MATERIALS WITH CRACKS AND PORES: MICROMECHANICS, CROSS-PROPERTY CORRELATIONS AND APPLICATIONS

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ABSTRACT

Explicit correlations between two groups of anisotropic effective properties - conductivity and elasticity - are established for porous materials with anisotropic microstructures (non-randomly oriented pores of non-spherical shapes). In the present work, the correlations are derived in the framework of the non-interaction approximation. The elasticity tensor is expressed in terms of the conductivity tensor in the closed form.. Applications to realistic microstructures, containing mixtures of diverse pore shapes are discussed.

KEYWORDS

Elasticity, conductivity, effective properties, porous, cross-property

INTRODUCTION

An intriguing fundamental, as well as practical, question concerning anisotropic porous materials is the following one: can different effective physical properties be explicitly linked to one another? Such cross-property correlations become especially important for applications if one property (say, electric conductivity) is more easily measured than another property (full set of anisotropic elastic constants). The importance of such correlation has been pointed out by Berryman and Milton [1] and was particularly emphasized by Gibiansky and Torquato [2].

We consider solids with anisotropic microstructures formed by non-randomly oriented pores of non-spherical shapes, including mixtures of diverse shapes. The matrix material is assumed isotropic. The microstructures of this kind are relevant for many realistic materials, both man-made and naturally occurring. We examine cross-property correlations between two groups of anisotropic effective properties: elastic compliances and thermal conductivities. Note, that the problem of thermal conductivity is mathematically equivalent to the ones of electric conductivity, dielectric and

magnetic permeabilities or diffusion coefficients; therefore, our results apply to the mentioned physical properties as well.

We show that the correlations can be established in the explicit form that directly express the tensor of effective elastic compliances in terms of the conductivity tensor. These expressions are approximate, with the accuracy that remains good for a wide range of pore geometries.

Cross-property correlations between various effective properties of heterogeneous materials have been examined in several works. The most relevant for the present work is the classical paper of Bristow [3] in which an explicit connection between the effective conductivity and effective elastic moduli of a solid with cracks was derived. The derivation was done in the framework of the non-interaction approximation and for the case of random crack orientations (overall isotropy).

The conductivity – elasticity correlations were further investigated in the work of Berryman and Milton [1] on the two-phase composites, where the cross-property bounds (that are narrower than the classical Hashin-Shtrikman's ones) were established. The cross-property bounds were substantially advanced by Gibiansky and Torquato [4,5], who narrowed them under additional restrictions on the composite microgeometry and on the properties of constituents. Gibiansky and Torquato [4] also considered the transversely isotropic material (fiber reinforced composite) and established bounds for two of the five effective elastic constants in terms of the effective conductivities. Gibiansky and Torquato [5] established the cross-property bounds for the isotropic solid with cracks; this result is particularly valuable since neither upper nor lower non-trivial bounds for the effective elastic constants of cracked solids in the classical sense (i.e. in terms of the crack density) cannot be established [6].

It should be mentioned that correlations between other pairs of effective properties were considered in a number of works. Levin [7] interrelated the effective bulk modulus and the effective thermal expansion coefficient of the two phase isotropic composites. Milton [8] established cross-property bounds for the transport and the optical constants of isotropic composites. Similar bounds for the electrical and the magnetic properties were given by Cherkaev and Gibiansky [9]. The general approach to establishing various cross-property correlations was outlined by Milton [10], see also the recent review of Markov [11].

The present work focuses on the conductivity-elasticity correlations for the anisotropic porous materials (an isotropic matrix containing spheroidal pores of arbitrary orientational distribution and generally diverse aspect ratios). In contrast with the works that focus on bounds, our work derives the explicit cross-property correlations for the full set of effective anisotropic constants. In this sense, the present work can be viewed as an extension of Bristow's [3] explicit cross-property correlation for the isotropic cracked media.

The results of the present work are derived in the non-interaction approximation. Strictly speaking, it applies to the case of low concentration of pores (although, as far as materials with cracks are concerned, computer simulations of Kachanov [6] show that the predictions of the non-interaction approximation remain valid at relatively high crack densities). The key to our analysis is the recent finding of Shafiro and Kachanov [12] that the fourth rank effective elasticity tensor S_{ijkl} for the anisotropic porous microstructures can be represented, with good accuracy, in terms of a certain symmetric second rank tensor ω_{ij} and unit tensor δ_{ij}. The present work establishes a connection between ω_{ij} and the effective conductivity tensor.

ON THE EFFECTIVE ELASTIC PROPERTIES OF POROUS MATERIALS.

We briefly summarize the results on the effective elasticity of materials with pores of diverse shapes and orientations that are relevant for our analyses (see [12,13] for details).

