Extremal structures of multiphase heat conducting composites

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Abstract

In this paper we construct microstructures of multiphase composites with unusual properties: their heat conductivity in one direction is equal to the harmonic or arithmetic mean of the phases' heat conductivities and the conductivity in an orthogonal direction does not equal either arithmetic or harmonic mean. Two dimensional three-phase structures are studied, but the results can be easily generalized for the three-dimensional composites with arbitrary number of phases.

1 Introduction

The paper is concerned with the structures of *multicomponent* composites with extremal effective properties. To explain what the "extremal" properties are we use the concept of the G_m-closure set. The G_m-closure is the set of the effective properties tensors of all mixtures (composites) that can be assembled from the given amounts of the given materials. For the heat conductivity problem, each effective conductivity tensor is determined by its eigenvalues (principal heat conductivities) $(\lambda_1, \lambda_2, ..,)$, and the G_m-closure is presented as a set of these vectors. The G_m-closure set is definitely bounded; its boundary corresponds to the composites with extremal properties. Now we call "extremal" the composite structures which correspond to the boundary of the G_m-closure.

The G_m-closure problem has attracted a lot of attention in recent years. The most complete results have been obtained for two-phase composites. Namely, the problem for the heat conducting materials has been completely solved for the mixtures of two

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isotropic phases, which means that all structures with extremal properties have been determined. The isotropic component of the G_m-closure has been obtained by Hashin and Shtrikman (1962); the full set of anisotropic composites has been found by Lurie & Cherkaev (1984b,1986), and Tartar (1985). The set of all pairs of electrical and magnetic permeability tensors of two-dimensional two-phase composites has been determined by Cherkaev & Gibiansky (1992) (the isotropic component of this set has been described earlier by Milton (1981a,b)). Here the coupling effect has been detected. Bounds on the complex conductivity of an isotropic two-dimensional composite have been obtained by Milton (1981a).

In elasticity, Hashin and Shtrikman have found the smallest rectangle in the bulk-shear moduli plane that contains the isotropic component of the G_m-closure for a two-phase composite. Milton and Phan-Thien (1982) and Cherkaev & Gibiansky (1993) have described a smaller set inside of this rectangle which represents more restrictive coupled bounds on the effective elastic moduli. The viscoelasticity problem has been studied by Gibiansky & Milton (1993), etc.

Most of the previously mentioned results have been obtained by using variational techniques (the Hashin-Shtrikman method, the Translation Method or their modifications) for constructing geometrically independent bounds for composite properties. These inequalities restrict the G_m-closure from outside. The optimality of the bounds has been proved by consideration of the special classes of microstructures which allow explicit calculation of their effective properties. The set of the effective properties of those classes restricts the G_m-closure from inside. When these two sets coincide, the complete description of the G_m-closure is achieved.

Relevant results for the multiphase composites are much weaker; there exists a gap between the already obtained bounds and the set of the properties of the known classes of microstructures. We mention here some papers where reader can find results and further references: the bounds for the conductivity of isotropic multiphase mixtures have been found by Hashin & Shtrikman (1962), attainability of the Hashin-Shtrikman bounds has been studied by Milton (1981c) and by Kohn & Milton (1988). Microstructures of optimal isotropic conductors have been studied by Lurie & Cherkaev (1985). Bounds on the effective properties of an anisotropic multiphase composite have been found by Zhikov (1986). The most complete analyses of the bounds and their attainability for the anisotropic mixtures can be found in the paper by Kohn & Milton (1988). The complex conductivity case has been studied by Golden & Papanicolaou (1985) and Milton & Golden (1990). Some bounds for the complex conductivity of multiphase composites have been given by Golden (1986) and by Milton (1987). Recent progress in the problem has been achieved by Nesi (1984). He has obtained a set of geometrically independent bounds on the conductivity of multiphase two-dimensional composites that improve upon the Hashin-Shtrikman results. The idea of his approach is close to the translation method. It is based on exploiting the special regularity properties of the solution of the conductivity equations in two dimensions that have been proved in the same paper.

However, in spite of numerous efforts, even the simplest problem of the exact bounds on the effective conductivity of a two-dimensional composite made of three isotropic materials is still mainly open: the gap between the bounds and the set of the known structures still exists.

