

## Three-phase plane composites of minimal elastic stress energy

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### 1. Abstract

In this work we seek a linearly elastic, three-phase anisotropic microstructural composite that stores minimal energy for a given homogeneous plane stress field. Our method consists of two steps: (i) determining the lower bound for effective stress energy accumulated in a particle of composite material, and (ii) proving that the bound is exact, i.e. it is achieved on a certain microstructure. Formulae for the energy bound are derived using a combination of the *translation method* and additional inequalities linking the components of a locally periodic stress field. Optimal layout of phases in a composite takes the form of a high-rank laminate. Its geometrical properties are obtained by the *field matching method* that enforces stress equilibrium in the optimal microstructure. It is shown that the applied technique leads to significant improvement of the Hashin-Shtrikman bounds on the effective constitutive properties of a three-phase composite material.

**2. Keywords:** Composites, Effective properties, Laminates, Optimal bounds.

### 3. Introduction

The vast majority of available results in the optimization of composite microstructures deals with a two-material case. Meanwhile, numerous applications call for optimal design of multimaterial composites, or even porous composites from several elastic materials and void, especially applications that utilize multi-physics, i.e. elastic and electromagnetic properties and those that deal with structures best adapted to variable environment such as natural morphologies perfected by evolution.

Optimal microstructures of two-phase and multiphase composites are drastically different. In contrast with the steady and intuitively expected topology of two-material optimal mixture (a strong material always surrounds weak inclusions), optimal multimaterial structures show the large variety of patterns. Topologies of these structures depend on volume fractions and their configurations reveal a geometrical essence of optimality, see [3, 4, 5, 6]. Geometries of multimaterial optimal structures are not unique, pieces of the same material may occur in different places of an optimal structure and they may correspond to different fields inside them.

In the last decades, the multimaterial, optimal elastic composites were studied by Gibiansky and Sigmund [7], Cherkaev and Zhang [5] and Cherkaev [4] among others. In our present work we generalize that results by investigating the case of arbitrarily anisotropic homogeneous stress field acting on a composite of two, well-ordered isotropic materials and a void. By this, we propose a next step from the well-elaborated *topology optimization* - a problem of optimal layout of one material and void.

Formally, the problem of optimal structures can be formulated as a question of minimizers of a variational problem with nonquasiconvex multiwell Lagrangians; the wells represent components' energies plus their costs. The minimizers (Young measures) are stress fields in the materials of an optimal composite. The challenging open problem is to build the quasiconvex envelope for Lagrangian with three or more wells. The problem is addressed by (i) finding exact bound (the lower bound for the quasiconvex envelope) and (ii) approximating these bounds by special class of minimizers. By building the lower bound, we also obtain sufficient conditions on optimal fields in materials that hint on the search for geometric patterns determining optimal structures.

Clearly, the method for finding optimal multiphase geometries differs from those for optimal two-material structures. Existing techniques for the bound such as Hashin-Shtrikman method, translation method, or analytic method of Bergman-Milton produced a number of results for two-material mixtures. These techniques, however, do not provide exact solutions for multimaterial composites. This, in turn, poses a mathematical challenge that needs to be addressed. In the last years, a new technique for finding optimal bounds for multimaterial mixtures was suggested in [3, 4, 6]. Its essence is to couple the translation method with the Alessandrini-Nesi inequality, see [2], that order and restrain values of the fields in any optimal composite. Roughly speaking, in the case tackled in the present research (elastic

2D microstructures of maximal stiffness for a mixture of two materials and void), it states that the sign of a stress field is constant in the whole microstructure. The technique was used to find the bounds of isotropic 2D elastic composites, see [4, 5] and anisotropic conducting composites made from two materials and void, see [6].

#### 4. Problem setting

Consider a domain  $\Omega \subset \mathbb{R}^2$  filled with two linearly elastic materials and a void. Non-homogeneous distribution of phases in  $\Omega$  is determined by its division into three disjoint subsets  $\Omega_i$ ,  $i = 1, 2, 3$ . Suppose that a boundary value problem (BVP) of linearized elasticity is posed in  $\Omega$ . If non-homogeneity of material layout is given by a fine partition of the domain then a solution to the BVP may be difficult to obtain even numerically. In such case, it is convenient to make use of the homogenization theory of periodic media in determining the simplified, effective Hooke's law in  $\Omega$  prior to solving the BVP. Due to local character of homogenization, in the sequel we consider arbitrary  $x \in \Omega$  which is sufficiently distant from the boundary  $\partial\Omega$ .

##### 4.1. Notation

Let  $Y = [0, 1]^2$  denote a unit cell corresponding to  $x \in \Omega$  and periodically extended to  $\mathbb{R}^2$ . Assume that  $Y$  is divided into three disjoint subcells  $Y_i$ ,  $i = 1, 2, 3$ , whose areas  $m_i$  are fixed. Write

$$Y = \bigcup_{i=1,2,3} Y_i, \quad |Y_i| = m_i, \quad \sum_{i=1}^3 m_i = 1 \quad (1)$$

and set  $(e_1, e_2)$  for a Cartesian basis in  $Y$ . Let  $\mathbb{E}_s^2$  stand for a space of plane, second-order symmetric tensors, and  $\mathbb{E}_s^4$  for the space of plane Hooke's tensors. Next, choose

$$E_1 = \frac{1}{\sqrt{2}}(e_1 \otimes e_1 + e_2 \otimes e_2), \quad E_2 = \frac{1}{\sqrt{2}}(e_1 \otimes e_1 - e_2 \otimes e_2), \quad E_3 = \frac{1}{\sqrt{2}}(e_1 \otimes e_2 + e_2 \otimes e_1) \quad (2)$$

for the basis in  $\mathbb{E}_s^4$ .

