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On the effective properties of polycrystals with intergranular cracks

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1. Introduction

In conventional models of effective properties of materials with inhomogeneities, the locations of inhomogeneities are usually unrestricted (with the exception of some models that prohibit inhomogeneities from entering certain regions surrounding their neighbors, see review in the book of Torquato (2002). In applications, however, both intergranular and intragranular cracks may appear in dependence on the strength of the interfaces between the grains (Paggi et al., 2018). In the present work, we analyze the case of the weak interfaces, when most of the cracks nucleate and propagate along the grain boundaries and, therefore, the inhomogeneity sites are restricted to specific locations. For example, microcracks in polycrystalline ceramics and metals caused by cooling from the molten state usually nucleate and propagate along intergranular boundaries (Fig. 1a, b); geomaterials provide yet another example of materials with weak intergranular boundaries and intergranular microcracking (Fig. 1c, d).

In such cases, the conventional effective media schemes may fail. Indeed, in cases of extensive microcracking (produced, for example, by cooling of ceramics having relatively large grains) the effective stiffness may be reduced by microcracks *by the factor of* 8-10 (see, for example, Bruno and Kachanov, 2013). An attempt to identify the microcrack density ρ causing such a dramatic drop, by using one of the conventional schemes, runs into difficulties: the drop of Young's modulus $E/E_0 = 0.1 - 0.12$ corresponds to very high values of microcrack density, of about 1.3 in the Differential Scheme (Zimmerman, 1991) or 4.6 in the Mori-Tanaka-Benveniste

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ABSTRACT

The effective properties, elastic and conductive, of a polycrystalline material with intergranular cracks are considered. The specifics of intergranular cracking are that crack locations are restricted to intergranular boundaries. This necessitates re-examination of the usual homogenization schemes (where crack locations are unrestricted). The model developed here addresses this issue.

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scheme (Mori and Tanaka, 1973; Benveniste, 1986). However, such values cannot be realized: if microcracking is *restricted to grain boundaries*, the crack density cannot exceed its cut-off value ρ_* at the point of losing coherence. An obvious upper bound for ρ_* corresponds to *all* grain boundaries being fully cracked; for grains of the cubic shape, for example, this implies $\rho_* = 0.54$ (since a square-shaped crack has approximately the same compliance as the circular crack of the same area, see (Fabrikant, 1989) and each crack is "shared" by two adjacent crystals). Smaller values of ρ_* may, possibly, be also relevant.

The intergranular microcracking in polycrystalline materials has been discussed in literature rather extensively. Most attention has been paid to the nucleation and propagation of intergranular cracks, particularly in the context of metals and in connection with dislocation activity (see, for example, Wu and He, 1999). The effective properties have received less attention; they have been modeled, mostly, by using one of the usual effective media schemes, disregarding the fact that crack locations are constrained to intergranular boundaries; see, for example, the review of Bruno and Kachanov (2016). Paggi and Wriggers (2012) discussed the effect of imperfect interfaces on the stiffness and strength of hierarchical polycrystalline materials. They obtained generalized expressions for the Voigt and Reuss estimates of the bounds to the effective elastic modulus of heterogeneous materials that account for finite thickness interfaces between the constituents undergoing damage up to final debonding. They showed that the interface nonlinearity significantly contributes to the deformability of the material in tensile tests. Increasing the number of hierarchical levels, the deformability increases. They also established a condition for scale separation, which corresponds to the independence of the material tensile strength from the properties of the interfaces in the second

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Fig. 1. Intergranular cracks in various materials: (a) aluminum titanate (Bruno and Kachanov, 2016); (b) Ti-10Mo-8V-1Fe-3.5Al alloy (Zhang et al., 2016); (c) quartz (van Noort et al., 2008); (d) silesian granite (Kožušníková et al., 2017).

level of microstructure. Benabou and Sun (2015) proposed an approximate analytical model for macroscopic behavior of polycrystals accounting for single crystal plasticity and interface debonding at the grain boundaries (through an exponential cohesive law).

An attempt to introduce this constraint, in the context of ceramics, was made by Fertig and Nickerson (2015). They used the following formula that expresses the effective Young's modulus in terms of a "damage parameter" $n = N_C/N_S$ where N_C and N_S seem to denote the number of cracked boundaries and the saturation level of this number, respectively (their definitions, given both in terms of crack density and the number of grains, are not fully clear):

$$E/E_0 = (1 + \xi n)^{-1} \tag{1.1}$$

where E_0 refers to uncracked material (presumably representing the effective modulus of a polycrystalline material) and ξ is a constant. The structure of formula (1.1) is the one of the noninteraction approximation (NIA), but, being expressed in terms of n – rather than crack density – it leads to serious inconsistencies; we mention some of them. Firstly, formulas of this kind should be expressed in terms of crack density and not n (in the 2-D case – that corresponds to the modeling considered in their paper – it is $(1/A)\Sigma a^{(k)2}$ where $2a^{(k)}$ are lengths of rectilinear cracks and A is the reference area; in the 3-D case of circular cracks, it is $(1/V)\Sigma a^{(k)3}$ where $a^{(k)}$ are radii of circular cracks and V is the reference volume). We emphasize that crack density parameter in formulas of the type of (1.1) is defined without regard to its saturation level (an attempt to introduce correction for the saturation level by adjusting the value of factor ξ would lead to incorrect results in the limit of low crack density where exact results are available). Secondly, being defined in terms of *n*, the ratio E/E_0 is predicted to be non-zero (in fact, quite substantial) at the saturation point n = 1. We add that the discussed model is not fully clear regarding the 2-D vs 3-D modeling. For example, crack coalescence in 3-D case – that is of main interest – may proceed quite differently from a simple 2-D sketch given by the authors; also, whereas the authors use the 3-D version of formula (1.1), their FEM modeling is two-dimensional.

