsymbol{H^i}$ can be specified as to explicitly reflect ellipses' geometries and the matrix anisotropy. This yields some non-trivial insights. For example, the effect of circular holes is anisotropic (the potential Δf is anisotropic); the compliance contribution of the elliptical hole can be represented as a sum of compliances of a circular hole and two cracks.

4.8. Three-dimensional solid with ellipsoidal inhomogeneities

For the ellipsoids of diverse shapes and orientations, $\boldsymbol{H}$-tensors that enter the proper parameter of inhomogeneities' concentration $\sum \boldsymbol{H^i}$ can be expressed in terms of inhomogeneities' Eshelby's tensors s_{ijkl}:

$$H_{ijkl} = \frac{V_*}{V}\left[(S^*_{ijkl} - S^0_{ijkl})^{-1} + C^0_{ijmn}(J_{mnkl} - s_{mnkl})\right]^{-1} \tag{27}$$

where $J_{ijkl} = (\delta_{ik}\delta_{lj} + \delta_{il}\delta_{kj})/2$ is the fourth rank unit tensor, C_{ijmn} and S_{mnkl} are stiffness and compliance tensors, correspondingly. The properties of the inclusion and of the matrix are denoted by an asterisk and by "0", respectively.

We note that a tensor that is dual to the compliance contribution tensor $\boldsymbol{H}$ can be introduced—a stiffness contribution tensor $\boldsymbol{N}$ that enters the change (due to inhomogeneities) in the elastic potential in strains $g(\boldsymbol{\varepsilon})$:

$$g = g_0 + \Delta g = g_0 + \frac{1}{2}\boldsymbol{\varepsilon} : \sum \boldsymbol{N^i} : \boldsymbol{\varepsilon} \tag{28}$$

Tensor $\boldsymbol{N}$ of an inhomogeneity is related to Eshelby's tensor as follows:

$$N_{ijkl} = \frac{V_*}{V}\left[(C^*_{ijkl} - C^0_{ijkl})^{-1} + s_{ijmn}S^0_{mnkl}\right]^{-1} \tag{29}$$

In the case of small concentration of inhomogeneities, the two potentials, $f(\boldsymbol{\sigma})$ and $g(\boldsymbol{\varepsilon})$, yield the same effective elastic constants. In the case of finite concentration, there appears to be no rigorous criterion for preferring one of the two potentials to the other. A seemingly reasonable suggestion is as follows: the choice between potentials is made in such a way as to ensure that its change, Δf or Δg, due to inhomogeneities is a positive definite function (of $\boldsymbol{\sigma}$ or $\boldsymbol{\varepsilon}$, correspondingly). For pores, for example, potential $f(\boldsymbol{\sigma})$ and $\boldsymbol{H}$-tensors are to be used, whereas for rigid inclusions the choice is $g(\boldsymbol{\varepsilon})$ and $\boldsymbol{N}$-tensors. This recipe would be a sufficient

(although not a necessary) condition for the *entire* potential ($f = f_0 + \Delta f$ or $g = g_0 + \Delta g$) to remain positive definite for any approximate scheme based on "one-particle" approximation (self-consistent, differential, Mori-Tanaka's).

In the case of identical shapes and random orientations, the general tensor parameter $\sum \boldsymbol{H}^i$ can be replaced simply by a volume fraction (Hill, 1965), with the shape factor as a multiplier; in the case of two families of spheroids (of two different shapes), all of them parallel, it can be replaced by partial volume fractions, with shape factors as multipliers (Taya and Chou, 1981). A somewhat surprising simplification is possible for the *spheroidal* shapes (of arbitrary distribution over orientations and aspect ratios), as outlined in the text to follow.

4.9. Inhomogeneities of the spheroidal shapes

An unexpected simplification is possible for spheroids (as compared to general ellipsoids): for an arbitrary mixture of spheroids of diverse aspect ratios and orientations, the general fourth rank tensor parameter $\sum \boldsymbol{H}^i$ can be replaced, with some approximation, by a symmetric second rank tensor. More precisely, terms $\boldsymbol{\sigma} : \sum \boldsymbol{H}^i : \boldsymbol{\sigma}$ in potential Δf can be replaced by terms of the form $\boldsymbol{\sigma} \cdot \boldsymbol{\sigma} : \boldsymbol{\Omega}$ where $\boldsymbol{\Omega}$ is a certain second rank tensor.

The accuracy of this approximation is generally good for pores (Shafiro and Kachanov, 1999). For spheroids of different elastic properties, the accuracy is good in most cases, although it worsens considerably for the case when contrast (with the matrix) in the bulk moduli is very different from the one for the shear moduli (Sevostianov and Kachanov, 2002a). The possibility of such a replacement has important consequences of physical character: (1) it implies the overall orthotropy (for any orientation distribution), and (2) it makes it possible to establish explicit elasticity–conductivity cross-property connections.

4.10. Pores of strongly oblate shapes (aspect ratios smaller than 0.10–0.15)

Such pores are frequent in many microstructures (rocks and sprayed coatings being examples). The key result is that their effect on the elastic and conductive properties is very close to the one of cracks. Therefore, they can be replaced by cracks and characterized by the crack density parameters. An important consequence is that porosity is an irrelevant parameter for such microstructures. Yet another implication concerns processing of microphotographical data: information on pore aspect ratios is unnecessary.

5. Inhomogeneities of irregular shapes

Being frequent in actual microstructures, such inhomogeneities do not always resemble ellipsoids, even approximately. This calls for analyses of relative importance of various "irregularity factors". This difficult, and largely incomplete, task needs both the theoretical guidance and numerical studies.

5.1. Applications of Hill's theorem

One of the basic theoretical tools is given by the comparison (or "auxiliary") theorem of Hill (1965). He formulated it in energy terms; we rephrase it here in terms of compliances/stiffnesses. The theorem focuses on changes in the effective properties of a material with inhomogeneities caused by replacing their shapes by the inscribed/circumscribed ones.

In the context of matrices with inhomogeneities, the theorem's statement is as follows. Let $\boldsymbol{C}^0$, $\boldsymbol{S}^0$ and $\boldsymbol{C}^*$, $\boldsymbol{S}^*$ be stiffness/compliance tensors of the matrix and of the inhomogeneities, correspondingly (both, generally, anisotropic), and $\boldsymbol{\omega}$—the space occupied by all inhomogeneities. To be specific, we assume that the material of inhomogeneities is 'softer' than the one of the matrix; more precisely, that eigenvalues of the 6×6 matrix $S^*_{ijkl} - S^0_{ijkl}$ are non-negative (or, equivalently, that eigenvalues of the matrix $C^*_{ijkl} - C^0_{ijkl}$ are non-positive). Let us enlarge $\boldsymbol{\omega}$ (some of the inhomogeneities are replaced by *circumscribed* ones). Then the effective properties become 'softer': eigenvalues of the change $\Delta S^{\text{eff}}_{ijkl}$ are non-negative. The opposite inequality signs will hold, of course, if $\boldsymbol{\omega}$ is shrunk (some of the inhomogeneities are replaced by *inscribed* ones).