Suppose that  $Y_1$  and  $Y_2$  are filled with elastic isotropic materials whose constitutive properties are given by  $K_i = 1/k_i$ ,  $L_i = 1/\mu_i$ ,  $i = 1, 2$ , where  $k_i$  and  $\mu_i$  stand for bulk and shear moduli of  $i$ -th phase. Let  $K_3 = L_3 = +\infty$  which means that the third phase corresponds to void. Introduce a set  $A = \{A_1, A_2, A_{\text{void}}\}$  where

$$A_i = \frac{K_i}{2} E_1 \otimes E_1 + \frac{L_i}{2} (E_2 \otimes E_2 + E_3 \otimes E_3) \quad (3)$$

represents Hooke's compliance tensor of  $i$ -th non-degenerate isotropic phase. In the sequel we assume that the materials are well-ordered, i.e.  $K_1 < K_2 < K_3 = +\infty$  and  $L_1 < L_2 < L_3 = +\infty$ .

Set

$$\tau_0 = 1 e_1 \otimes e_1 + \varrho e_2 \otimes e_2 \quad (4)$$

for the average stress tensor in  $Y$ . Components 1 and  $\varrho$  denote principal values of  $\tau_0$  and  $(e_1, e_2)$  stands for its principal basis. It follows that

$$\tau_0 = S_0 E_1 + D_0 E_2, \quad S_0 = \frac{1+\varrho}{\sqrt{2}}, \quad D_0 = \frac{1-\varrho}{\sqrt{2}} \quad (5)$$

and  $S_0$ ,  $D_0$  represent spherical and deviatoric components of  $\tau_0$ . Without loss of generality we may assume  $|\varrho| \leq 1$ . It is understood that  $\tau_0$  denotes a value (calculated at  $x \in \Omega$ ) of a stress field solving the homogenized BVP.

Next, define a set of stress fields statically admissible in  $Y$

$$\Sigma = \left\{ \tau: \tau \in L_{\#}^2(Y, \mathbb{E}_s^2), \operatorname{div} \tau = 0 \text{ in } Y, \int_Y \tau(y) dy = \tau_0 \right\} \quad (6)$$

where  $L_{\#}^2(Y, \mathbb{E}_s^2)$  stands for the space of  $L^2$ -functions with values in  $\mathbb{E}_s^2$  and  $Y$ -periodic in  $\Omega$ . Fields  $\tau = \tau(y)$  belonging to this space are thus uniquely represented in the basis set in Eq.(2) by one spherical and two deviatoric components, respectively given by  $s = s(y)$  and  $d_1 = d_1(y)$ ,  $d_2 = d_2(y)$ , such that

$$s = \frac{\tau_{11} + \tau_{22}}{\sqrt{2}}, \quad d_1 = \frac{\tau_{11} - \tau_{22}}{\sqrt{2}}, \quad d_2 = \sqrt{2} \tau_{12} \quad (7)$$

hence  $\tau(y) = s(y) E_1 + d_1(y) E_2 + d_2(y) E_3$ .

Due to  $Y$ -periodicity,  $\tau \in \Sigma$  is endowed with two properties:

– function  $\det \tau(y)$ ,  $y \in Y$ , is quasilinear hence

$$\int_Y \det \tau(y) dy = \det \tau_0 = \varrho; \quad (8)$$

– function  $\det \tau(y)$ ,  $y \in Y$ , is locally univalent with  $\det \tau_0$ , that is

$$\det \tau(y) \geq 0 \text{ a.e. in } Y \text{ if } \det \tau_0 = \varrho \geq 0 \quad (9)$$

and the latter remains valid if “ $\geq$ ” is replaced by “ $\leq$ ”,

see [2]. The above-mentioned properties do not result in any restrictions on  $\tau \in \Sigma$ , they simply unveil certain characteristics of the stress fields related to assumed  $Y$ -periodicity. Nevertheless, Eq.(8) and Eq.(9) are of great significance in bounding the stress energy which is the central part of the study.

Decomposing the determinant function of a stress field according to

$$2 \det \tau = s^2 - (d_1^2 + d_2^2) \quad (10)$$

and considering  $\varrho \in [-1, 1]$ , allows for rewriting Eq.(9) in the form

$$\begin{aligned} s^2(y) &\geq d_1^2(y) + d_2^2(y) \text{ a.e. in } Y \text{ if } \varrho \in [0, 1], \\ s^2(y) &\leq d_1^2(y) + d_2^2(y) \text{ a.e. in } Y \text{ if } \varrho \in [-1, 0]. \end{aligned} \quad (11)$$

For further considerations, let us rephrase the requirements imposed on  $\tau \in \Sigma$ . First, define a set

$$\Sigma_{\text{uni}} = \left\{ \tau : \tau \in L^2_{\#}(Y, \mathbb{E}_s^2) \text{ with univalence property as in Eq.(11), } \right\}. \quad (12)$$

Next, write the restriction on the mean stress ( $\int_Y \tau = \tau_0$ ) in a form

$$\Sigma_{\text{av}} = \left\{ \begin{aligned} S_i, D_{ij}, \quad i, j = 1, 2: \quad & m_1 S_1 + m_2 S_2 = S_0, \\ m_1 D_{11} + m_2 D_{12} = D_0, \quad & m_1 D_{12} + m_2 D_{22} = 0, \\ S_i^2 \geq D_{i1}^2 + D_{i2}^2, \quad & \text{if } \varrho \in [0, 1], \\ S_i^2 \leq D_{i1}^2 + D_{i2}^2, \quad & \text{if } \varrho \in [-1, 0] \end{aligned} \right\} \quad (13)$$

where

$$S_i = \frac{1}{m_i} \int_{Y_i} s(y) dy, \quad D_{ij} = \frac{1}{m_i} \int_{Y_i} d_j(y) dy, \quad i, j = 1, 2, \quad (14)$$

denote average spherical and deviatoric stresses in non-degenerate phases. It follows that  $\Sigma \subseteq \Sigma_{\text{rel}}$  where

$$\Sigma_{\text{rel}} = \left\{ \tau : \tau \in \Sigma_{\text{uni}} \text{ and such that } S_i, D_{ij} \in \Sigma_{\text{av}}, \quad i, j = 1, 2 \right\} \quad (15)$$

stands for the set of relaxed stress fields, i.e. fields with neglected differential constraint  $\text{div} \tau = 0$  in  $Y$ .