We develop an alternative model that utilizes the basic idea of the differential scheme (that has been shown to be relatively accurate for cracked solids, Saenger et al., 2006) but is modified to account for a limited supply of intergranular area available for cracking. It has correct asymptotics at both low crack densities and near the saturation limit. We focus on the case of overall isotropy that corresponds to microcracking caused by cooling the polycrystalline material from the molten state (rather than by mechanical loading).

2. Background results on the differential scheme

The differential scheme introduces inhomogeneities in increments of concentration, until the final concentration is reached, with homogenization of the background matrix after each increment. Since the increments are infinitesimal the corresponding increments of the effective constants are found from the dilute limit results. This leads to first-order differential equations for the effective constants as functions of concentration, with the initial condition that, at zero concentration, the constants are the ones of the bulk material. This scheme was first formulated by Bruggeman (1935, 1937) for the effective dielectric and elastic constants of an isotropic matrix with spherical inhomogeneities. It was applied to the elastic properties of cracked solids by Vavakin and Salganik (1975) and Hashin (1988); for the ellipsoidal inhomogeneities, the equations were given by McLaughlin (1977) who solved them explicitly for spherical inhomogeneities; this solution was further analyzed by Zimmerman (1991).

2.1. Conductive properties

We consider the isotropic case of a matrix of isotropic conductivity k_0 containing randomly oriented inhomogeneities of generally diverse shapes having the isotropic conductivity k_1 . In this case, the differential equation for the overall conductivity k_{eff} has the form (Sevostianov and Kachanov, 2013):

$$\frac{dk_{eff}}{d\phi} = \sum_{i} \phi_{i} K_{mm}^{(i)} \left(k_{1}, k_{eff} \right) \equiv \Psi k_{eff}$$
(2.1)

where φ is the total volume fraction of the inhomogeneities, φ_i is the volume fraction of the *i*-th inhomogeneity; and $K_{qr}^{(i)}(k_1, k_{eff})$ is the conductivity contribution tensor of the *i*-th inhomogeneity (Sevostianov and Kachanov, 2002; see Appendix 1), so that Ψ depends on inhomogeneity shapes and on the ratio k_1/k_{eff} . In the limiting cases of perfectly insulating or superconducting inhomogeneities, the dependence of Ψ on the ratio k_1/k_{eff} vanishes and Ψ can be treated as parameter that depends on the geometry only. In these limiting cases, Eq. (2.1) has the exponential solution:

$$k_{eff} = k_0 e^{\phi \Psi} \tag{2.2}$$

If all inhomogeneities have the same shape (more precisely, it is sufficient that the trace $K_{mm}^{(i)}$ is the same for all *i*),

$$\Psi = K_{mm}/k_{eff} \tag{2.3}$$

McLaughlin (1977) suggested to modify the differential scheme by disregarding the part of the newly introduced inhomogeneities that overlaps with the volume occupied by the ones introduced earlier. Then, instead of the exponential solution, one obtains a power-law one (see the review of Markov, 2000):

$$k_{eff} = k_0 (1 - \phi)^{\Psi}$$
 (2.4)

It has the advantage of having the proper limit at $\phi \rightarrow 1$. The exponent $\Psi(\gamma)$ has the meaning of shape factor that can be determined from consistence with the non-interaction approximation in the limit of small φ .

Note that, starting with the work of Archie (1942), the power law of the (2.4) type (as well as similar law for the effective elastic stiffness) has been used in materials science literature, often on empirical grounds – in which case the micromechanical meaning of Ψ remains unclear and it is treated as a fitting constant. In fact, Ψ is a shape parameter (as is clear from the low concentration limit) and its best-fit value that provides information on inhomogeneity shapes.