Remark. In the case when the matrix and the inhomogeneities have the same type of elastic anisotropy and their anisotropy axes coincide, non-negative eigenvalues of the difference in the compliance tensor $\boldsymbol{S}^* - \boldsymbol{S}^0$ imply that eigenvalues of $\boldsymbol{S}^* \geqslant$ eigenvalues of $\boldsymbol{S}^0$ (with a similar statement for the stiffness tensor).

In the isotropic case (both the matrix and the inhomogeneities are isotropic and inhomogeneity shapes/orientation distribution are such that the overall properties are isotropic), assuming, for example, for the shear and bulk moduli, that $\mu_{\text{inhomogeneity}} < \mu_{\text{matrix}}$, $K_{\text{inhomogeneity}} > K_{\text{matrix}}$, Hill's theorem implies that enlargement of inhomogeneities results in decrease of μ_{eff} and increase in K_{eff}.

Taking the "comparison" circumscribed/inscribed shapes as ellipsoids generates bounds that can be explicitly calculated. The bounds are tight in the important case of irregularly shaped inhomogeneities of the strongly oblate type, since the compliance/stiffness contribution tensors of strongly oblate ellipsoids are only weakly dependent on the aspect ratio, In general, however, the bounds formed by ellipsoids may be wide and hence less useful (particularly in the case of strongly concave shapes).

A further step in using Hill's theorem can be suggested as follows. The space in-between the original shape and the circumscribed/inscribed ellipsoids is filled with smaller ellipsoids, with their contributions subtracted/added. However, as demonstrated on *cracks* of irregular shapes, the resulting narrowing of the bounds may be only moderate (Sevostianov and Kachanov, 2002b), due to a strong effect of the remaining ligaments.

Hill's theorem has useful implications of general character:

- Slight "jaggedness" of inhomogeneity boundaries can be ignored, as far as the effective properties are concerned. (In case of crack-like pores, "jaggedness" is unimportant only if does not produce contacts between crack faces, say, under compressive loading.)
- It is unimportant whether "corner" points of inhomogeneities are sharp or blunted, since this difference can be tightly bounded.
- The difference between the convex and the concave shapes (of the same volume) cannot be tightly bounded and may, in fact, have a strong effect on the contribution to the effective properties (as illustrated by 2-D calculations on convex vs concave polygons by Kachanov et al., 1994).

5.2. "Islands" of partial contacts between crack faces

Such "islands" are common, for example, in sprayed coatings. They produce a very strong effect *even if the "islands" are very small*: their presence reduces the compliance contribution of a crack quite drastically (several times).

The "islands" factor can be accounted for in the framework of the usual crack density parameters (2) and (3) by reducing the "effective" crack radii. Importantly, the effects of "islands" on the elastic and on the conductive properties are very close (this implies that their presence does not affect the cross-property connections, Sevostianov, 2003).

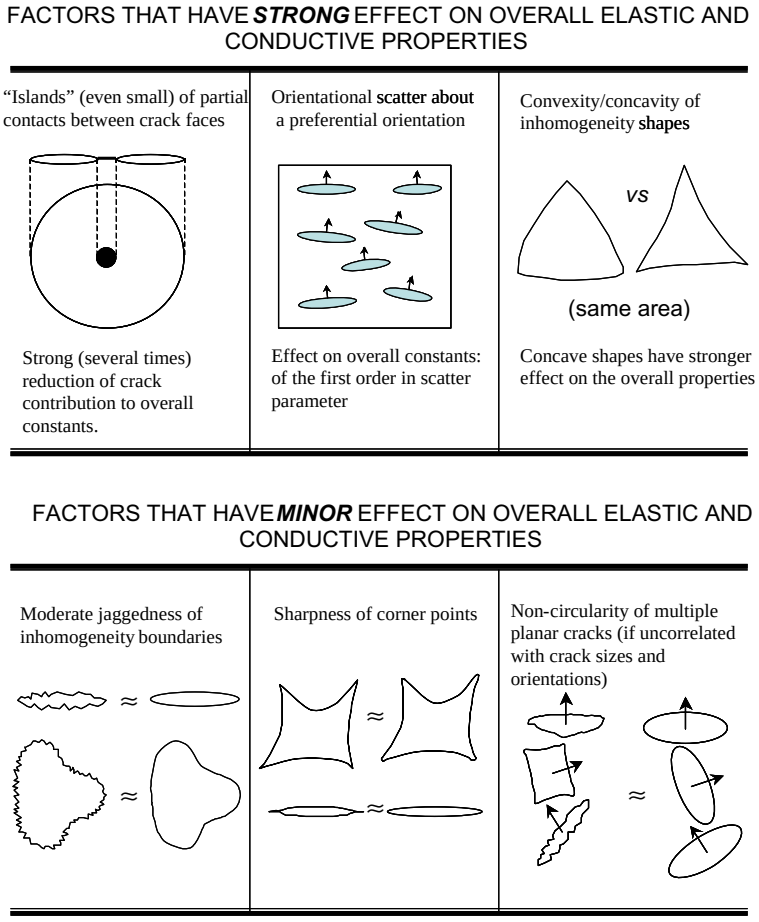

Fig. 1. Influence of various "irregularity factors" on the elastic and conductive properties.

The discussion of this section is summarized in Fig. 1.

6. Proper microstructural parameters are different for different physical properties

As discussed above, the proper microstructural parameters represent individual inhomogeneities in accordance with their contributions to the physical property considered. For different properties, these contributions may be different. Therefore, the proper microstructural parameters will, generally, be different. The preceding section discussed proper parameters for the *elastic* properties. We now discuss this problem in the context of conductive, transport and fracture-related properties.

6.1. Effective conductive properties (thermal or electric)

Proper quantitative characterization of a microstructure in the context of conductivity is somewhat similar, but not identical to the one for elasticity. The following results should be mentioned (they are summarized in Fig. 2).