#### 4.2. Composite materials of minimal stress energy

The (quadrupled) stress energy density in  $Y_i$ ,  $i = 1, 2$ , is calculated according to

$$U_i(\tau) = 4 [\tau : (A_i \tau)] = K_i s^2 + L_i (d_1^2 + d_2^2) \quad (16)$$

and we set  $U_3(\tau) = 0$  due to assumed  $\tau = 0$  in void. The contraction  $\tau : (A_i \tau)$  is realized by a standard operation  $[\tau]^T (A_i) [\tau]$  in the basis set in Eq.(2). Here  $[\tau]$  and  $(A_i)$  stand for a vector and matrix representations of respective quantities and  $[\tau]^T$  denotes a transpose of  $[\tau]$ . Effective energy is thus calculated according to

$$U_0(\varrho) = \inf \left\{ \sum_{i=1}^3 \int_{Y_i} U_i(\tau) dy \mid \tau \in \Sigma \right\} \quad (17)$$

and  $U_0(\varrho)$  is bounded from below by

$$U_*(\varrho) = \inf \left\{ U_0(\varrho) \mid Y_i \text{ as in Eq.(1)} \right\}. \quad (18)$$

Bounding the stress energy allows for restricting the values of effective constitutive properties. Indeed, by introducing  $K_*$ ,  $L_*$  and  $A_*$  linked similarly as in Eq.(3) one may claim  $U_*(\varrho)$  in the form

$$U_*(\varrho) = 4 [\tau_0 : (A_* \tau_0)] = K_* S_0^2 + L_* D_0^2 = \frac{1}{2} \left( K_* (1 + \varrho)^2 + L_* (1 - \varrho)^2 \right). \quad (19)$$

With this notation,  $K_*$  and  $L_*$  represent coupled bounds on effective moduli of a composite for fixed  $\varrho$ . They may be understood as constitutive properties of a homogenized medium adjusted to the external stress  $\tau_0 = S_0 E_1 + D_0 E_2$  in a sense of storing the minimal amount of energy in two directions  $E_1$ ,  $E_2$  simultaneously.

Note that in light of the above, the requirement of isotropy imposed on the effective medium is redundant. Indeed, the component of  $A_*$  related to the direction  $E_3 \otimes E_3$  may be arbitrary as  $\tau_0 : E_3 = 0$ . Non-isotropic microstructures are thus optimal if the amount of stress energy stored in them equals  $U_*(\varrho)$ .

Let us find formulae for  $K_*$  and  $L_*$ . To this end, note that by varying  $\varrho \in [-1, 1]$  on the r.h.s. of Eq.(19) we obtain a family of functions that are quadratic in  $\varrho$  and  $U_*(\varrho)$  represents an envelope of this family. Solving the system

$$\begin{aligned} U_*(\varrho) - \frac{1}{2} \left( K_* (1 + \varrho)^2 + L_* (1 - \varrho)^2 \right) &= 0, \\ \frac{d}{d\varrho} \left[ U_*(\varrho) - \frac{1}{2} \left( K_* (1 + \varrho)^2 + L_* (1 - \varrho)^2 \right) \right] &= 0, \end{aligned} \quad (20)$$

allows for determining the coefficients of  $U_*(\varrho)$ . They read

$$\begin{aligned} K_*(\varrho) &= \frac{U_*(\varrho)}{1 + \varrho} + \frac{1 - \varrho}{2(1 + \varrho)} \frac{dU_*(\varrho)}{d\varrho}, \\ L_*(\varrho) &= \frac{U_*(\varrho)}{1 - \varrho} - \frac{1 + \varrho}{2(1 - \varrho)} \frac{dU_*(\varrho)}{d\varrho}. \end{aligned} \quad (21)$$

Functions in Eq.(21) are extremal if their values belong to  $\partial G_m A$ , i.e. the boundary of  $G$ -closure of set  $A$ . Recall that  $G_m A$  contains all effective Hooke's tensors obtained by homogenization of components belonging to  $A$ , taken with arbitrary microstructure and fixed volume fractions  $m_i$ .

For determining  $U_*(\varrho)$  we make use of *the translation method* which proved to be an efficient tool in solving problems regarding energy and effective property bounds posed in various settings. The method starts from introducing *a translation parameter*  $\alpha \in \mathbb{T} \subset \mathbb{R}$  and rephrasing Eq.(16) in the form

$$U_i(\tau) = F_i(\tau, \alpha) - 2\alpha \det \tau, \quad i = 1, 2, \quad (22)$$

where

$$F_i(\tau, \alpha) = (K_i + \alpha) s^2 + (L_i - \alpha) (d_1^2 + d_2^2). \quad (23)$$

With Eq.(8) taken into consideration we calculate

$$\sum_{i=1}^3 \int_{Y_i} U_i(\tau) dy = \sum_{i=1}^3 \int_{Y_i} F_i(\tau, \alpha) dy - 2\varrho \alpha. \quad (24)$$

Next, we neglect the differential constraints on the stress field in  $Y$  which allows for taking the infimum in Eq.(17) on the set enlarged from  $\Sigma$  to  $\Sigma_{\text{rel}}$ . Another effect of dropping  $\text{div } \tau = 0$  in  $Y$  is that the optimal stress field  $\tau \in \Sigma_{\text{rel}}$  can be determined independently in each phase. Moreover, the search can be reduced to non-degenerate phases only as  $\tau = 0$  in void. Consequently, one obtains

$$\begin{aligned} U_0(\varrho) &\geq \Phi(\varrho, \alpha) - 2\varrho \alpha, \\ \Phi(\varrho, \alpha) &= \inf \left\{ \sum_{i=1}^2 \int_{Y_i} F_i(\tau, \alpha) dy \mid \tau \in \Sigma_{\text{rel}} \right\}. \end{aligned} \quad (25)$$