In the present paper we consider one part of this problem: we explicitely construct anisotropic heat conducting structures (special laminates) which possess the extremal value of one of the principal heat conductivities. Therefore, these structures are certainly optimal: they belong to the boundary of the G_m-closure. Suggested structures correspond to the boundary points; the existance of these structures proves that the boundary component is exact.

Also we formulate some rules of assembling extremal mixtures. The construction of the microstructures exploits the idea of an "imitation" that was suggested by Schulgasser (1976) and then used by Milton (1981c,1987), and by Lurie & Cherkaev (1985).

For the sake of brevity we restrict ourselves in this paper to the particular case of a three-phase two-dimensional heat conducting composite. We focus our attention on composites with extremal value of one of the principal conductivities (they clearly form a component of the G_m-closure boundary) and we compare extremal two- and three-phases mixtures. Two-phase mixtures in two dimensions possess the following property: if the heat conductivity of the composite in some direction is equal to the harmonic or the arithmetic mean, then the conductivity in an orthogonal direction is equal to the arithmetic or the harmonic mean, respectively. Surprisingly, this is not true for multicomponent mixtures. We construct the heat conducting multiphase composites of a special structure with the following properties: the conductivity in one direction is extreme and equal to the harmonic mean of the phases' conductivities while the conductivity in an orthogonal direction is less than an arithmetic mean!

Although we consider the simplest problem, the results obtained have more general significance. First of all, they can be immediately applied to the anti-plane strain problem which is formally identical to the heat conductivity problem in two dimensions (the equations of these problems coincide if the heat conductivities are replaced by the inverse shear moduli, and the temperature is replaced by the stress potential). Also, the plane elasticity problem for materials with equal bulk moduli can be reduced to the problem discussed here, see Lurie & Cherkaev (1984a) for details. But even more important here seems to be a demonstration of principles of construction of optimal geometries for multicomponent composites. These principles are definitely not limited to the considered example but are applicable to any multicomponent mixture. The optimal structures that we have found, have no analogues for two-component mixtures.

The plan of the paper is the following: in section 2 we give the statement of the problem, section 3 summarizes known results, section 4 contains the main results of the paper, namely, the description of extremal microstructures that form a component of the G_m-closure boundary.

2 Statement of the problem

Consider a three-phase heat conducting composite with periodic structure. Suppose that each cell of periodicity is divided into three parts that have relative volume fractions m_1, m_2, and m_3, $m_1 + m_2 + m_3 = 1$. Suppose now that these parts are filled by three isotropic heat conducting materials with specific heat conductivities $\kappa_1,\ \kappa_2,\ \kappa_3$. Assume also that

$$\kappa_1 \le \kappa_2 \le \kappa_3. \tag{2.1}$$

The heat conductivity in this heterogeneous material is described by the Fourier law:

$$\boldsymbol{q}(x) = \kappa(x)\boldsymbol{e}(x), \tag{2.2}$$

where $\kappa(x)$ takes the values $\kappa_1,\ \kappa_2,\ \kappa_3$, $\boldsymbol{q}(x)$ and $\boldsymbol{e}(x)$ are the heat flux and temperature gradient, respectively, i.e.,

$$\operatorname{div}\, \boldsymbol{q} = 0, \quad \boldsymbol{e}(x) = \nabla T. \tag{2.3}$$

Homogenization of the heat conductivity in such a media leads to the relationship

$$\langle \boldsymbol{q}(x) \rangle = \boldsymbol{\kappa}_* \langle \boldsymbol{e}(x) \rangle, \tag{2.4}$$

where $\langle \cdot \rangle$ denotes averaging over the periodic cell, $\boldsymbol{\kappa}_*$ is the effective heat conductivity tensor. This tensor $\boldsymbol{\kappa}_*$ depends on the conductivity constants κ_i of the phases, on their volume fractions m_i in the mixture, and on the microstructure.