PROPER PARAMETERS OF CONCENTRATION OF INHOMOGENEITIES FOR THE ELASTIC AND THE CONDUCTIVE PROPERTIES

MICROSTRUCTURE	PARAMETERS FOR ELASTICITY	PARAMETERS FOR CONDUCTIVITY
1 — 2-D isotropic matrix with cracks. Random orientations.	Scalar crack density $\rho = (1/A)\sum (a^2)^i$	Same
2 — 2-D isotropic matrix with cracks. Non-random orientations.	Second rank symmetric crack density tensor $\alpha = (1/A)\sum (a^2 \boldsymbol{nn})^i$	Same
3 — 3-D isotropic matrix with circular cracks. Random orientations.	Scalar crack density $\rho = (1/V)\sum (a^3)^i$	Same
4 — 3-D isotropic matrix with circular cracks. Non-random orientations.	Two parameters: Second rank crack density tensor $\alpha = (1/V)\sum (a^3 \boldsymbol{nn})^i$ Fourth rank tensor $(1/V)\sum (a^3 \boldsymbol{nnnn})^i$ (can be neglected in the first approximation)	$\alpha = (1/V)\sum (a^3 \boldsymbol{nn})^i$
5 — 3-D isotropic matrix with sliding (closed) circular cracks. Non-random orientations.	Two parameters: Second rank crack density tensor $\alpha = (1/V)\sum (a^3 \boldsymbol{nn})^i$ Fourth rank tensor $(1/V)\sum (a^3 \boldsymbol{nnnn})^i$ (cannot be neglected)	Closed cracks do not affect conductivity.

PROPER PARAMETERS OF CONCENTRATION OF INHOMOGENEITIES FOR THE ELASTIC AND THE CONDUCTIVE PROPERTIES (continuation)

MICROSTRUCTURE	PARAMETERS FOR ELASTICITY	PARAMETERS FOR CONDUCTIVITY
6 — 3-D isotropic matrix with crack-like pores of diverse aspect ratios filled with compressible fluid. Non-random orientations.	Two parameters: Second rank crack density tensor $\alpha = (1/V)\sum (a^3 \boldsymbol{nn})^i$ Fourth rank tensor $(1/V)\sum \left(\frac{2+\nu\delta}{2(1+\delta)} a^3 \boldsymbol{nnnn}\right)^i$ (cannot be neglected)	See line 10
7 — 2-D isotropic matrix with elliptical holes of diverse eccentricities. Random orientations.	Two scalar parameters: Porosity $p = (\pi/A)\sum (ab)^i$ Average eccentricity $q = (\pi/A)\sum (a^2 - b^2)^i$	One scalar parameter: $r \equiv tr\beta = (\pi/A)\sum (a^2 + b^2)^i = 2p + q$
8 — 2-D isotropic matrix with elliptical holes of diverse eccentricities. Non-random orientations.	Second rank hole concentration tensor $\beta = (1/A)\sum (a^2 \boldsymbol{nn} + b^2 \boldsymbol{mm})^i$	Same
9 — 3-D isotropic matrix with spherical inhomogeneities	Volume fraction of inhomogeneities $c = (1/V)\sum V^i$	Same
10 — 3-D isotropic matrix with spheroidal inhomogeneities of diverse aspect ratios. General case of non-random orientations.	Fourth rank compliance (or stiffness) contribution tensor H_{ijkl} (or N_{ijkl}) In certain cases may be expressed with good accuracy in terms of symmetric second rank tensor $\omega = \frac{1}{V}\sum (V_* \boldsymbol{nn})^i$	Second rank resistivity (or conductivity) contribution tensor. Expressed in terms of tensor $\omega = \frac{1}{V}\sum (V_* \boldsymbol{nn})^i$

Fig. 2. Proper microstructural parameters for various microstructures.

- For a 3-D material containing non-conducting cracks (or strongly oblate pores, with aspect ratios smaller than 0.10–0.15), second rank crack density tensor $\boldsymbol{\alpha}$ is the *sole* proper crack density parameter (no fourth rank tensor emerges, in contrast with the elasticity problem).
- "Islands" of partial contacts between the crack faces produce the effect on the conductive properties that is very close to the one for the elastic properties (Sevostianov, 2003). Therefore, adjustments to the crack density tensor $\boldsymbol{\alpha}$, via reducing the "effective" crack radii, are very close for these two properties.
- The effect of *ellipsoidal* inhomogeneities on the conductive properties is characterized by a second rank symmetric tensor, with components explicitly linked to ellipsoid's characteristics (Sevostianov and Kachanov, 2002a).
- Estimates of the role of various "irregularity factors" ("jagged" boundaries, etc.), that follow from Hill's comparison theorem are similar to the ones for the elasticity problem, as outlined by Zohdi et al. (1999). Namely, let K_{ij}^0 and K_{ij}^1 be the conductivity tensors of the matrix and of the inhomogeneities and $\boldsymbol{\omega}$—the region occupied by inhomogeneities. We assume, to be specific, that the material of inhomogeneities is more conductive (in the sense that eigenvalues of $K_{ij}^1 - K_{ij}^0$ are non-negative). Then, enlargement of inhomogeneities leads to non-negative eigenvalues of the change $\Delta K_{ij}^{\text{eff}}$. If both the matrix and the inhomogeneities are isotropic (although the overall conductivity may be anisotropic, due to anisotropy of the inhomogeneity shapes), then enlargement of inhomogeneities leads to non-negative change in the effective conductivity in any direction. Similar conclusions, with opposite inequality signs, would apply to the resistivity tensors.

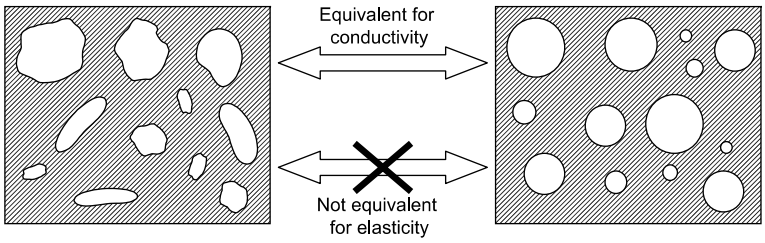

Fig. 3. For the *conductive* properties, any isotropic mixture of diverse inhomogeneities is equivalent to a certain volume fraction of spheres. This equivalence does not hold for the *elastic* properties.

The differences between the proper parameters to be used for the elastic and for the conductive properties are best seen in the case of *overall isotropy* (Fig. 3). For conductivity, the effect of inhomogeneities (on *one* effective constant) is characterized by *one* microstructural parameter (that reduces to volume fraction, for the spherical shapes, to crack density, for cracks, and reflects a certain average shape, in the case of mixtures). This means that any isotropic mixture of diverse shapes is equivalent, in its effect on conductivity, to a certain volume fraction of *spheres*. For *elasticity*, there is no such equivalence, since the effect of inhomogeneities (on *two* effective elastic constants) is characterized by *two* parameters. This is best illustrated by the example of elliptical holes (Section 4.6) where these two parameters are p and q (porosity and average eccentricity); matching one of the two elastic constants by an appropriate concentration of *circles* would leave the other constant unmatched.