By Eq.(15) it is possible to split the latter task into two steps. First, we set

$$\Phi_i(S_i, D_{i1}, D_{i2}, \alpha) = \inf \left\{ \int_{Y_i} F_i(\tau, \alpha) dy \mid \tau \in \Sigma_{\text{uni}} \right\}, \quad i = 1, 2, \quad (26)$$

and we continue with

$$\Phi(\varrho, \alpha) = \min \left\{ \Phi_1 + \Phi_2 \mid S_i, D_{ij} \in \Sigma_{\text{av}} \right\}. \quad (27)$$

Stress energy estimation predicted by the translation method is thus given by

$$U_*(\varrho) \geq U_{\text{tr}}(\varrho) = \max \left\{ \Phi(\varrho, \alpha) - 2 \varrho \alpha \mid \alpha \in \mathbb{T} \right\} \quad (28)$$

and the equality  $U_*(\varrho) = U_{\text{tr}}(\varrho)$  holds if  $\tau \in \Sigma_{\text{rel}}$  solving Eq.(25), or equivalently Eq.(26) and Eq.(27), proves to be statically admissible, i.e.  $\tau \in \Sigma$ . This requirement is fulfilled if the stress field components in neighboring materials are consistent with  $\text{div } \tau = 0$  in  $Y$ . If this is the case then formula for  $U_{\text{tr}}(\varrho)$  is *optimal*, as it corresponds to the boundary of  $G_m A$  and it may be substituted in Eq.(21) for calculating extremal coupled effective properties of a three-phase composite.

## 5. Lower bound on the stress energy

Explicit calculation of  $\tau \in \Sigma_{\text{rel}}$  in two steps defined by Eq.(26) and Eq.(27) allows for determining  $U_{\text{tr}}(\varrho)$  by proper adjustment of the translation parameter  $\alpha$  in Eq.(28). Consequently, bounds on effective constitutive properties  $K_*(\varrho)$  and  $L_*(\varrho)$  related to  $\partial G_m A$  are obtained through Eq.(21) under the assumption that energy bound predicted by the translation method is optimal, i.e. that  $U_*(\varrho) = U_{\text{tr}}(\varrho)$  holds.

Assuming that  $K_i, L_i, i = 1, 2$ , are given, the sufficient condition of optimality of  $U_{\text{tr}}(\varrho)$  turns out to be dependent on mutual relations among  $m_1, m_2$  and  $\varrho$ . It results in the division of a polyhedron  $\Pi = \{(\varrho, m_1, m_2) : \varrho \in [-1, 1], m_1 \in [0, 1 - m_2], m_2 \in [0, 1]\}$  into several regions of optimality. Figure 1 shows an exemplary cross-section of  $\Pi$  by a plane  $m_2 = \text{const}$ .

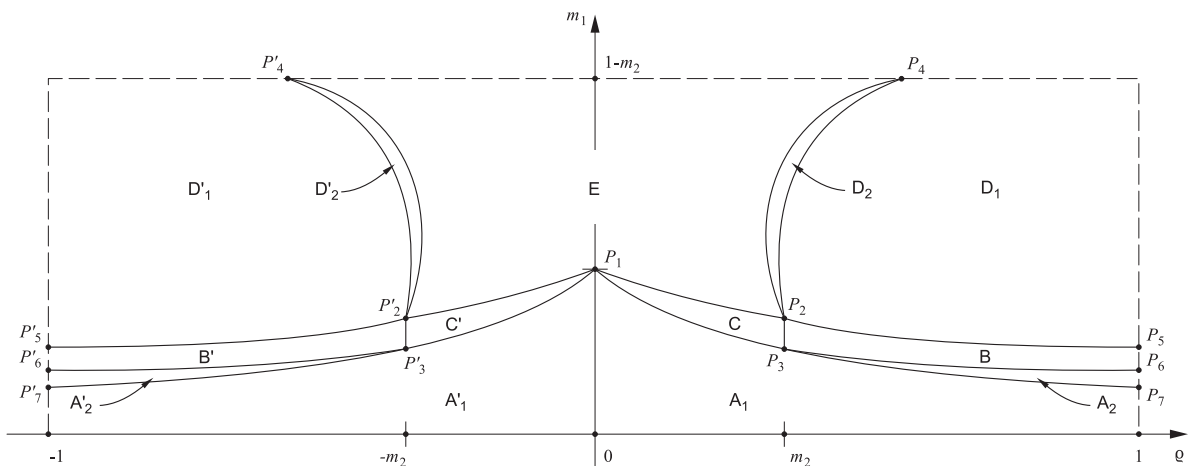


Figure 1: Regions of optimality related to a cross-section of a polyhedron  $\Pi$  by a plane  $m_2 = 0.35$ . Constitutive properties of nondegenerate materials are fixed to  $K_1 = 1, L_1 = 2, K_2 = 3, L_2 = 4$ .

### 5.1. Solving Eq.(26)

In Eq.(26) we wish to obtain  $\Phi_i(S_i, D_{i1}, D_{i2}, \alpha) > -\infty$  for  $i = 1, 2$ , as such property is crucial in subsequent derivation of a nontrivial energy bound  $U_{\text{tr}}(\varrho)$ . To this end, one should first determine a convex function that bounds the integrand  $F_i(\tau, \alpha)$  from below. Next, optimal relaxed stress fields  $\tau \in \Sigma_{\text{uni}}$  may be calculated by making use of the Jensen inequality. Applied to our case, it states that if  $F_i(\tau, \alpha)$  is convex in  $\tau$  then its integral over  $Y_i$  takes a minimum value on a constant stress field being the average of  $\tau$  over  $Y_i$ . Thus, with  $\tau$  decomposed into spherical and deviatoric parts, we expect the minimizers on the r.h.s. of Eq.(26) to be expressed in terms of averages  $S_i, D_{i1}, D_{i2}$ .