The tensor $\boldsymbol{\kappa}_*$ (which is second order, possibly anisotropic, symmetric, and positive definite) is characterized by its eigenvalues λ_1 and λ_2 and the eigenvectors (these have no importance for us). It has the representation:

$$\kappa_* = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} \tag{2.5}$$

in the basis associated with the eigenvectors of this tensor. The eigenvalues λ_1 and λ_2 are bounded by the arithmetic and harmonic means of the components conductivities, i.e.,

$$\kappa_h \le \lambda_i \le \kappa_a, \quad i = 1,\ 2, \tag{2.6}$$

where

$$\kappa_h = \left[\frac{m_1}{\kappa_1} + \frac{m_2}{\kappa_2} + \frac{m_3}{\kappa_3} \right]^{-1}, \qquad \kappa_a = m_1\kappa_1 + m_2\kappa_2 + m_3\kappa_3. \tag{2.7}$$

These bounds are known were proved by Wiener (1912) (see also Christensen (1979)). We call them arithmetic - harmonic mean (AHM) bounds because they bound the effective heat conductivity by the harmonic or arithmetic means of the components' conductivities. The set of the pairs (λ_1, λ_2) that satisfy the bounds (2.6) is represented by a square in the λ_1-λ_2 plane. We call it AHM square. The AHM bounds are optimal in the following sense: they describe the minimal rectangle in the plane λ_1-λ_2 which contains the G_m-closure set. To demonstrate this, consider a laminate structure which represents a point of the G_m-closure. One of the eigenvalues of the effective conductivity tensor of the laminates (the one that describes the conductivity in the direction $\boldsymbol{n}$ across the laminates) is equal to the harmonic mean of the components conductivities:

$$\lambda_n = \left[\frac{m_1}{\kappa_1} + \frac{m_2}{\kappa_2} + \frac{m_3}{\kappa_3}\right]^{-1}. \tag{2.8}$$

The other one, corresponding to the conductivity in the direction $\boldsymbol{t}$ along the laminates, is equal to the arithmetic mean of the components conductivities:

$$\lambda_t = m_1\kappa_1 + m_2\kappa_2 + m_3\kappa_3. \tag{2.9}$$

This shows that two symmetric corners (κ_h, κ_a) and (κ_a, κ_h) of the AHM square correspond to the laminate structure and that the AHM square is the minimal one, indeed.

Remark: The simple rules (2.8) and (2.9) for calculation of the effective conductivity of the laminates are the key (and the only one!) tool of our analyses. We call them harmonic and arithmetic mean rules, respectively. Note, that they are valid also for a laminate of anisotropic phases if the direction of lamination coincides with one of the principal axis of the phase's conductivity tensors.

There is a natural physical explanation of the laminates extremal properties. If one applies an external temperature gradient $\boldsymbol{e}$ *along* the layers then the local field $\boldsymbol{e}(x)$ in the laminates takes the same value in each point of the structure:

$$\boldsymbol{e}(x) = \mathrm{const}(x) = \boldsymbol{e}. \tag{2.10}$$

and

$$\boldsymbol{q}(x) = \kappa(x)\boldsymbol{e}. \tag{2.11}$$

Therefore the effective conductivity along the laminates (which relates $\langle \boldsymbol{e}(x)\rangle$ and $\langle \boldsymbol{q}(x)\rangle$) is given by the arithmetic mean rule (as for the conductivity of conductors in parallel), i.e.,

$$\langle \boldsymbol{q}(x)\rangle = \langle \kappa(x)\boldsymbol{e}\rangle = \langle \kappa(x)\rangle\boldsymbol{e}. \tag{2.12}$$

Similarly, the external heat flux applied *across* the layers causes the constant local heat flux $\boldsymbol{q}(x)$ =const(x) $= \boldsymbol{q}$. Then the effective conductivity across the laminates is given by the harmonic mean rule (as for the conductivity of conductors in series):

$$\langle \boldsymbol{e}(x) \rangle = \langle \frac{1}{\kappa(x)} \rangle \boldsymbol{q}. \tag{2.13}$$

We are interesting to find extremal composites that correspond to the bounds of the AHM square.

3 Known bounds

3.1 The G_m-closure for the two-phase composite

The G_m-closure set for the two-component mixtures was found by Lurie & Cherkaev (1984b), (1986) and Tartar (1985). In particular, in two-dimensional space it is described by the following inequalities:

$$1 + \frac{\kappa_1}{\lambda_1 - \kappa_1} + \frac{\kappa_1}{\lambda_2 - \kappa_1} \leq \frac{1}{m_2} \left(1 + \frac{2\kappa_1}{\kappa_2 - \kappa_1} \right), \tag{3.1}$$

$$1 + \frac{\kappa_2}{\lambda_1 - \kappa_2} + \frac{\kappa_2}{\lambda_2 - \kappa_2} \leq \frac{1}{m_1} \left(1 + \frac{2\kappa_2}{\kappa_1 - \kappa_2} \right), \tag{3.2}$$

and is illustrated in Fig.1. (The previously mentioned Hashin & Shtrikman (1962) bounds on the effective conductivity of a two-phase isotropic composite coincide with the inequalities (3.1)-(3.2) restricted to the case $\lambda_1 = \lambda_2$). These bounds are optimal in a sense that they correspond to special microstructures, see Lurie & Cherkaev (1984b) and Tartar (1985).