In the case of randomly oriented perfect insulators of the spheroidal shape of aspect ratio γ , we have:

$$k = k_0 (1 - \phi)^{\Psi(\gamma)}$$
(2.5)

where the shape factor $\Psi(\gamma)$ is given by (A2.2). In particular, in the limit of randomly oriented, very thin platelets ($\gamma \rightarrow 0$) that are



Fig. 2. Effective conductivity of a material with randomly oriented microcracks, as predicted by the non-interaction approximation and by the differential scheme.

perfectly insulating (that, in particular, covers cracks provided the conductivity across them is neglected), $f_0(\gamma) \rightarrow -\pi\gamma/4$, $\eta(\gamma) \rightarrow -2/(3\pi\gamma)$ and the volume fraction can be expressed in terms of the crack density parameter ρ (Bristow, 1960) as $\varphi = (4/3)\pi\gamma\rho$ provided all platelets have identical aspect ratios γ . In this limit, the overlap prohibition $d\phi \rightarrow (1-\phi)d\phi$ disappears (since it is formulated in terms of volume fraction) and one obtains the exponential solution:

$$k = k_0 e^{-8\rho/9} \tag{2.6}$$

Remark 1. Formally, the transition from (2.5) to (2.6) can be obtained by solving the indeterminacy 1^{∞} in Eq. (2.5):

$$(1-\varphi)^{\Psi(\gamma)} \to 1 - \frac{8}{9}\rho + \frac{1}{2!} \left(\frac{8}{9}\rho\right)^2 - \frac{1}{3!} \left(\frac{8}{9}\rho\right)^3 + \dots = e^{-8\rho/9}$$
(2.7)

Remark 2. Although the assumption on identical aspect ratios was used to derive (2.6) from (2.5) via limiting transition, formula (2.6) remains valid in the case of diverse aspect ratios as long as they are small (γ is smaller than 0.08–0.10). Indeed the crack density parameter ρ entering (2.6) contains no reference to γ . Fig. 2 shows dependence of the effective conductivity on crack density calculated by the differential scheme and the non-interaction approximation.

2.2. Elastic properties

In the isotropic case of random orientations, assuming that all inhomogeneities have the same isotropic compliance tensor S^1 , we have two coupled differential equations for the effective bulk and shear moduli (Zimmerman, 1991):

$$\begin{cases} \frac{1}{K} \frac{dK}{d\varphi} = -B(\gamma, \nu) \\ \frac{1}{G} \frac{dG}{d\varphi} = -C(\gamma, \nu) \end{cases}$$
(2.8)

where $B(\gamma, \nu)$ and $C(\gamma, \nu)$ are obtained from the expression (A2.4) in the Appendix by replacing ν_0 for components of the compliance contribution tensor by the effective Poisson's ratio ν . As shown by Zimmerman (1991), these two equations yield the following decoupled equation for the effective Poisson's ratio:

$$\frac{d\nu}{d\varphi} = \frac{(1-2\nu)(1+\nu)}{3} [-C(\gamma,\nu) + B(\gamma,\nu)]$$
(2.9)

Remark. A major simplification concerning the system (2.8) is possible if the inhomogeneities are pores: in formula for the effective Young's modulus (but not for other moduli!), replacement $v \rightarrow v_0$ produces errors smaller than 1% (Sevostianov et al., 2006). In this approximation,

$$E \approx E_0 (1 - \phi)^{D(\gamma, \nu_0)}$$
 (2.10)

where $D(\gamma, \nu)$ is given by (A2.4).



Fig. 3. Effective elastic constants of a material with randomly oriented microcracks, as predicted by the non-interaction approximation, by the differential scheme and by the simplified solution (2.15).

Had solution of the Eq. (2.9) been known, its substitution into the system (2.8) would have decoupled it. However, Eq. (2.9) cannot generally be solved in closed form.

In the case of randomly oriented cracks, we have:

$$\frac{1}{K}\frac{dK}{d\rho} = -B(\nu, 0) = -\frac{16}{9}\frac{(1-\nu^2)}{1-2\nu}$$
$$\frac{1}{G}\frac{dG}{d\rho} = -C(\nu, 0) = -\frac{32}{45}\frac{(1-\nu)(5-\nu)}{2-\nu}$$
(2.11)

where ρ is crack density. These equations were integrated by Zimmerman (1985) producing an implicit expression of the effective Poisson's ratio ν in terms of ρ :

$$\rho = \frac{5}{8} \ln \frac{\nu_0}{\nu} + \frac{15}{64} \ln \frac{1-\nu}{1-\nu_0} + \frac{45}{128} \ln \frac{1+\nu}{1+\nu_0} + \frac{5}{128} \ln \frac{3-\nu}{3-\nu_0}$$
(2.12)

and the following expressions of the effective bulk and shear moduli in terms of ν :

$$\frac{G}{G_0} = \left(\frac{1+\nu_0}{1+\nu}\right) \left(\frac{\nu}{\nu_0}\right)^{10/9} \left(\frac{3-\nu_0}{3-\nu}\right)^{1/9} \\ \frac{K}{K_0} = \left(\frac{1-2\nu_0}{1-2\nu}\right) \left(\frac{\nu}{\nu_0}\right)^{10/9} \left(\frac{3-\nu_0}{3-\nu}\right)^{1/9}$$
(2.13)

A significant simplification is possible for calculation of the effective Young's modulus.

$$\frac{1}{E}\frac{dE}{d\rho} = -D(0, v_0) = -\frac{16}{45}\frac{(1-v^2)(10-3v)}{2-v}$$
(2.14)

Note that the dependence of the right hand part of (2.14) on Poisson's ratio is relatively weak provided $v_0 < 0.4$ so that the right hand part does not change much in this interval and, with accuracy that is satisfactory for rough estimates (that are sufficient for "irregular", and somewhat uncertain, 3-D microgeometries),

$$E \approx E_0 e^{-D_0 \rho} \tag{2.15}$$

where
$$D_0 = D(0, v_0) = -\frac{16}{45} \frac{(1-v_0^2)(10-3v_0)}{2-v_0}$$
.