Full discussion of the topic is omitted here. We report the results of calculations of  $\Phi_i(S_i, D_{i1}, D_{i2}, \alpha)$  assuming that  $S_i, D_{ij}, i, j = 1, 2$ , are prescribed and  $K_i \neq L_i$ .

(I) For  $\alpha \in (-K_i, L_i)$  and  $\varrho \in [-1, 1]$  we obtain

$$\Phi_i(S_i, D_{i1}, D_{i2}, \alpha) = m_i(K_i + \alpha) S_i^2 + m_i(L_i - \alpha) (D_{i1}^2 + D_{i2}^2). \quad (29)$$

(II) For  $\alpha \geq L_i$  and  $\varrho \in [0, 1]$  it follows that

$$\Phi_i(S_i, D_{i1}, D_{i2}, \alpha) = m_i(K_i + L_i) S_i^2. \quad (30)$$

(III) For  $\alpha \leq -K_i$  and  $\varrho \in [-1, 0]$  we have

$$\Phi_i(S_i, D_{i1}, D_{i2}, \alpha) = m_i(K_i + L_i) (D_{i1}^2 + D_{i2}^2). \quad (31)$$

Other relations between  $\varrho$  and  $\alpha$  are not discussed here as they are irrelevant in our study.

5.2. Solving Eq.(27) and Eq.(28).

Having  $\Phi_i = \Phi_i(S_i, D_{i1}, D_{i2}, \alpha)$ ,  $i = 1, 2$ , explicitly calculated, we now turn to the problem of determining  $\Phi(\varrho, \alpha)$  and  $U_{\text{tr}}(\varrho)$  through (27) and (28). The details of calculations are omitted here due to their length. Let us mention that

$$U_{\text{tr}}(\varrho) = \begin{cases} \frac{(1+\varrho)^2}{2} \frac{(K_1+L_1)(K_2+L_2)}{m_1(K_2+L_2)+m_2(K_1+L_1)} - 2\varrho L_2 & \text{in A,} \\ \frac{(1+\varrho-2\sqrt{\varrho m_2})^2}{2m_1} (K_1+L_1) + 2\varrho K_2 & \text{in B,} \\ \frac{(K_2+L_2)\varrho^2}{2m_2} + (K_2-L_2)\varrho + \frac{(K_1+L_1)(1-m_2)^2 + (K_2+L_2)m_1m_2}{2m_1} & \text{in C,} \\ \frac{(1+\varrho)^2}{2} \frac{(K_1+L_1)(K_2+L_1)}{m_1(K_2+L_1)+m_2(K_1+L_1)} - 2\varrho L_1 & \text{in D,} \\ \frac{(1-\varrho)^2}{2} \frac{(K_1+L_1)(K_2+L_2)}{m_1(K_2+L_2)+m_2(K_1+L_1)} + 2\varrho K_2 & \text{in A',} \\ \frac{(1-\varrho-2\sqrt{-\varrho m_2})^2}{2m_1} (K_1+L_1) - 2\varrho L_2 & \text{in B',} \\ \frac{(K_2+L_2)\varrho^2}{2m_2} + (K_2-L_2)\varrho + \frac{(K_1+L_1)(1-m_2)^2 + (K_2+L_2)m_1m_2}{2m_1} & \text{in C',} \\ \frac{(1-\varrho)^2}{2} \frac{(K_1+L_1)(K_1+L_2)}{m_1(K_1+L_2)+m_2(K_1+L_1)} + 2\varrho K_1 & \text{in D'.} \end{cases} \quad (32)$$

Technically, determining  $U_{\text{tr}}(\varrho)$  in region E requires similar algorithm to the one used for the energy bound in other regions. However, explicit formula is not presented here due to its complexity.

5.3. Bounds on effective isotropic properties. Relation to Hashin-Shtrikman bounds.

Making use of Eq.(21) allows for calculating bounds on effective isotropic properties in each optimality region where  $U_*(\varrho)$  is determined. From the results obtained in the preceding Section and by assuming that  $U_{\text{tr}}(\varrho) = U_*(\varrho)$  it follows that formulae for  $K_*(\varrho)$  and  $L_*(\varrho)$  can be derived in any region except E. It also has to be pointed out that the equality of energy formulae in regions D<sub>1</sub> and D'<sub>1</sub> is not fully proved but it is strongly conjectured, see the discussion in Sec. 6.3. Recall that  $K_*(\varrho)$  and  $L_*(\varrho)$  are related to  $\partial G_m A$  (boundary of the  $G$ -closure of the set of effective properties) only if optimal stress fields predicted in the previous Section are statically admissible.

Region A:

$$K_*(\varrho) = \left( \frac{m_1}{K_1+L_1} + \frac{m_2}{K_2+L_2} \right)^{-1} - L_2, \quad L_*(\varrho) = L_2. \quad (33)$$

Region B:

$$\begin{aligned} K_*(\varrho) &= K_2 - \frac{[(1+\varrho)\sqrt{\varrho m_2} - 2\varrho][1+\varrho-2\sqrt{\varrho m_2}]}{2m_1\varrho(1+\varrho)} (K_1+L_1), \\ L_*(\varrho) &= \frac{\sqrt{\varrho m_2}(1+\varrho-2\sqrt{\varrho m_2})}{2m_1\varrho} (K_1+L_1) - K_2. \end{aligned} \quad (34)$$

Regions C and C':

$$\begin{aligned} K_*(\varrho) &= \frac{1}{2} \left[ (K_2 - L_2) + \frac{(1 - m_2)^2}{m_1(1 + \varrho)}(K_1 + L_1) + \frac{m_2^2 + \varrho}{m_2(1 + \varrho)}(K_2 + L_2) \right], \\ L_*(\varrho) &= \frac{1}{2} \left[ \frac{(1 - m_2)^2}{m_1(1 - \varrho)}(K_1 + L_1) + \frac{m_2^2 - \varrho}{m_2(1 - \varrho)}(K_2 + L_2) - (K_2 - L_2) \right]. \end{aligned} \quad (35)$$