6.2. Effective transport properties

In the problem of fluid filtration through a porous/cracked media, the issues of interconnectedness and percolation are of primary importance. Therefore, volume average parameters, like (1)–(3), are, generally, insufficient (see books of Adler and Thovert, 1999; Torquato, 2002 for recent reviews).

However, such volume average characterization is sufficient for one class of microstructures that occur in rock materials, and *it is different from the one used in the context of elastic/conductive properties*. We consider fluid filtration through a system of planar fissures (with unit normals $\boldsymbol{n}^{i}$) that fully intersect representative volume V. We assume that the usual Darcy's law governs filtration, i.e. the overall flow is proportional to the applied pressure gradient ∇p. In the general anisotropic case (non-randomly oriented fissures),

$$\boldsymbol{q} = -\frac{1}{\mu}\boldsymbol{K}\cdot\nabla p \tag{30}$$

where $\boldsymbol{q}$ is the overall filtration rate, μ is the viscosity coefficient and $\boldsymbol{K}$ is a symmetric second rank permeability tensor. Assuming that the "background" permeability in the absence of fissures is isotropic (equal to $k_0\boldsymbol{I}$), we aim at expressing the change of permeability due to cracks $\boldsymbol{K} - k_0\boldsymbol{I}$ as a function of the proper microstructural parameter.

It is usually assumed that permeability due to several families of fissures is a simple superposition of the individual permeabilities, the underlying assumption being that energy losses at intersections can be neglected (Wittke, 1990). This implies that $\boldsymbol{\alpha}$-type tensor that sums up the individual fissure contributions, is adequate.

However, tensor $\boldsymbol{\alpha}$, as defined by (3), should be substantially modified, to account for the fact that, according to the hydrodynamics laws, the contribution of a given fissure to $\boldsymbol{v}$ is proportional to its area S and to its width *w cubed* (in contrast with the elastic properties, where such a contribution is independent of the width and is proportional to $S^{3/2}$). This leads to the following proper microstructural parameter:

$$\boldsymbol{\gamma} = \frac{1}{V}\sum_i (Sw^3 \boldsymbol{nn})^{(i)} \tag{31}$$

Its identification readily yields the effective permeability $\boldsymbol{K} - k_0\boldsymbol{I}$ in terms of $\boldsymbol{\gamma}$. Indeed, $\boldsymbol{K} - k_0\boldsymbol{I}$ is the isotropic function of $\boldsymbol{\gamma}$ (if both ∇p and $\boldsymbol{\gamma}$ undergo a certain orthogonal transformation, say, rotation, then $\boldsymbol{q}$ undergoes the same transformation). Then Cayley–Hamilton theorem implies that $\boldsymbol{K} - k_0\boldsymbol{I}$ is a tensorly quadratic polynomial in $\boldsymbol{\gamma}$—a combination of $\boldsymbol{I}$, $\boldsymbol{\gamma}$ and $\boldsymbol{\gamma}\cdot\boldsymbol{\gamma}$, with coefficients—functions of invariants of $\boldsymbol{\gamma}$. Since $\boldsymbol{q}$ is a sum of the individual fissure contributions, the polynomial should be linearized in $\boldsymbol{\gamma}$. Finally, we require that a family of parallel fissures does not contribute to $\boldsymbol{v}$ in the normal to the fissures direction. These considerations yield the permeability

$$\boldsymbol{K} - k_0\boldsymbol{I} = C[(\mathrm{tr}\,\boldsymbol{\gamma})\boldsymbol{I} - \boldsymbol{\gamma}] \tag{32}$$

to within constant C of the hydrodynamic nature. Result equivalent to (32) was derived by Romm and Pozinenko (1963) by lengthier means and without identifying the proper microstructural parameter $\boldsymbol{\gamma}$. The derivation above was given by Kachanov (1975).

Proper microstructural parameter $\boldsymbol{\gamma}$ identifies the principal axes of orthotropy of filtration (they are the principal axes of $\boldsymbol{\gamma}$). They are generally different from the principal axes of the *elastic* orthotropy (the principal axes of $\boldsymbol{\alpha}$). The two orthotropies are coaxial only if all the fissures are identical—have the same width w and the same area S.

6.3. Fracture—related properties of a brittle–elastic material containing multiple cracks

An important problem—still waiting for an in-depth analysis—is to identify proper microstructural parameters that would characterize the proximity of the specimen to fracture.

Here, we briefly discuss the connection of such fracture-related characterization to the characterization for the effective elastic properties. We note that the usual crack density, scalar (1) or tensor (3)—that is appropriate for the effective elastic (and conductive) properties—cannot be used for this purpose. Indeed,

- The usual crack density is insensitive to the *mutual positions* of cracks, whereas the fracture-related properties (such as the maximal, among the crack tips, stress intensity factors, SIFs) are highly sensitive to them.
- For a solid with strongly oblate, crack-like pores, the fact whether the crack tips are *sharp or blunt* makes almost no difference as far as the effective elastic properties are concerned (as follows from Hill's comparison theorem, Section 5). This difference is of obvious importance for the fracture-related properties.

7. Benefits of identifying the proper microstructural parameters

Identification of the proper microstructural parameters yields a number of benefits relevant for materials science applications.

7.1. Guidance in intelligent reading of various microstructural data

This means identifying those microstructural features that have a dominant effect on the property considered and distinguishing them from less important "details". It can be applied to intelligent processing of microphotographs. Examples are as follows.

- The proper microstructural parameters for the elastic/conductive properties take the individual inhomogeneities' contributions proportionally to their sizes *cubed*. This implies that *small inhomogeneities can be ignored*, as compared to the dominant larger ones, unless they vastly outnumber the larger ones (for example, by 2–3 orders of magnitude in the case their sizes are one order of magnitude smaller).
- For *pores of strongly oblate shapes* (aspect ratios smaller than 0.10–0.15), the knowledge of aspect ratios is unnecessary in the context of the elastic/conductive properties, and their concentration can be characterized by the crack density parameters. For a material with such pores, *porosity is not a relevant parameter*.
- The following details of microgeometries are unimportant, for the effective elastic/conductive properties:
  - slightly "jagged" inhomogeneity boundaries;
  - moderate non-planarity of cracks;
  - sharp vs blunted corners of inhomogeneities.
- *"Islands" of partial contacts* between crack faces are of primary importance: they produce a strong effect on the elastic/conductive properties, even if they are very small (the effect can be incorporated into the usual crack density parameters by appropriately reducing the "effective" crack sizes). Therefore, their detection—in cases when their presence is suspected—is essential.
- The difference in effects on the elastic/conductive properties between the *convex* and the *concave* shapes of inhomogeneities (of the same volume) may be substantial. Therefore, the convexity/concavity factor is important.
- Knowledge of proper microstructural parameters substantially simplifies the reconstruction of 3-D microstructural data from 2-D images. For example, in the cases of isotropic distribution of spherical pores or cracks, the 2-D defect densities coincide with 3-D ones (Sevostianov et al., 2004).