Fig. 4. An almost linear dependence of $\frac{\nu E_0}{\nu_0 E}$ on crack density ρ , for various Poisson's ratios of the matrix ν_0 .

Remark. The above statement on weak dependence on Poisson's ratio does not apply to other elastic constants. Fig. 3 shows dependencies of the elastic constants on crack density calculated three different ways: (1) the non-interaction approximation, (2) numerical solution of the system (2.11), and (3) by the simplified solution (2.15). It also illustrates the above observation concerning dependencies of *E*, *K* and *G* on the effective Poisson's ratio.

An important observation is that the ratio of the effective Poisson's ratio to the effective Young's modulus, as calculated numerically from the system (2.11), is almost linear, with the proportionality coefficient almost independent of ν_0 (Fig. 4). This means that a simplified solution (2.14) for the Young's modulus implies an equally simple approximate solution for the effective Poisson's ratio:

$$\frac{\nu}{\nu_0} \approx \frac{E}{E_0} (1 + k\rho) = e^{-D_0\rho} (1 + k\rho)$$
(2.16)

where the proportionality coefficient *k* is only weakly dependent on v_0 ; approximately k = 0.22.

Thus, we have constructed an approximate solution for both elastic constants that has satisfactory accuracy in the range $\nu_0 < 0.4.$

3. Modeling the effect of intergranular cracking on the overall properties

We now modify the system (2.11) for intergranular microcracking. The latter is characterized by two specific features:

- (A) Certain saturation value ρ_* of crack density exists; it can be associated with fully cracked intergranular boundaries (that, in case of grains of the cubic shape, is about 0.54); it may also be somewhat lower;
- (B) A rather specific arrangement of cracks: prior to crack coalescence, there are substantial spacings between them so that crack interactions are relatively weak; they become strong only when the remaining ligaments become small.

Modeling of factor (B) is difficult, particularly in 3-D case, and is not undertaken in the present work. We modify the differential scheme with the account of factor (A) following the basic idea of McLaughlin (1977) that we reformulate for cracks: that only limited area is available for new cracks, so that, of the newly introduced increment $d\rho$, only $d\rho(1 - \rho/\rho_*)$ falls onto the intergranular surface that is still available. Hence we replace $d\rho \rightarrow \frac{d\rho}{(1-\rho/\rho_*)}$ in the system (2.11). Introducing the normalized crack density $\bar{\rho} = \rho/\rho_*$ we have

$$\frac{1}{K}\frac{dK}{d\bar{\rho}} = -\frac{19}{6}\frac{(1-\nu^2)}{1-2\nu}\frac{1}{\rho^*(1-\bar{\rho})}$$
$$\frac{1}{G}\frac{dG}{d\bar{\rho}} = -\frac{32}{45}\frac{(1-\nu)(5-\nu)}{2-\nu}\frac{1}{\rho^*(1-\bar{\rho})}$$
(3.1)

Closed form solution of this system is difficult to obtain. However, as far as the Young's modulus is concerned, the modification $d\rho \rightarrow d\rho(1 - \rho/\rho_*)$ leads to the following simple solution

$$E = E_0 (1 - \bar{\rho})^{D_0 \rho_*} \tag{3.2}$$

having satisfactory accuracy in the range $\nu_0 < 0.4$.

Remark. One can also arrive at (3.2) in a different way, as the microcrack density increases and the saturation value ρ_* that remains available for the introduction of new cracks gets smaller, the effect of newly introduced increment of crack density $d\rho$ obviously increases, and becomes infinite as $\bar{\rho} \rightarrow 1$. The simplest way to account for this factor is to assume that this increase can be described by the factor $(1 - \bar{\rho})^{-1}$ so that Eq. (2.14) is modified as follows:

$$\frac{1}{E}\frac{dE}{d\rho} = -\frac{D_0}{1-\bar{\rho}} \tag{3.3}$$

yielding the solution (3.2) that agrees with the non-interaction asymptotics at small ρ and has correct limit at $\bar{\rho} \rightarrow 1$.

The obtained result also implies a simple solution for the effective Poisson's ratio that follows from Eq. (2.16) by introducing (3.2) into this equation:

$$\frac{\nu}{\nu_0} = (1 - \bar{\rho})^{D_0 \rho_*} (1 + k \rho_* \bar{\rho})$$
(3.4)

In the conductivity problem, similar considerations yield

$$k = k_0 (1 - \bar{\rho})^{(8/9)\rho_*} \tag{3.5}$$

Fig. 5 illustrates the approximate results (3.2), (3.4) and (3.6) and compares them with the ones imply by the conventional differential scheme Eqs. (2.12), (2.14), and (2.6).