Region D<sub>1</sub>:

$$K_*(\varrho) = \left( \frac{m_1}{K_1 + L_1} + \frac{m_2}{K_2 + L_1} \right)^{-1} - L_1, \quad L_*(\varrho) = L_1. \quad (36)$$

Region A':

$$K_*(\varrho) = K_2, \quad L_*(\varrho) = \left( \frac{m_1}{K_1 + L_1} + \frac{m_2}{K_2 + L_2} \right)^{-1} - K_2. \quad (37)$$

Region B' (note that  $\varrho < 0$  in B'):

$$\begin{aligned} K_*(\varrho) &= -\frac{\sqrt{-\varrho m_2}(1 - \varrho - 2\sqrt{-\varrho m_2})}{2m_1\varrho}(K_1 + L_1) - L_2, \\ L_*(\varrho) &= L_2 + \frac{[(1 - \varrho)\sqrt{-\varrho m_2} + 2\varrho][1 - \varrho - 2\sqrt{-\varrho m_2}]}{2m_1\varrho(1 - \varrho)}(K_1 + L_1). \end{aligned} \quad (38)$$

Region D'<sub>1</sub>:

$$K_*(\varrho) = K_1, \quad L_*(\varrho) = \left( \frac{m_1}{K_1 + L_1} + \frac{m_2}{K_1 + L_2} \right)^{-1} - K_1. \quad (39)$$

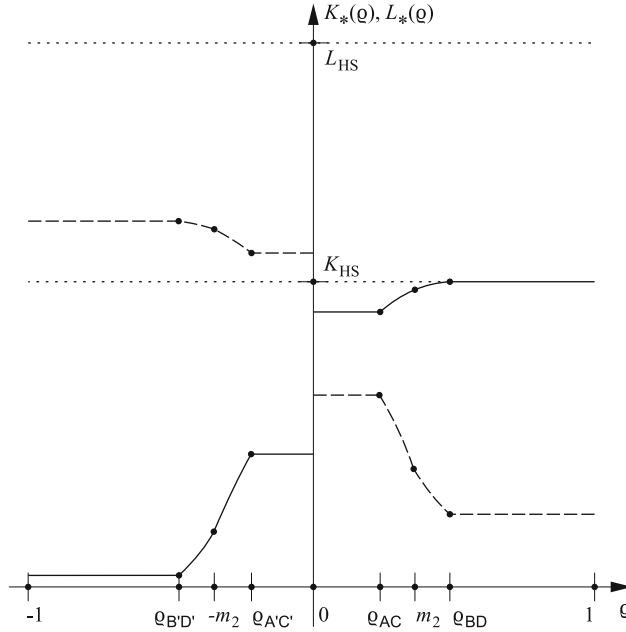


Figure 2: Comparison of optimal bounds  $K_*(\varrho)$  (solid lines),  $L_*(\varrho)$  (dashed lines) and the Hashin-Shtrikman estimates  $K_{HS}$ ,  $L_{HS}$  (dotted lines). Values of functions are calculated for  $m_1 = 0.17$ ,  $m_2 = 0.35$  and  $K_1 = 1$ ,  $L_1 = 2$ ,  $K_2 = 3$ ,  $L_2 = 4$ . Symbols  $\varrho_{AC}$ ,  $\varrho_{BD}$ ,  $\varrho_{A'C'}$ ,  $\varrho_{B'D'}$  refer to the anisotropy level of  $\tau_0$  at the interfaces between respective regions;  $\varrho = 0$  at the interface between A and A',  $\varrho = m_2$  at the interface between C and B,  $\varrho = -m_2$  at the interface between C' and B'.

Figure 2 illustrates the comparison of functions  $K_*(\varrho)$  and  $L_*(\varrho)$  representing coupled lower bounds on isotropic properties of a three-phase composite in different regions with the Hashin-Shtrikman uncoupled

bounds

$$\begin{aligned} K_{\text{HS}} &= \left( \frac{m_1}{K_1 + \alpha_K} + \frac{m_2}{K_2 + \alpha_K} \right)^{-1} - \alpha_K, & \alpha_K &= L_1, \\ L_{\text{HS}} &= \left( \frac{m_1}{L_1 + \alpha_L} + \frac{m_2}{L_2 + \alpha_L} \right)^{-1} - \alpha_L, & \alpha_L &= 2K_1 + L_1. \end{aligned} \quad (40)$$

Estimates  $K_{\text{HS}}$ ,  $L_{\text{HS}}$  are independent of  $\varrho \in [-1, 1]$ , as they do not incorporate an information on the anisotropy of  $\tau_0$ . Note that  $K_*(\varrho) \leq K_{\text{HS}}$  for all  $\varrho \in [-1, 1]$  and  $K_*(\varrho) = K_{\text{HS}}$  in region D while the inequality  $L_*(\varrho) < L_{\text{HS}}$  is slack in all regions.

At the boundary of regions B and C that correspond to maximal allowed volume fraction  $m_1$ , see Fig. 1, the optimal translation parameter reaches the value of  $L_1$ . The energy bound  $U_{\text{tr}}(\varrho)$  in region B transforms into the classical translation bound which corresponds to the Hashin-Shtrikman estimate on the bulk modulus for isotropic composites. This bound is realizable, see [4]. Similarly, at the boundary of regions B' and C', the optimal translation parameter reaches the value of  $-K_1$ . However, in this case, the energy bound  $U_{\text{tr}}(\varrho)$  in region B' *does not* give rise to the Hashin-Shtrikman bound on the shear modulus for isotropic composites.

Indeed,  $U_{\text{tr}}$  measures the energy of a composite subjected to an arbitrary stress field whose anisotropy is controlled by  $\varrho \in [-1, 1]$ . Consequently, if we set  $\varrho = 1$  then the effective energy is optimized only in a direction of the applied field  $\tau_0 = [(1 + \varrho)/2] E_1$  which is spherical, i.e. isotropic. On the contrary, setting  $\varrho = -1$  does not lead to a similar conclusion because applying the deviatoric field  $\tau_0 = [(1 - \varrho)/2] E_2$  and retaining the isotropy of a composite medium by controlling its response in the direction  $E_3$  at the same time is impossible.