7.2. Identification of the overall anisotropy

The effective elastic anisotropy is determined by the tensor rank and symmetry of the proper microstructural parameters. Below, we discuss the anisotropy issue for several microstructures. (For the *conductive* properties, that always possess the orthotropic symmetry, relating the orthotropic constants to microstructure is similarly rooted in microstructural parameters that are proper in the context of conductivity.)

- For *cracks in a 2-D isotropic material*, the proper microstructural parameter is a symmetric second rank tensor $\boldsymbol{\alpha}$. Therefore such a material is orthotropic—a somewhat counterintuitive result, since it applies to an arbitrary orientation distribution of cracks (for example, to two families of parallel cracks inclined at an arbitrary angle to each other).
- This result on orthotropy extends to a 2-D isotropic material with *elliptical holes*, since their concentration is characterized by a symmetric second rank tensor $\boldsymbol{\beta}$ given by (24).
- Orthotropy also holds for a 3-D isotropic material with *circular cracks*. Moreover, the orthotropy is of a simplified type—it is characterized by only four independent constants (Kachanov, 1980). However, in contrast with 2-D, these results are approximate, since they are based on neglecting a relatively small contribution of fourth rank tensor (4). The same is true for a 3-D isotropic material with *irregularly shaped* cracks, as long as the irregularities are random (not correlated with crack orientations and sizes).
- Orthotropy holds, with some approximation, for a material with 3-D spheroidal inhomogeneities in the isotropic matrix (Sevostianov and Kachanov, 2002a,b). This follows from an approximate representation of the potential Δf due to inhomogeneities in terms of a symmetric second rank tensor.
- For *cracks constrained against the normal opening* and for *fluid-filled cracks*, the fourth rank tensors (4) or (16) emerges as a second, in addition to $\boldsymbol{\alpha}$, crack density parameter. In contrast with "freely opening" cracks, its contribution cannot be neglected. This leads to violation of orthotropy.

- In the case of *anisotropic matrix* with cracks or other inhomogeneities, the overall anisotropy is determined both by the matrix anisotropy (part f_0 of the potential in representation (6)) and by the orientation distribution of defects with respect to the matrix anisotropy axes (part Δf of the potential). If symmetries of these two parts are not coaxial, the overall anisotropy, generally, has no symmetry elements.

Remark. In general, if the proper microstructural parameter is a symmetric second rank tensor, the material is not only orthotropic, but the orthotropy is of a substantially simplified type, characterized by a reduced number of constants (the simplified orthotropy was discussed in more detail by Kachanov (1980) and Kachanov et al. (1994)).

7.3. Design of microstructures for the prescribed effective properties

An example is given by plasma-sprayed thermal barrier coatings, that should have low thermal conductivity in the direction normal to the coating and high elastic compliance in the direction parallel to the coating. Such a design requires identification of the microstructural parameters that actually control the said properties.

7.4. Recovery of information on microstructure from the effective properties

Such information recovery is, obviously, non-unique. Nevertheless, certain information can be extracted (Sevostianov et al., 2001). Identification of the proper microstructural parameters is crucial, since the recovered quantities are these very parameters. In the case of the *isotropic* material, the elasticity data provide more information than the conductivity data. Indeed, in the conductivity problem, an isotropic mixture of diverse shapes can be replaced by an appropriate concentration of *spheres*, whereas in the *elasticity* problem, there is no such equivalence (Fig. 3). Hence, no information on inhomogeneity shapes can be recovered from the isotropic conductivity data, but certain shape information *can* be recovered from the isotropic elasticity data.

7.5. Establishing explicit elastic–conductive cross-property connections

Establishing explicit elastic–conductive cross-property connections is, perhaps, one of the most significant benefits of identifying the proper microstructural parameters. This issue is discussed in the section to follow.

8. Proper microstructural parameters imply cross-property connections

Cross-property connections—when they are possible—interrelate changes in two different physical properties (say, elastic and conductive ones) due to the presence of inhomogeneities. The possibility of such connections is actually rooted in similarity between the proper microstructural parameters for these two properties.

As mentioned in the Introduction, proper microstructural parameters are generally different for different physical properties. The differences can be essential. For example, for a material with crack-like fissures, the effect of fissure openings on the *elastic* properties is minor, whereas the *transport* properties are highly sensitive to them. Therefore, parameters used for these two properties have to be essentially different, and a connection cannot, generally, be established between the two properties.

As far as *elastic and conductive* properties are concerned, the proper parameters for these two properties are either identical or similar (in spite of differences in their tensor ranks in some cases, they have similar dependencies on sizes and shapes of inhomogeneities). This leads to explicit cross-property connections obtained by eliminating the mentioned parameters. Depending on the extent of the similarity, the connections may have different forms.

(A) If the mentioned parameters are *identical* (lines 1–3, 8, 9 of Fig. 2), the cross-property connections are exact and do not depend on any microstructural information. An example is given by 2-D cracks of any (generally anisotropic) orientation distribution. In this case, the connection between effective Young's modulus E_i in a certain direction x_i and effective conductivity k_i in the same direction has the form

$$\frac{E_0 - E_i}{E_i} = 2\frac{k_0 - k_i}{k_i} \tag{33}$$

(E_0, k_0 are constants of the bulk material). This connection does not contain any reference to the density of cracks or their orientation distribution.

(B) In certain cases, the microstructural parameters for elasticity require more parameters, or parameters of a higher tensor rank, as compared to conductivity. At the same time, both properties have identical dependencies of the defect sizes and somewhat similar dependencies on defect shapes. Then the cross-property connections may hold only approximately and may have some sensitivity to microstructural information. The following situations can be identified:

- The elastic properties require an *extra parameter* (lines 4, 7 of Fig. 2). The cross-property connection (obtained by eliminating the parameter that is common for both properties) will be sensitive to the microstructural information expressed by this parameter.