Cavity compliance tensors. For a solid of volume V containing *one* cavity, the total strain per V under remotely applied stress tensor $\boldsymbol{\sigma}$ is a sum:

$$\boldsymbol{\varepsilon} = \boldsymbol{S}^0 : \boldsymbol{\sigma} + \Delta\boldsymbol{\varepsilon} \tag{1}$$

where $\boldsymbol{S}^0$ is the compliance tensor of the matrix (a colon denotes contraction over two indices). In the case of the isotropic matrix, $S^0_{ijkl} = \dfrac{1}{2G_0}\left\{\dfrac{1}{2}\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right) - \dfrac{v_0}{1+v_0}\delta_{ij}\delta_{kl}\right\}$.

Due to linear elasticity, strain $\Delta\boldsymbol{\varepsilon}$ is a linear function of the applied stress:

$$\Delta\boldsymbol{\varepsilon} = \boldsymbol{H}^E : \boldsymbol{\sigma} \tag{2}$$

where fourth rank tensor $\boldsymbol{H}^E$ - a *cavity compliance tensor* - was calculated for *3-D* ellipsoidal pores by Kachanov *et al* (1994). Superscript "E" indicates the elasticity problem (in contrast with $\boldsymbol{H}^C$, introduced in Section 3 in connection with the conductivity problem).

Let us consider a *3-D* cavity of the shape that possesses three mutually orthogonal planes of geometric symmetry, with unit normals $\boldsymbol{l}, \boldsymbol{m}, \boldsymbol{n}$ (this case covers ellipsoids but is not restricted to them). Cavity compliance tensor $\boldsymbol{H}^E$ has, due to symmetry, the following structure:

$$
\begin{aligned}
\boldsymbol{H}^E = \frac{2V_{cav}}{VE_0}\big[& \xi_1\boldsymbol{llll} + \xi_2\boldsymbol{mmmm} + \xi_3\boldsymbol{nnnn} + \eta_1(\boldsymbol{lm}+\boldsymbol{ml})(\boldsymbol{lm}+\boldsymbol{ml}) \\
& + \eta_2(\boldsymbol{mn}+\boldsymbol{nm})(\boldsymbol{mn}+\boldsymbol{nm}) + \eta_3(\boldsymbol{nl}+\boldsymbol{ln})(\boldsymbol{nl}+\boldsymbol{ln}) + \\
& + \zeta_1(\boldsymbol{llmm}+\boldsymbol{mmll}) + \zeta_2(\boldsymbol{mmnn}+\boldsymbol{nnmm}) + \zeta_3(\boldsymbol{nnll}+\boldsymbol{llnn})\big]
\end{aligned} \tag{3}
$$

where the three groups of components of $\boldsymbol{H}^E$-tensor - dimensionless coefficients ξ_i, η_i, ζ_i - represent the normal, shear and Poisson's ratio compliances of the cavity. For the ellipsoidal shape, they are given in the appendix in terms of Eshelby's tensor.

Further analysis is best done in terms of the *elastic potential,* rather than compliances: for a solid with many cavities, such a formulation identifies the proper parameters of pore density (that may not reduce to porosity if pores are non-spherical) and establishes the overall anisotropy in the cases of non-random pore orientations.

For volume V containing a cavity, the potential in stresses - such a function $f(\boldsymbol{\sigma})$ that (1) can be written as $\varepsilon_{ij} = \partial f / \partial \sigma_{ij}$ - is a sum of two terms:

$$f(\sigma) = (1/2)\sigma:\varepsilon(\sigma) = (1/2)\sigma:S^0:\sigma + (1/2)\sigma:H^E:\sigma \equiv f_0 + \Delta f \tag{4}$$

where f_0 is the potential in the absence of cavity In the case of the isotropic matrix $f_0 = (1/2E_0)\left\{(1+v_0)tr(\sigma \cdot \sigma) - v_0(tr\sigma)^2\right\}$ and Δf is the change due to cavity.

For a solid with *many* cavities,

$$\Delta f = (1/2)\sigma:\sum_k \Delta\varepsilon^{(k)} \tag{5}$$

where $\Delta\varepsilon^{(k)}$ are linear functions of applied stress σ. These functions reflect pore shapes, as well as elastic interactions between pores; their determination constitutes the most difficult part of the problem. Provided the mentioned functions are specified, the effective compliances S_{ijkl} are found from the relation

$$\varepsilon_{ij} = \partial f/\partial\sigma_{ij} = S^0_{ijkl}\sigma_{kl} + \partial(\Delta f)/\partial\sigma_{ij} \equiv S_{ijkl}\sigma_{kl} \tag{6}$$

We consider the approximation of non-interacting cavities. It is of the fundamental importance: besides being rigorous at small defect densities, it is the basic building block for various effective field methods. In this approximation, each cavity is placed in remotely applied stress σ and is not influenced by other cavities. Then, $\Delta\varepsilon_{ij}^{(m)} = H_{ijkl}^{E(m)}\sigma_{kl}$ and

$$\Delta f = \sum_k \Delta f^{(k)} = \frac{1}{2}\sigma:\sum_k H^{E(k)}:\sigma \tag{7}$$

where summation over cavities may be replaced by integration over orientations,

Representation of a cavity compliance tensor in terms of a second rank symmetric tensor.