## 6. Optimal high-rank laminates

The task of proving that optimal relaxed stress fields determined in regions A, B, C and A', B', C' coincide with statically admissible stress fields  $\tau \in \Sigma$  is two-fold. First, one should make use of the differential constraint  $\text{div}\tau = 0$  in deriving additional requirements on  $\tau \in \Sigma_{\text{rel}}$ . Next, it is necessary to show that these requirements are fulfilled in certain microstructures, so-called laminates of high rank.

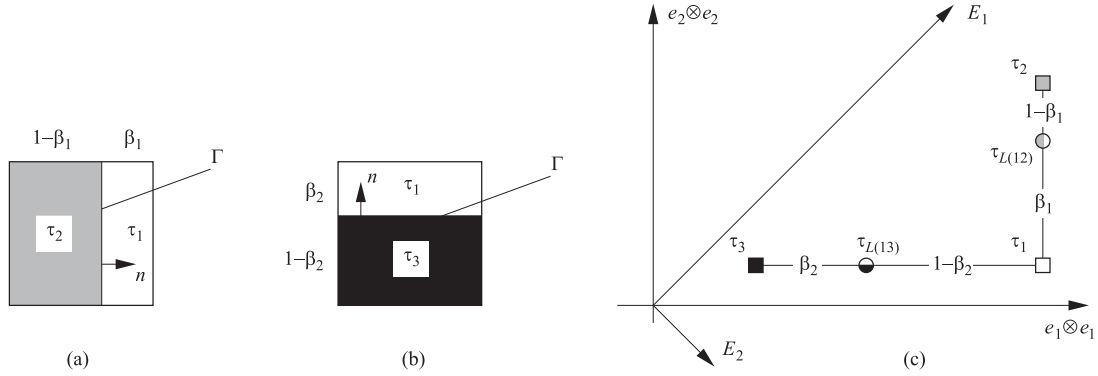


Figure 3: Rank-one connectivity of stress fields  $\tau_m$ ,  $m = 1, 2, 3$ : (a) simple laminate  $L(12)$  with phases taken in proportions  $\beta_1$ ,  $1 - \beta_1$ , a normal to the interface  $\Gamma$  given by  $n = e_1$  and stress fields  $\tau_1$  and  $\tau_2$ ; (b) simple laminate  $L(13)$  with phases taken in proportions  $\beta_2$ ,  $1 - \beta_2$ , a normal to the interface  $\Gamma$  given by  $n = e_2$  and constant stress fields  $\tau_1$  and  $\tau_3$ ; (c) graphical interpretation of compatibility conditions and mean fields  $\tau_{L(12)}$  in laminate  $L(12)$ ,  $\tau_{L(13)}$  in laminate  $L(13)$ . Vectors  $E_1$ ,  $E_2$  are defined in Eq.(2).

### 6.1. Field matching method

In calculations of optimal  $\tau \in \Sigma_{\text{rel}}$ , the differential constraint  $\text{div}\tau = 0$  in  $Y$  (equilibrium equation) is neglected. Consequently, energy-minimizing stress fields are determined in each phase independently. It follows that components of optimal relaxed fields may be incompatible with  $\text{div}\tau = 0$  on material interfaces which in turn means that  $\tau \notin \Sigma$ .

Suppose that two materials meet in a given microstructure at a line  $\Gamma$  and let  $n$  and  $t$  denote a normal and tangent to  $\Gamma$ . In our research we consider microstructures where phases are arranged in layers hence



$\Gamma$  takes a form of a straight line. Moreover, we assume that stress field in each layer is constant. By this we claim that if a given non-degenerate phase  $Y_i$ ,  $i = 1, 2$ , is distributed in  $p$  layers  $Y_{i,1}, Y_{i,2}, \dots, Y_{i,p}$ , then optimal  $\tau$  is *layer-wise constant* in  $Y_i$ . It follows that if  $p = 1$  then  $\tau$  is constant in entire  $Y_i$ . Equilibrium equation is thus fulfilled identically in each phase.

Here we discuss stresses  $\tau_1, \tau_2$  in two materials arranged in a rank-one laminate  $L(12)$ . Compatibility of stress fields in  $L(12)$  is also referred to as *rank-one connectivity* at  $\Gamma$ . Let  $\tau_1$  and  $\tau_2$  denote rank-one connected stress fields in materials layered in proportions  $\beta$  and  $1 - \beta$  respectively. Resulting mean field takes a value  $\tau_{L(12)} = \beta \tau_1 + (1 - \beta) \tau_2$ . Examples of rank-one connected stress fields and their mean values in simple laminates are sketched in Fig. 3. High-rank laminates are constructed by repeated rank-one layering scheme under the assumption that the materials resulting from previous laminations are homogeneous. These type of structures are considered in the subsequent Section.

## 6.2 Optimal microstructures in high-porosity regions A, B, C, A', B' and C'

The field matching method introduced in the previous Section allows for calculating the geometrical properties of optimal microstructures in high-porosity regions A, B, C, A', B' and C' with  $A = A_1 \cup A_2$  and  $A' = A'_1 \cup A'_2$ . Layering schemes determining the system of equations for the volume fractions of phases in each region of optimality of the translation bound  $U_{tr}$  is presented below. In this scheme  $\tau_{1,p}$  represents stress field in  $p$ -th layer of non-degenerate phase 1 and  $\tau_{2,q}$  refers to  $q$ -th layer of phase 2, while in void (phase 3) the stress field is constant and  $\tau_3 = 0$ .