This situation is illustrated by the 2-D example of elliptical holes, of an arbitrary distribution over orientations, aspect ratios and sizes (line 7 of Fig. 2). Microstructural parameter that is common to both elastic and conductive properties is the second rank symmetric tensor

$$\boldsymbol{\beta} = \frac{1}{A}\sum_i (a^2 \boldsymbol{nn} + b^2 \boldsymbol{mm})^i \tag{34}$$

where a, b are ellipses' semiaxes, $\boldsymbol{n}, \boldsymbol{m}$ are unit vectors along them and A is the area of averaging. However, the elastic properties require an extra parameter—scalar porosity $p = (\pi/A)\sum(ab)^i$. This has interesting physical implications that are best seen in the simplest case of overall isotropy (random orientations of ellipses). In this case, the elastic properties are expressed in terms of two scalar parameters, porosity p and "average eccentricity" $q = (\pi/A)\sum[(a-b)^2]^i$ (or, alternatively, $r = (\pi/A)\sum(a^2+b^2)^i = 2p + q$. Namely, for the effective Young's and bulk moduli we have

$$\frac{E}{E_0} = \frac{1}{1+p+r}; \qquad \frac{K}{K_0} = \frac{1}{1+r} \tag{35}$$

The effective conductivity requires only one parameter, r:

$$\frac{k}{k_0} = \frac{1}{1+r} \tag{36}$$

so that, although the effective conductivity can be uniquely related to the bulk modulus:

$$\frac{k}{k_0} = \frac{K}{K_0} \tag{37}$$

relating it to *Young's* modulus

$$\frac{E}{E_0} = \frac{1}{(k_0/k) + p} \tag{38}$$

requires knowledge of a microstructural parameter—porosity p.

- Elastic properties require a fourth rank tensor parameter as compared to a second rank one for conductivity (lines 4, 6, 10 of Fig. 2). Then the cross-property connections are possible if the fourth rank parameter can be replaced, with some approximation, by a second rank one, as discussed throughout Section 4. An example is given by 3-D circular cracks when the exact connection (33) changes to an approximate one

$$\frac{E_0 - E_i}{E_i} = \frac{4(1 - \nu_0^2)}{2 - \nu_0} \frac{k_0 - k_i}{k_i} \tag{39}$$

Generally, the accuracy of such connections depends on the average shapes of inhomogeneities and on Poisson's ratio ν_0 of the matrix (see Sevostianov and Kachanov (2002a,b) for cross-property connections for materials with spheroidal inhomogeneities).

Remark 1. In connection with the last statement, we mention a related result of Zimmerman and Lutz (2004) that connects the effective bulk modulus of the isotropic material (randomly oriented spheroidal pores) and the effective conductivity, in the case $\nu_0 = 0$. The results above appear to put his result in a more general context, since in the case $\nu_0 = 0$ for the spheroidal pores, the fourth rank parameter can be replaced by a second rank one exactly in the general anisotropic case (and, if $\nu_0 \neq 0$, the error can be estimated, see Shafiro and Kachanov, 1999).

Remark 2. In certain cases, a cross-property connection can be established in spied of the fact that the fourth rank tensor determining the elastic properties cannot be replaced by a second rank one. For example, if the case of parallel fluid-filled cracks (situation typical for hydrothermal aging of thin-walled structures), fourth rank crack density tensor may be represented as $(1/V)\sum(a^3 \boldsymbol{nnnn})^i = \boldsymbol{\alpha\alpha}/\rho$ (where $\boldsymbol{\alpha\alpha}$ is a dyadic product of second rank crack density tensors and ρ is scalar crack density. This results in a non-linear cross-property connection, Sevostianov et al., 2003).

9. Fabric tensor approach

> Give me five adjustable parameters and I will draw an elephant; give me a sixth and I will make its trunk wave—L. Landau

The terminology. The term "fabric" has been used in literature in different senses. Therefore, we start with clarification of the terminology.

- In a loose sense, "fabric" may simply mean that a certain texture is present. For example, in structural geology it often indicates preferred crystallographic orientations (Law, 1990).
- The term "fabric tensors" may indicate a specific technique of quantitative characterization of orientation distributions of various geometric features (Kanatani, 1984).
- In the context of *granular* materials, "fabric tensors" are introduced in such a way that they explicitly reflect orientations of grain contacts and, possibly, other microstructural features (Satake, 1978 and works that followed, e.g. Oda et al., 1982). In the terminology of the present paper, this constitutes the micromechanical approach (rather than the fabric tensor one). Therefore, the comments made below do not apply to this case.

Most often, however, this terminology indicates a certain approach to the effective elastic properties that is discussed in the text to follow. (Note that a similar approach has also been applied to anisotropic *strength* criteria, see Cowin, 1986.) Here, we focus on "fabrics" constituted by inhomogeneities (cracks, pores,

foreign particles) in a matrix. Similar arguments may be applied, though, to "fabrics" of other morphologies.

This approach has been taken by several authors. Leaving aside works on granular materials (for the reason indicated above), we mention the works of Cowin (1985), Litewka (1985), Talreja (1994) (where the matrix containing inhomogeneities is assumed anisotropic), Zysset and Curnier (1995) and Kuna-Ciskal and Skrzypek (2004) for the latest one.

A number of works on the elastic properties of *trabecular bone* belong to this framework, starting, probably, with work of Cowin and Mehrabadi (1989); see Hamminga et al. (2003) for the latest one. We note that, as far as (highly porous) trabecular bone is concerned, modeling its microstructure by a continuum with voids may not be the best route. Therefore, restrictions imposed by consistency with the known results on elastic continua with pores/cracks that are discussed below may not apply to such bone; instead, it may be more appropriate to require consistency with micromechanics of cellular materials.

One of the present authors (MK) has also taken this approach in his earlier work (Vakulenko and Kachanov, 1971) where the basic formulas (40) and (41) were used in the micromechanical context, perhaps, for the first time. The fact that the "fabric tensor" was introduced there in connection with cracks is irrelevant in the context of the present discussion, since constructions (40) and (41) are independent of the microstructural interpretation of the "fabric tensor".

The basic logic is as follows.