Comparison of the results for the elastic and conductive effective properties yields the following *cross-property connection*:

$$\frac{E}{E_0} = \left(\frac{k}{k_0}\right)^{9D_0/8} \tag{3.6}$$

This connection does not depend on ρ_* and coincides with the one obtained from the conventional differential scheme applied, separately, to the effective elastic and conductive properties of a solid with randomly oriented cracks (with the simplification (2.15) taken into account). Thus, the existence of saturation value ρ_* , and its exact value, do not affect the connection.

4. Discussion and conclusions

In intergranular microcracking, crack locations are limited to the intergranular area, i.e. there exists certain "saturation" crack density ρ_* . It can be associated with the state where all intergranular surfaces are fully cracked, implying $\rho_* \approx 0.54$ (it may also be somewhat smaller); at $\rho \rightarrow \rho_*$ the effective stiffnesses, and the effective conductivity, must tend to zero. This necessitates revision of the conventional effective media theories where crack locations can be arbitrary.

Such revision is applied to the differential scheme, DS, in the case of overall isotropy (as has been shown in computational simulations, the DS yields relatively accurate predictions for cracked solids). We first re-examine the usual formulation of the DS and construct simple closed-form expressions for the effective elastic moduli. Then we revise the DS with the account of the "saturation" crack density so that the effective moduli tend to zero as $\rho \rightarrow \rho_*$; similar revision is done in the context of effective conductivity.

This revision, aimed at the case of intergranular cracking, can be viewed as material-specific homogenization method. As such, it can be applied to other cases where positions of inhomogeneities (cracks, pores, inclusions) are limited to certain specific locations (for example, delamination cracks at boundaries of foreign particles).

The curves of Fig. 5 predicted by the developed scheme Eqs. (3.2), (3.4) and (3.6) have upward convexity; in particular the rate of change xxx become infinite on approach to the saturation point - in contrast with predictions of the differential scheme. This reflects the nature of the softening effect of interactions between intergranular cracks as the remaining ligaments get smaller: the interaction effects remain weak up to quite small ligaments, at which point they rapidly become strong. Note that the predicted rapid drop of stiffness upon approach to the critical point seems to be in agreement with experimental observations of Doncieux et al. (2008) and Fertig and Nickerson (2015) although the stiffness data were plotted there against temperature rather than crack density.

Note that, in the 2-D case, (2-D crack density is $\rho = (1/A) \sum l^{(k)2}$ where $2l^{(k)}$ is the length of *k*-th crack and *A* is reference area), an analogue of the system (2.11) has the form $dE/E = d\nu/\nu = -\pi d\rho$ and is easily integrated: in terms of normalized crack density $\bar{\rho} = \rho/\rho_*$

$$E/E_0 = \nu/\nu_0 = (1 - \bar{\rho})^{\pi \rho_*} \tag{4.1}$$

where, in the case of hexagonal grains, $\rho_* = 0.29$.

We note, in conclusion, that the cut-off point ρ_* for the effective properties is also predicted in the conventional self-consistent scheme (Budiansky and O'Connell, 1976). It may seem, therefore, that the self-consistent scheme can be used, instead of the above developed model. However, this scheme cannot be applied, for the following reason: the values of ρ_* predicted by it for the elastic and for the conductive properties are very different ($\rho_* = 9/16$ and $\rho_* = 9/8$, respectively) whereas they should obviously coincide.



Fig. 5. Effective elastic and conductive properties of a material with randomly oriented microcracks, as predicted by the conventional differential scheme and by its modification according to Eqs. (3.2), (3.4) and (3.6).

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Appendix

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A1. Property contribution tensors of inhomogeneities

This tensor, first introduced by Horii and Nemat-Nasser (1983) for ellipsoidal pores and cracks the context of elastic compliance, describes the inhomogeneity contribution to the overall property of interest. Referring to the book of Kachanov and Sevostianov (2018) for details, we outline the basic definitions and facts relevant for the present work.

We consider a representative volume element V containing an isolated inhomogeneity of volume V_1 . In the context of *elastic* properties, the average, over V strain is a sum

$$\varepsilon = \mathbf{S}^{\mathsf{o}}: \sigma^{\mathsf{o}} + \Delta \varepsilon \tag{A1.1}$$

where S^0 is the compliance tensor of the matrix and σ^0 is the farfield or "remotely applied" stress (that would have been uniform, at the site of the inhomogeneity, in its absence). The material is linear elastic, hence the extra strain due to inhomogeneity is a linear function of σ^0 :

$$\Delta \varepsilon = \frac{V_1}{V} \mathbf{H} : \sigma^0 \tag{A1.2}$$

where **H** is a fourth-rank *compliance contribution tensor* of the inhomogeneity normalized to its volume fraction. In the case of a *flat* crack (unit normal $\mathbf{n} = const$ along the crack surface), $\mathbf{H} = Sn\mathbf{Bn}$ where **B** is the displacement discontinuity tensor that gives the displacement discontinuity vector averaged over the crack surface *S* in terms of vector $\mathbf{t} = \boldsymbol{\sigma} \cdot \mathbf{n}$; $< \mathbf{u}^+ - \mathbf{u}^- > = \mathbf{B} \cdot \mathbf{t}$.