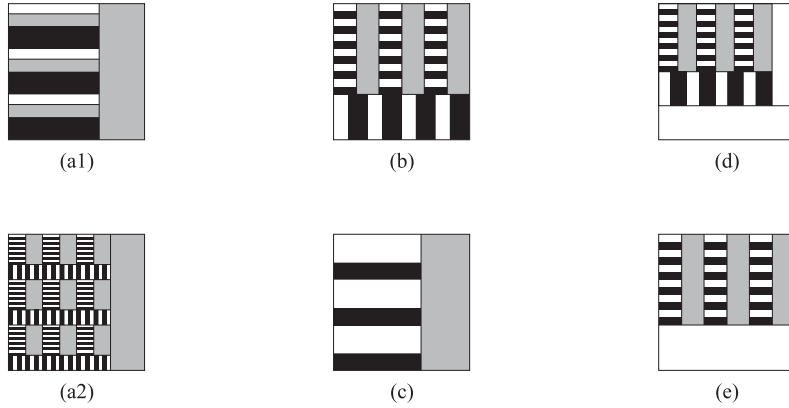


Figure 4: Optimal microstructures in different regions of optimality shown in Fig. 1: (a1) structure in  $A_1$  and  $A'_1$ , (a2) structure in  $A_2$  and  $A'_2$ , (b) structure in B and B', (c) structure in C and C', (d) structure in  $D_1$  and  $D'_1$ , (e) conjectured structure in  $D_2, D'_2$  and E.

Regions B and B': Substructures  $L(13_1)$  and  $L(13_2)$  are formed. In  $L(13_1)$ , the first layer of phase 1 (field  $\tau_{1,1}$ ) and void are laminated with  $n_1 = e_2$  and volume fractions  $\beta_1, 1 - \beta_1$  respectively. Stress field in  $L(13_1)$  is given by  $\tau_{L(13_1)} = \beta_1 \tau_{1,1}$ . In  $L(13_2)$ , the second layer of phase 1 (field  $\tau_{1,2}$ ) and void are laminated with  $n_2 = e_1$  and volume fractions  $\beta_2, 1 - \beta_2$ . Stress field in  $L(13_2)$  reads  $\tau_{L(13_2)} = \beta_2 \tau_{1,2}$ . Substructure  $L(13_1, 2)$  is formed: phase 2 and  $L(13_1)$  are laminated with  $n_3 = e_1$  and volume fractions  $\beta_3, 1 - \beta_3$ . Stress field in the substructure is given by  $\tau_{L(13_1,2)} = \beta_3 \tau_2 + (1 - \beta_3) \tau_{L(13_1)}$ . Final structure  $L(13_1, 2, 13_2)$  is formed: laminates  $L(13_2)$  and  $L(13_1, 2)$  are layered with  $n_4 = e_2$  and volume fractions  $\beta_4$  and  $1 - \beta_4$ , see Fig. 4(b).

Regions  $A_1$  and  $A'_1$ : Substructure  $L(123)$  is formed in two steps: (i) phase 1 and void are layered with  $n_1 = e_2$  and volume fractions  $\beta_1$  and  $1 - \beta_1$  (in this way  $L(13)$  with  $\tau_{0,1} = \beta_1 \tau_1$  is obtained), (ii) first layer of phase 2 and  $L(13)$  are laminated in the same direction with volume fractions  $\beta_2$  and  $1 - \beta_2$ ; this leads to  $L(123)$  with  $\tau_{L(123)} = \beta_2 \tau_{2,1} + (1 - \beta_2) \beta_1 \tau_1$ . Final structure  $L(123, 2)$  is formed: second layer of phase 2 (field  $\tau_{2,2}$ ) and  $L(123)$  are laminated with  $n_3 = e_1$  and volume fractions  $\beta_3$  and  $1 - \beta_3$ , see Fig. 4(a1). Stress field  $\tau_{L(123,2)} = \beta_3 \tau_{2,2} + (1 - \beta_3) \tau_{L(123)}$ .

Regions  $A_2$  and  $A'_2$ : We make use of “the coating principle”, see [1, Th. 9], in determining optimal microstructure. Laminate  $L(13_1, 2, 13_2)$  (optimal in regions B and B') is coated with a layer of phase 2, in the direction  $n_5 = e_1$  normal to the interface, and volume fractions  $1 - \beta_5$  and  $\beta_5$ . In this way,  $L(13_1, 2, 13_2, 2)$  is obtained, see Fig. 4(a2).

Regions C and C': Substructure  $L(13)$  is formed: phase 1 and void are laminated with  $n_1 = e_2$  and vol-

ume fractions  $\beta_1, 1 - \beta_1$  respectively. Homogenized stress field in  $L(13)$  is given by  $\tau_{L(13)} = \beta_1 \tau_1$ . Final structure  $L(13, 2)$  is formed: phase 2 and  $L(13)$  are laminated with  $n_2 = e_1$  and volume fractions  $\beta_2, 1 - \beta_2$  respectively. Stress field in the final structure, see Fig. 4(c), is given by  $\tau_{L(13,2)} = \beta_2 \tau_2 + (1 - \beta_2) \tau_{L(13)}$ .

### 6.3 Remarks on low-porosity regions D, D', and E

Following the discussion in [6] one may conclude that the anisotropic translation bound  $U_{tr}$  in regions D and D' is attained on certain microstructures only when the anisotropy level is not too large. The optimal structures for both conducting and elastic composites are similar, they are determined by high-rank orthogonal laminates  $L(13_1, 2, 13_2, 1, 1)$  obtained by enveloping the nucleus laminate  $L(13_1, 2, 13_2)$  - optimal for the region B - with two orthogonal layers of the first material. It is shown in [1] that such enveloping is stable with respect to the translation bound: if the nucleus satisfies this bound, then the enveloped nucleus also satisfies it. Microstructures shown in Fig. 4(d) are optimal in subregions  $D_1$  and  $D'_1$ . They reduce to those shown in Fig. 4(e) at the interfaces  $D_1$ - $D_2$  and  $D'_1$ - $D'_2$ . We conjecture that these microstructures are also most efficient high-rank laminates in regions  $D_2, D'_2$  and E.

## 7. Acknowledgements

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