One can see that the G_m-closure set is smaller than the AHM square. Only the corner point $B = (\kappa_h, \kappa_a)$ and the symmetric point $D = (\kappa_a, \kappa_h)$ correspond to structures. The only structure which belongs to the boundary of the AHM square is the laminate (we recall that the conductivity along the laminates is equal to κ_a and the conductivity across them is equal to κ_h).

The slopes of the boundary curves (3.1), (3.2) are strictly negative and finite. This implies, in particular, that the arithmetic mean rule for the effective conductivity in any direction implies the harmonic mean rule for the effective conductivity in the orthogonal direction and vice versa. This observation corresponds to the fact that an increase of the maximal possible conductivity of the extremal mixture in one direction necessarily leads to a decrease of the conductivity in the orthogonal direction and vice versa. It is surprising that the last conclusion is not true for the multiphase mixtures. In this work we present the microstructures that correspond to some other (not corner) points on the boundary of the AHM square for the three-phase mixture.

3.2 The trace bounds for the multiphase composite

Bounds on the effective conductivity of an isotropic multiphase composite have been found by Hashin & Shtrikman (1962).

Namely, they found that the effective conductivity κ_* of such a mixture is restricted by the inequalities

$$\kappa^L \le \kappa_* \le \kappa^U, \tag{3.3}$$

where (for the two-dimensional three-phase problem)

$$\kappa^L = \left[\sum_{i=1}^{3} \frac{m_i}{\kappa_i + \kappa_1}\right]^{-1} - \kappa_1, \qquad \kappa^U = \left[\sum_{i=1}^{3} \frac{m_i}{\kappa_i + \kappa_3}\right]^{-1} - \kappa_3. \tag{3.4}$$

However, the attainability of the bounds for multicomponent structures is subject to some additional constrains. Namely, the lower bound (3.3) is exact and corresponds to some composite if $\kappa^L \le \kappa_2$, whereas the upper bound (3.3) is attainable if $\kappa^U \ge \kappa_2$, (see Milton (1981c), Lurie & Cherkaev (1985)).

An anisotropic version of the Hashin-Shtrikman bounds has been obtained by Zhikov (1986) and Kohn & Milton (1988) who called them trace bounds. They have the form:

$$\left[1 + \frac{\kappa_1}{\lambda_1 - \kappa_1} + \frac{\kappa_1}{\lambda_2 - \kappa_1}\right]^{-1} \ge m_2 \frac{\kappa_2 - \kappa_1}{\kappa_2 + \kappa_1} + m_3 \frac{\kappa_3 - \kappa_1}{\kappa_3 + \kappa_1}, \tag{3.5}$$

$$\left[1 + \frac{\kappa_3}{\lambda_1 - \kappa_3} + \frac{\kappa_3}{\lambda_2 - \kappa_3}\right]^{-1} \le m_1 \frac{\kappa_1 - \kappa_3}{\kappa_1 + \kappa_3} + m_2 \frac{\kappa_2 - \kappa_3}{\kappa_2 + \kappa_3}. \tag{3.6}$$

The point (λ_1, λ_2) on the lower bound (3.5) is known to be attainable if

$$\kappa_2 \ge \lambda_{\max} \ge \lambda_{\min} \ge \kappa_1, \quad (\lambda_{\max} - \kappa_1)\lambda_{\min} \le (\lambda_{\min} - \kappa_1)\kappa_2, \tag{3.7}$$

where $\lambda_{\max} = \max\{\lambda_1, \lambda_2\}$ and $\lambda_{\min} = \min\{\lambda_1, \lambda_2\}$; the point (λ_1, λ_2) on the upper bound (3.6) is attainable if

$$\kappa_3 \ge \lambda_{\max} \ge \lambda_{\min} \ge \kappa_2, \quad (\kappa_3 - \lambda_{\max})\lambda_{\min} \ge (\kappa_3 - \lambda_{\min})\kappa_2, \tag{3.8}$$

(see Kohn & Milton (1988)).