Alternatively, one can consider the extra average stress $\Delta \sigma$ due to the inhomogeneity under displacement boundary conditions (such that strains would have been uniform at the site of the inhomogeneity, in its absence). This defines the *stiffness contribution tensor N* of an inhomogeneity:

$$\Delta \sigma = \frac{V_1}{V} \mathbf{N} \cdot \varepsilon^0 \tag{A1.3}$$

The **H**- and **N**-tensors are functions of the inhomogeneity shape and elastic constants of the matrix and the inhomogeneity. They are interrelated: $\mathbf{N} = -\mathbf{C}^0$:**H**: \mathbf{C}^0 or $\mathbf{H} = -\mathbf{S}^0$:**N**: \mathbf{S}^0 .

In the context of conductivity (thermal or electric), analogues of **H** and **N**-tensors are the extra flux (thermal or electric), per volume *V*, under given imposed gradient of temperature or electric potential, or the extra gradient needed to maintain the same flux when the inhomogeneity is introduced. Thus, in the thermal conductivity problem, assuming the Fourier conduction law and homogeneous boundary conditions (the field of **U** would have been uniform in *V* in absence of the inhomogeneity), the change in **G** required to maintain the same heat flux when the inhomogeneity can be written as

$$\Delta \mathbf{G} = \frac{V_1}{V} \mathbf{R} \cdot \mathbf{U} \tag{A1.4}$$

where the symmetric second-rank tensor \mathbf{R} can be called the *resis*tivity contribution tensor of an inhomogeneity. Alternatively,

$$\Delta \mathbf{U} = \frac{V_1}{V} \mathbf{K} \cdot \mathbf{G} \tag{A1.5}$$

where **K** is the *conductivity contribution tensor* of an inhomogeneity. The two tensors are interrelated: $\mathbf{K} = -\mathbf{k}^0 \cdot \mathbf{R} \cdot \mathbf{k}^0$ or $\mathbf{R} = -\mathbf{r}^0 \cdot \mathbf{K}$ $\cdot \mathbf{r}^0$ where \mathbf{k}^0 and $\mathbf{r}^0 = (\mathbf{k}^0)^{-1}$ are the conductivity and resistivity tensors of the matrix.

In the context of *conductivity*, tensor **R** for *pores of the ellipsoidal shape* (and for them only) can be expressed in terms of Eshelby's tensor for conductivity problem \mathbf{s}^{C} as follows:

$$\mathbf{R} = \frac{V^*}{V} \frac{1}{k_0} \left(\mathbf{I} - \mathbf{s}^C \right)^{-1} \tag{A1.6}$$

where **I** is the second rank unit tensor. In particular, for a *spheroidal* pore of aspect ratio γ , tensor **s**^{*C*} is expressed in elementary functions:

$$\mathbf{s}^{\mathbf{K}} = f_0(\gamma)(\mathbf{I} - \mathbf{nn}) + (1 - 2f_0(\gamma))\mathbf{nn}$$
(A1.7)
where

$$f_0 = \frac{\gamma^2 (1-g)}{2(\gamma^2 - 1)}$$
(A1.8)

and the shape factor g is expressed in terms of the aspect ratio γ as follows

$$g(\gamma) = \begin{cases} \frac{1}{\gamma\sqrt{1-\gamma^2}} \arctan\frac{\sqrt{1-\gamma^2}}{\gamma}, & \text{oblate shape } (\gamma < 1) \\ \frac{1}{2\gamma\sqrt{\gamma^2-1}} \ln\frac{\gamma+\sqrt{\gamma^2-1}}{\gamma-\sqrt{\gamma^2-1}}, & \text{prolate shape } (\gamma > 1) \end{cases}$$
(A1.9)

Then one obtains the following relation for **R**:

$$\mathbf{R} = \frac{V^*}{V_0} \frac{1}{k_0} (A_1 \mathbf{I} + A_2 \mathbf{n} \mathbf{n})$$
(A1.10)

where

$$A_1 = \frac{1}{1 - f_0(\gamma)}, \ A_2 = \frac{1 - 3f_0(\gamma)}{2f_0(\gamma) \left[1 - f_0(\gamma)\right]}$$
(A1.11)

In the context of *elasticity*, tensor **H** for *pores of the ellipsoidal shape* (and for them only) can be expressed in terms of Eshelby's tensor for the elasticity problem s as follows:

$$\mathbf{H} = \begin{bmatrix} \mathbf{C}^0 : (\mathbf{J} - \mathbf{s}) \end{bmatrix}^{-1}$$
(A1.12)

where $J_{ijkl} = (1/2)(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$ is the fourth-rank unit tensor. For a general ellipsoid, components H_{ijkl} are expressed in terms of elliptic integrals. They reduce to elementary functions for the spheroidal shapes, as follows:

$$\begin{split} \tilde{H}_{1111} &\equiv G_0 H_{1111} = \frac{\kappa (f_0 - f_1)}{2(4\kappa - 1) \left[2\kappa (f_0 - f_1) - (4\kappa - 1)f_0^2 \right]} \\ &+ \frac{1}{4[1 - (2 - \kappa)f_0 - \kappa f_1]}; \\ \tilde{H}_{1122} &\equiv G_0 H_{1122} = \frac{\kappa (f_0 - f)_1}{2(4\kappa - 1) \left[2\kappa (f_0 - f_1) - (4\kappa - 1)f_0^2 \right]} \\ &+ \frac{1}{4[1 - (2 - \kappa)f_0 - \kappa f_1]} \\ \tilde{H}_{1133} &\equiv G_0 H_{1133} = \frac{-(2\kappa f_0 - f_0 + 2\kappa f_1)}{4(4\kappa - 1) \left[2\kappa (f_0 - f_1) - (4\kappa - 1)f_0^2 \right]}; \\ \tilde{H}_{3333} &\equiv G_0 H_{3333} = \frac{4\kappa - 1 - 6\kappa f_0 + 2f_0 - 2\kappa f}{4(4\kappa - 1) \left[2\kappa (f_0 - f_1) - (4\kappa - 1)f_0^2 \right]} \\ \tilde{H}_{1313} &\equiv G_0 H_{1313} = \frac{1}{4[f_0 + 4\kappa f_1]}; \quad \tilde{H}_{1313} \equiv G_0 H_{1313} = \frac{1}{4[f_0 + 4\kappa f_1]}; \end{split}$$

$$(A1.13)$$

where

$$\kappa = \frac{1}{2(1-\nu_0)}, \ f_1 = \frac{\gamma^2}{4(\gamma^2-1)^2} \Big[(2\gamma^2+1)g - 3 \Big]$$
(A1.14)

and f_0 , g are given by (A1.8) and (A1.9), respectively.

In the case of circular crack, $\gamma \to 0$, $g(\gamma) \approx (\pi/2)/\gamma$, $f_0(\gamma) \approx (\pi/4)\gamma$, $f_1(\gamma) \approx (\pi/8)\gamma$, and

$$\mathbf{H} = \frac{32(1-\nu^2)}{3(2-\nu_0)E_0} \frac{a^3}{V} \underbrace{\left(nIn - \frac{\nu_0}{2}nnnn\right)}_{\tilde{\mathbf{H}}}$$
(A1.15)

A2. Non-interaction approximation for the effective elastic and conductive properties

For randomly distributed spheroidal pores of identical aspect ratio γ , the effective (isotropic) conductivity of a porous material is given by

$$k = \frac{\kappa_0}{1 + \phi \Psi} \tag{A2.1}$$

where

$$\Psi = A_1 + A_2/3 \tag{A2.2}$$

and A_1 and A_2 are given by (A1.11) and ϕ is the volume fraction. For the effective elastic properties of the same material, the effective bulk, shear, and Young's moduli are:

$$K = \frac{K_0}{1 + \varphi B}, \ G = \frac{G_0}{1 + \varphi C} \ E = \frac{E_0}{1 + \varphi D}$$
 (A.2.3)

where *B* and *C* are shape factors expressed in terms of **H**-tensor given by (A1.13):

$$B = 3K_0 \frac{10H_{1111} + 10H_{1122} + 16H_{1133} + 5H_{3333}}{15}$$

$$C = 2G_0 \frac{13\tilde{H}_{1111} - 11\tilde{H}_{1122} - 8\tilde{H}_{1133} + 96\tilde{H}_{1313} + 8\tilde{H}_{3333}}{30}$$

$$D = E_0 \frac{3\tilde{H}_{1111} - \tilde{H}_{1122} + 4\tilde{H}_{1313} + \tilde{H}_{3333}}{3}$$
(A2.4)

Note that there are *two* shape factors in the elasticity problem – in contrast with one shape factor in the conductivity problem – since there are two independent isotropic elastic constants.

In the case of randomly oriented cracks,

$$B(\nu, 0) = \frac{16}{9} \frac{(1 - \nu^2)}{1 - 2\nu}; \ C(\nu, 0) = \frac{32}{45} \frac{(1 - \nu)(5 - \nu)}{2 - \nu};$$

$$D(0, \nu_0) = \frac{16}{45} \frac{(1 - \nu^2)(10 - 3\nu)}{2 - \nu}$$
(A2.5)