1. It is postulated that a microstructure is characterized by a certain "fabric" tensor $\boldsymbol{A}$ of an a priori postulated rank. Most often, it is taken as a symmetric second rank tensor (the possibilities of higher rank fabric tensors, or more than one fabric tensor, have also been discussed; the basic scheme would then remain the same, but the algebraic expressions would involve even larger numbers of terms and parameters).
2. The effective elastic potential is treated as a function of *two* variables: stress $\boldsymbol{\sigma}$ and tensor $\boldsymbol{A}$: $f = f(\boldsymbol{\sigma}, \boldsymbol{A})$. In equivalent formulations, the potential in strains, $f = f(\boldsymbol{\varepsilon}, \boldsymbol{A})$ is considered, or the effective compliance (or stiffness) tensor is constructed as a function of $\boldsymbol{A}$.
3. If the matrix material is isotropic in absence of inhomogeneities, then $\boldsymbol{\sigma}$ and $\boldsymbol{A}$ enter f *only through their invariants*, including the joint ones (since any orthogonal transformation, for example, rotation, applied to *both* $\boldsymbol{\sigma}$ and $\boldsymbol{A}$ should not affect the potential). Using general tensor representations (see, for example, Green and Adkins, 1960; or Spencer, 1971) and imposing the requirement that f is quadratic in stresses (linear elasticity), yields the potential as a sum of nine terms:

$$f(\boldsymbol{\sigma}, \boldsymbol{A}) = C_1(\operatorname{tr}\boldsymbol{\sigma})^2 + C_2\boldsymbol{\sigma} : \boldsymbol{\sigma} + C_3(\boldsymbol{\sigma} \cdot \boldsymbol{\sigma}) : \boldsymbol{A} + C_4(\operatorname{tr}\boldsymbol{\sigma})\boldsymbol{\sigma} : \boldsymbol{A} + C_5(\boldsymbol{\sigma} : \boldsymbol{A})^2 + C_6(\boldsymbol{\sigma} \cdot \boldsymbol{\sigma}) : (\boldsymbol{A} \cdot \boldsymbol{A}) + C_7[\boldsymbol{\sigma} : (\boldsymbol{A} \cdot \boldsymbol{A})]^2 + C_8 \operatorname{tr}\boldsymbol{\sigma}[\boldsymbol{\sigma} : (\boldsymbol{A} \cdot \boldsymbol{A})] + C_9[\boldsymbol{\sigma} : (\boldsymbol{A} \cdot \boldsymbol{A})]\boldsymbol{\sigma} : \boldsymbol{A} \tag{40}$$

   (a dot and a colon denote contraction over one and two indices). This representation contains nine factors $C_{1\text{–}9}$. Each of them is a function of three variables—invariants of $\boldsymbol{A}$.
4. Since this representation contains nine terms, with uncertain functions $C_{1\text{–}9}$, various simplifications have been suggested. Most of them fall into one of the two categories:
   - Linearization of $f = f(\boldsymbol{\sigma}, \boldsymbol{A})$ with respect to $\boldsymbol{A}$. A possible justification is that the linearity should hold, at least, in the limit of low density of inhomogeneities (although this argument is not fully clear, since $\boldsymbol{A}$ is not necessarily identified as the proper parameter of concentration of inhomogeneities). This yields:

$$f(\boldsymbol{\sigma}, \boldsymbol{A}) = (C_1' + C_1'' \operatorname{tr}\boldsymbol{A})(\operatorname{tr}\boldsymbol{\sigma})^2 + (C_2' + C_2'' \operatorname{tr}\boldsymbol{A})\boldsymbol{\sigma} : \boldsymbol{\sigma} + C_3(\boldsymbol{\sigma} \cdot \boldsymbol{\sigma}) : \boldsymbol{A} + C_4(\operatorname{tr}\boldsymbol{\sigma})\boldsymbol{\sigma} : \boldsymbol{A} \tag{41}$$

   where C', C''-factors are constants. Note that, had tensor $\boldsymbol{A}$ been a proper parameter of concentration of inhomogeneities, the linearized version (41) would have represented simply the low concentration limit. Since, however, this is generally not the case, such an association cannot be made.

- It is suggested that the C-factors can be treated as constants. This is done either (1) by claiming that they are "material constants" (this claim is discussed below), or (2) as an approximation, that is justified by the ability to fit specific sets of experimental data (note that a number of adjustable parameters required is usually rather large; for example, 18 adjustable parameters were used in the work of Hamminga et al., 2003).

5. If the matrix material is anisotropic, the number of terms in the potential—and, therefore, the number of C-factors—increases further. Indeed, in this case $\boldsymbol{\sigma}$ and $\boldsymbol{A}$ enter f through their invariants with respect to the group of symmetry of the material (rather than the full orthogonal group). This results in larger number of terms in $f(\boldsymbol{\sigma}, \boldsymbol{A})$. For the orthotropic matrix, this number is 14, even in the linearized formulation (41) (Talreja, 1994). We note that the question whether a second rank tensor $\boldsymbol{A}$ is adequate at all, as a parameter of microstructure is even more complex in the case of an anisotropic matrix. For example, whereas the concentration of 2-D elliptical holes in the *isotropic* matrix is adequately characterized by a second rank tensor (see formula (23)), their concentration in an *anisotropic* matrix is not (it requires a fourth rank tensor).

Discussion of the approach. The approach is aimed at a difficult problem of key importance—linking anisotropic microstructures to the effective elastic properties. However, the way it is done raises a number of objections, as follows.

1. *Linking the effective properties to microstructure*. For this purpose, the key problem is *to explicitly link $\boldsymbol{A}$ to relevant microstructural features*. This would involve (1) identifying those features (concentration of inhomogeneities, their shapes and orientations) that have dominant effects on the elastic properties; (2) quantifying these effects and incorporating them into $\boldsymbol{A}$. Most often, however, no such attempt is made. In several works, this link is suggested in a somewhat arbitrary way, without a micromechanical justification.

That such a linkage is non-trivial, is clearly shown, in the context of trabecular bones, in the review of Odgaard (1997). Several possible—and quite different—linkages between bone's microstructure and the fabric tensor are outlined in this work; they yield different fabric tensors. The problem of making a choice between these methodologies appears to remain unresolved. Note that one of these choices—based on the "mean intercept length"—that seems to be used most often (see, for example, Hamminga et al., 2003) produces isotropic fabric tensors in certain cases when the microstructure is clearly anisotropic.

2. *C-factors*. The presence of the mentioned nine functions (or six constants, in the linearized version) creates a major uncertainty—it appears that these factors cannot be specialized on the theoretical grounds (except for the requirement that, at $\boldsymbol{A} = 0$, the potential should reduce to the usual elastic potential of the matrix material). These uncertainties are the price paid for the fact that $\boldsymbol{A}$ is not explicitly linked to relevant microstructural features, i.e. for bypassing the micromechanical analysis.

It is sometimes hypothesized that C-factors are "material constants". Aside from the fact that these factors do not seem to represent any fundamental property of the matter, the following comments should be made. Had the C-factors been constants for a given material, formula (40) would have covered the limit of low concentration of inhomogeneities as a special case. From this point of view, let us examine two 2-D cases: the one of cracks and the one of elliptical holes, both in the limit of small concentration. In the first case, result (14) means that, of all the terms in (40), only the first three have non-zero C-factors; $C_{4\text{–}9}$ are zeros. Constancy of C's would then imply that $C_{4\text{–}9}$ remain zeros for the elliptical holes as well—in contradiction with result (23) that shows, for example, that $C_4 \neq 0$ (and that the value of C_2 should be changed).