For certain shapes of a cavity, its characterization by H^E - tensor can be reduced, with sufficient accuracy, to the one in terms of a certain second rank symmetric tensor $\boldsymbol{\Omega}$. Namely, we seek to approximate (uniformly with respect to all stress states) the potential change due to cavity $\Delta f = (1/2)\,\sigma : H^E : \sigma$ by the expression:

$$2\Delta f = \underbrace{B_1(tr\sigma)^2 + B_2 tr(\sigma \cdot \sigma)}_{\text{isotropic terms}} + \left[B_3\sigma \cdot \sigma + B_4(tr\sigma)\sigma\right]:\boldsymbol{\Omega} \tag{8}$$

where B_i are scalar coefficients that depend on the cavity shape and on v_0 (they are given in the Appendix and illustrated in Fig.2) and where $\boldsymbol{I}$ and $\boldsymbol{J}$ are the second rank and fourth rank unit tensors, respectively ($I_{ij} = \delta_{ij}$ and $2J_{ijkl} = \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}$). The "isotropic terms" in (8) are expressed in terms of stress invariants and do not depend on the cavity orientation. Symbols $\boldsymbol{nn}$ and $\boldsymbol{II}$ denote hereafter tensor (dyadic) products of vectors or tensors.

The condition for reduction of (3) to the simplified form (8) reduce to certain restrictions on components of tensor $\boldsymbol{H}^E$; see [12] for details. With the exception of a sphere, these conditions do not hold exactly, but they are satisfied, with good accuracy, for *spheroids*. In the case of a solid containing *many* pores, a similar condition is also satisfied.

EFFECTIVE CONDUCTIVITIES OF A MATERIAL WITH SPHEROIDAL PORES

We consider reference volume V of a material with the isotropic thermal conductivity k_0 containing an insulating ellipsoidal pore; a_1, a_2, a_3 are semi-axes of the pore and $\boldsymbol{l}, \boldsymbol{m}, \boldsymbol{n}$ are unit vectors along them. The change of heat flux vector $\Delta\boldsymbol{Q}$ (per volume V) due to the cavity is a linear function of the far-field temperature gradient $\boldsymbol{G}^0$ and hence can be written in the form:

$$\Delta\boldsymbol{Q} = \boldsymbol{H}^C \cdot \boldsymbol{G}^0 \tag{9}$$

where second rank tensor $\boldsymbol{H}^C$ is a function of the inclusion shape (superscript "C" indicates the conductivity problem). It has been derived in[14]. In the framework of the non-interaction approximation (each inclusion is subject to the same far-field temperature gradient, unperturbed by the presence of other inclusions), the effective conductivity tensor $\boldsymbol{K}$ is expressed in terms of a sum (or integral over orientations) $\sum_i \boldsymbol{H}^{C(i)}$ over individual inclusions:

$$\boldsymbol{K} = k_0\boldsymbol{I} + \sum_i \boldsymbol{H}^{C(i)} \tag{10}$$

where $k_0\boldsymbol{I}$ is the tensor of (isotropic) conductivity of the matrix.

CROSS-PROPERTY CORRELATIONS BETWEEN ANISOTROPIC COMPLIANCES AND CONDUCTIVITIES

Utilizing the above results we obtain the following explicit cross-property correlations that apply to an arbitrary mixture of pores of diverse aspect ratios – the central result of the present work::

$$E_0\left(\boldsymbol{S}-\boldsymbol{S}_0\right) = \left[\frac{b_1a_2 - b_4a_1}{a_2\left(a_2 + 3a_1\right)}\boldsymbol{II} + \frac{b_2a_2 - b_3a_1}{a_2\left(a_2 + 3a_1\right)}\boldsymbol{J}\right]\frac{tr\left(\boldsymbol{K}_0 - \boldsymbol{K}\right)}{k_0}$$

$$\tag{11}$$

$$+\frac{b_3}{a_2}\frac{1}{k_0}\left[\left(\boldsymbol{K}_0 - \boldsymbol{K}\right)\cdot\boldsymbol{J} + \boldsymbol{J}\cdot\left(\boldsymbol{K}_0 - \boldsymbol{K}\right)\right] + \frac{b_4}{a_2}\frac{1}{k_0}\left[\left(\boldsymbol{K}_0 - \boldsymbol{K}\right)\boldsymbol{I} + \boldsymbol{I}\left(\boldsymbol{K}_0 - \boldsymbol{K}\right)\right]$$

This relation covers all pore shapes (including mixtures of diverse shapes) and orientational distributions of pores in a unified way. It contains the matrix constants (elastic constants and conductivity) and does not contain any adjustable parameters. The shape dependent coefficients at tensorial terms in this basic relation are plotted in [13].

The presence of shape factors – coefficients at the tensorial terms in (11) – reflects the fact that pore shapes affect the elastic and the conductive properties differently. However, this difference is relatively mild, as seen from a relatively mild variation of these factors in the entire range of

possible shapes and vanishes altogether in the limiting cases of strongly oblate (aspect ratio smaller than 0.15) and strongly prolate (aspect ratio larger than 10) pores.

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