References

- Archie, G.E., 1942. The electrical resistivity log as an aid in determining some reservoir characteristics. Trans. AIME 146, 54–67.
- Benabou, L., Sun, Z., 2015. Analytical homogenization modeling and computational simulation of intergranular fracture in polycrystals. Int. J. Fract. 93, 59–75.
- Bristow, J.R., 1960. Microcracks, and the static and dynamic elastic constants of annealed heavily cold-worked metals. Br. J. Appl. Phys. 11, 81–85.
- Benveniste, Y., 1986. On the Mori–Tanaka method for cracked solids. Mech. Res. Commun. 13 (4), 193–201.
- Bruggeman, D.A.G., 1935. Berechnung verschiedener physikalisher Konstanten von heterogenen Substanzen. I. Dielectrizitätkonstanten und Leitfähigkeiten der Mischkörper aus isotropen Substanzen. Ann Physik Leipzig 24, 636–679.
- Bruggeman, D.A.G., 1937. Berechnung verschiedener physikalisher Konstanten von heterogenen Substanzen. III. Die elastische Konstanten der Quaiisotropen Mischkörper aus isotropen Substanzen. Ann Physik Leipzig 29, 160–178.
- Bruno, G., Kachanov, M., 2013. On modeling of microstresses and microcracking generated by cooling of polycrystalline porous ceramics. J. Eur. Ceram. Soc. 33, 1995–2005.
- Bruno, G., Kachanov, M., 2016. Microstructure-property connections for porous ceramics: the possibilities offered by micromechanics. J. Am. Ceram. Soc. 99, 3829–3852.
- Budiansky, B., O'Connell, R.J., 1976. Elastic moduli of a cracked solid. Int. J. Solids Struct. 12, 81–97.
- Doncieux, A., Stagnol, D., Huger, M., Chotard, T., Gault, C., Ota, T., Hashimoto, S., 2008. Thermo-elastic behaviour of a natural quartzite: itacolumite. J. Mater. Sci. 43, 4167–4174.
- Fabrikant, V.I., 1989. Applications of Potential Theory in Mechanics: A selection of New Results. Kluwer Academic Publishers, The Netherlands.
- Fertig, R.S., Nickerson, S.T., 2015. Towards prediction of thermally induced microcrack initiation and closure in porous ceramics. J. Am. Ceram. Soc. 99 (2), 581–588.
- Hashin, Z., 1988. The differential scheme and its application to cracked materials. J. Mech. Phys. Solids 36, 719–734.
 Horii, H., Nemat-Nasser, S., 1983. Overall moduli of solids with microcracks: load-
- Horii, H., Nemat-Nasser, S., 1983. Overall moduli of solids with microcracks: load--induced anisotropy. J. Mech. Phys. Solids 31, 155–171.
- Kachanov, M., Sevostianov, I., 2018. Micromechanics of Materials, with Applications. Springer 2018.

Kožušníková, A., Konecny, P., Plevovaa, E., Králováa, L., 2017. Changes of physical properties of silesian granite due to heat loading. Procedia Eng. 191, 426-433.

- Markov, K.Z., 2000. Elementary micromechanics of heterogeneous media. In: Markov, K.Z., Preziozi, L. (Eds.), Heterogeneous Media: Micromechanics Modeling Methods and Simulations. Birkhauser, Boston, pp. 1-162.
- McLaughlin, R., 1977. A study of the differential scheme for composite materials. Int. J. Eng. Sci. 15, 237-244.
- Mori, T., Tanaka, K., 1973. Average stress in matrix and average elastic energy of materials with misfitting inclusions. Acta Metall. 21, 571–574 (1973).
- Paggi, M., Corrado, M., Reinoso, J., 2018. Fracture of solar-grade anisotropic polycrystalline Silicon: a combined phase field-cohesive zone model approach. Comput. Methods Appl. Mech. Eng. 330, 123–148. Paggi, M., Wriggers, P., 2012. Stiffness and strength of hierarchical polycrystalline
- materials with imperfect interfaces. J. Mech. Phys. Solids 60, 557–572. Saenger, E.H., Krueger, O.S., Shapiro, S.A., 2006. Effective elastic properties of frac-
- tured rocks: dynamic vs. static considerations. Int. J. Fract. 139, 569-576.
- Sevostianov, I., Kachanov, M., 2002. Explicit cross-property correlations for anisotropic two-phase composite materials. J. Mech. Phys. Solids 50, 253–282. Chapter 1 in Sevostianov, I., Kachanov, M., 2013. Non-interaction approximation in
- the problem of effective properties. In: Kachanov, M., Sevostianov, I. (Eds.), Effective Properties of Heterogeneous Materials. Springer, pp. 1-96. Eds.

- Sevostianov, I., Kováčik, J., Simančík, F., 2006. Elastic and electric properties of closed-cell aluminum foams. Cross-property connection. Mater. Sci. Eng. A-420, 87-99.
- Torquato, S., 2002, Random Heterogeneous Materials: Microstructure and Macroscopic Properties. Springer.
- van Noort, R., Spiers, C.J., Pennock, G.M., 2008. Compaction of granular quartz under hydrothermal conditions: Controlling mechanisms and grain boundary processes. J. Geophys. Res. 113, 1-23 B12206.
- Vavakin, A.S., Salganik, R.L., 1975. Effective characteristics of nonhomogeneous media with isolated inhomogeneities. Mech. of Solids 10, 65-75 (English transl. of Izvestia AN SSSR, Mekhanika Tverdogo Tela).
- Wu, M.S., He, M.D., 1999. Prediction of crack statistics in a random polycrystal damaged by the pile-ups of extrinsic grain-boundary dislocations. Philos. Mag.-A 79 (2), 271–292.
- Zhang, W., Huang, Y., Dai, W., Jin, X., Yin, C., 2016. A fracture analysis of Ti-10Mo-8V-1Fe-3.5Al alloy screws during assembly. Materials 9 (852), 1–10.
- Zimmerman, R.W., 1985. The effect of microcracks on the elastic moduli of brittle materials. J. Mater. Sci. Lett. 4, 1457-1460.
- Zimmerman, R.W., 1991. Elastic moduli of solid containing spherical inclusions. Mech. Mater. 12, 17-24.