Note that the hypothesis on constancy of C-factors has sometimes been used in the context of cracks only. In this narrower context, the structure (40), having to be in agreement with rigorous results for low

crack densities, implies that $\boldsymbol{A}$ is the tensor crack density parameter (3) and that C-factors are identified from formulas (14) or (15). Then, constancy of C-factors would imply that the results obtained in the non-interaction approximation remain valid in general.

Thus, C-factors are not constants but must be treated as functions of invariants of $\boldsymbol{A}$ that have to be experimentally measured. This requires $\boldsymbol{A}$ to be explicitly linked to microstructural features in a micromechanically justified way, i.e. of several possible linkages (of the kind overviewed by Odgaard, 1997) the one that properly reflects the effect of the features on the overall property is chosen. Otherwise, C's will not be unique functions of their arguments. This brings us back to the focal point of micromechanical analyses—identification of contributions of individual micromechanical features to the overall properties.

3. *The rank of tensor* $\boldsymbol{A}$ is postulated a priori. Actually, this is not a trivial matter. For example, micromechanical analysis (Section 4) shows that for cracks in a 3-D solid, retaining second rank tensor $\boldsymbol{\alpha}$ as a sole crack density parameter is a good approximation (with accuracy dependent on Poisson's ratio). However, in cases of fluid-filled cracks, or cracks constrained against the normal opening, $\boldsymbol{\alpha}$ should be supplemented by fourth rank tensor (18). For the spheroidal inhomogeneities, whereas second rank tensor characterization is satisfactory in most cases, fourth rank tensor becomes necessary at certain combinations of the spheroid eccentricities and Poisson's ratios. These facts cannot be predicted in the framework of the "fabric" tensor approach.
4. *Overlooking possible simplifications*. If the rank of $\boldsymbol{A}$ is postulated correctly, the general structure (40) is, of course, correct. However, one may not be able to identify important simplifications.
   (A) For cracks, in those cases when second rank crack density tensor $\boldsymbol{\alpha}$ is adequate, the potential actually contains *only one* joint invariant, $(\boldsymbol{\sigma}\cdot\boldsymbol{\sigma}):\boldsymbol{\alpha}$ of tensors $\boldsymbol{\sigma}$ and $\boldsymbol{\alpha}$, see (14).
   (B) A substantial reduction of the number of independent constants (four constants, instead of nine, in the case of cracks) cannot be predicted.
   (C) In cases when *both* the second and the fourth rank tensors are needed, the general structure of f produced by the fabric tensor approach would be quite complex. However, the actual expression for f may be much simpler (formulas (15) and (16)).
   (D) In the case of an anisotropic matrix, the general fabric tensor representations contain a large number of terms. Again, the micromechanical analysis shows that the potential may actually be much simpler. For example, for a 2-D orthotropic matrix with arbitrarily oriented cracks, the change of potential due to cracks Δf reduces to *one term only*, formula (22).

Summing up, it appears that the basic result of the approach reduces to the following statement: if a certain "fabric" tensor $\boldsymbol{A}$ is postulated to characterize the microstructure, then its rank and symmetry determine the overall anisotropy.

10. Discussion and conclusions

We focus on microstructures that comprise a mixture of inhomogeneities of diverse shapes and orientations. The problem of effective properties is closely related to the one of quantitative characterization of such microstructures—identification of microstructural parameters, in whose terms the said properties are to be expressed.

The proper microstructural parameters should represent the individual inhomogeneities in accordance with their contributions to the effective property. Therefore, such parameters are, generally, different for different physical properties (elastic, conductive, transport).

The key problem in their identification is to find *the contribution of one isolated inhomogeneity* to the property considered, as a function of its shape and orientation. This is, generally, a challenging problem; we

overview the progress that has been made in this direction. For anisotropic microstructures, we identify the cases when second rank tensors are sufficient and the cases when fourth rank tensor parameters become necessary.

The microstructural parameters, that are identified this way, may be non-trivial, even in cases of overall isotropy they may not reduce to volume fractions. A relatively simple case of a 2-D material with randomly oriented elliptical holes is an example. Various shape "irregularities" further complicate the matter—the irregularity factors of dominant importance have to be distinguished from the ones of minor importance. It is found, for example, that "islands" of partial contacts between the faces of crack-like pores constitute a microstructural feature of primary importance; we show how to incorporate this factor into the microstructural parameters.

This approach, based on analyses on individual inhomogeneity contributions, can be called "micromechanical". Its advantages are as follows.

- Coverage of microstructures that involve *mixtures* of inhomogeneities of *diverse shapes and orientations*.
- "*Intelligent processing*" of various microphotographical data, namely, distinguishing between the microstructural features of primary importance (for example, small "islands" of partial contact between crack faces) from the ones that can be ignored (for example, "jaggedness" of inhomogeneity boundaries or sharpness of various corner points).
- *The overall anisotropy* is established—it is determined by a rank and symmetry of the proper tensor microstructural parameter.
- *Explicit cross-property connections* can be established between two physical properties (elasticity–conductivity, for example), if the proper parameters for these properties are sufficiently similar.

We contrast the micromechanical approach with the "fabric" tensor one, that is based on postulating, a priori, that a "fabric" tensor of a certain rank characterizes the microstructure. In most cases, this tensor is not linked, in a quantitative way, to relevant microstructural features (in several works on a trabecular bone, linkages have been suggested, but not in a unique, or a micromechanically justified way). The effective properties are then constructed using general tensor representations. This produces of a large number of uncertain factors—coefficients in these representations. They cannot be treated as material constants (and are, generally, functions of three, somewhat uncertainly defined, arguments). Yet another difficulty is that the rank of a tensor that characterizes a microstructure is actually not a trivial matter (for example, it may not be clear, without micromechanical analyses, when second rank tensors are sufficient and when the fourth rank ones are necessary).

We also mention rapid advances in computational techniques whereby the effective properties are directly computed for any particular microgeometry. Such computational tools are very valuable, since they allow one to directly examine various microstructural features and to solve numerically the interaction problem for particular arrangements of inhomogeneities. Their limitation is that the results they produce do not constitute a physical theory. More specifically, they do not provide guidance in recovery of information from various effective property data, in design of microstructures for given effective properties or in establishing cross-property connections.

Acknowledgements

The authors are grateful to Dr. T. Zohdi for comments. This work was partially supported by Sandia National Laboratories through contracts to Tufts University (#162729) and to New Mexico State University (#161754).

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