Figure 2 shows the λ_1-λ_2 plane where we draw the trace bounds (3.5)-(3.6) and mark the points (κ^L, κ^L) and (κ^U, κ^U) of the Hashin-Shtrikman bounds for the following values of parameters:

$$\kappa_1 = 1, \quad \kappa_2 = 5, \quad \kappa_3 = 25, \quad m_1 = 0.6, \quad m_2 = 0.2, \quad m_3 = 0.2. \tag{3.9}$$

The points on the bold part of the lower bound satisfy to the conditions (3.7) and, therefore, are attainable by some microstructures. At the same time one can check that the conditions (3.8) (for the upper bound) are never satisfied for the chosen values of the parameters, therefore the attainability of this bound is not established.

It should be noted, that the bounds (3.5)-(3.6) are definitely not exact in the sense that they cannot be achieved for all values of the parameters κ_1, κ_2, κ_3, m_1, m_2, m_3. For example, the lower bound does not satisfy natural limiting requirement

$$\hat{G}_m(\kappa_1, \kappa_2, \kappa_3, 0, m_2, m_3) = \hat{G}_m(\kappa_2, \kappa_3, m_2, m_3), \tag{3.10}$$

Here $\hat{G}_m(\kappa_1, \kappa_2, m_1, m_2)$ is the set of the pairs (λ_1, λ_2) satisfying the inequalities (3.1)-(3.2), and $\hat{G}_m(\kappa_1, \kappa_2, \kappa_3, m_1, m_2, m_3)$ is the set of the pairs (λ_1, λ_2) that satisfy to the bounds (3.5)-(3.6). In other words, the established lower bound of the G_m-closure does significantly depend on κ_1, even if the volume fraction of κ_1 tends to zero. When the volume fraction reaches zero, the inequality has a discontinuity: this contradicts the expected continuous dependence of the bounds on the volume fractions.

Remark: Note that the new bounds recently suggested by Nesi (1994) satisfy equalities of the type (3.10). They are more restrictive than the Hashin-Shtrikman bounds although the attainability of these bounds is also not stated.

The curves given by the bounds (3.5)-(3.6) do not pass through the corner points of the AHM square (unlike the two-component case); instead they pass through the points on the sides of this square (points E, F, G, H in Fig.2). It is important to emphasize that these bounds do not forbid the existence of the composites corresponding to the points on the sides of the AHM square. In the next section we demonstrate such structures.

4 Composite structures with extremal properties

In this section we find structures with one of their principal conductivities equal to the arithmetic mean bounds, $\lambda_1 = \kappa_a$, while the other one is bigger than the harmonic mean, $\lambda_2 \geq \kappa_h$. These structures correspond to points on the intervals DG and BF on the side of the AHM square, see Fig. 2. Then by using similar arguments we find structures with $\lambda_1 = \kappa_h$, $\lambda_2 \leq \kappa_a$ which correspond to points on the intervals BE and DH, see Fig. 2.

4.1 Structures that support constant temperature gradient

Let us begin with structures with principle conductivity in the direction x_1 equal to the arithmetic mean of the phase's conductivities. These structures must support a constant temperature gradient when exposed to an external field directed along x_1 axis: it guarantees the equality $\lambda_1 = \kappa_a$, see e.q. (2.11). On the other hand, they should not be able to support a constant heat flux in the orthogonal direction x_2. The last condition means that conductivity in the x_2 direction should not be equal to the harmonic mean, i.e. $\lambda_2 \geq \kappa_h$.

We construct the structure that consists of three sequential laminations in the following order:

1. First, we mix some amounts of the first and the third materials in proportions p and $1-p$ in the laminates parallel to the axis x_1, see Fig.3a. We choose the proportion p so that the conductivity of this laminate in the direction x_1 equals to the conductivity of the intermediate material κ_2, i.e.,

$$\lambda_1^{(1)} = p\kappa_1 + (1-p)\kappa_3 = \kappa_2. \tag{4.1}$$

Here and below the lower index in the notation $\lambda_i^{(k)}$ shows the direction, the upper index denotes the rank of the lamination. The required proportion p is equal to:

$$p = (\kappa_2 - \kappa_3)/(\kappa_1 - \kappa_3), \qquad \text{where} \quad p \in [0,1]. \tag{4.2}$$

The other eigenvalue $\lambda_2^{(1)}$ (in the direction x_2 across the laminates) is given by the harmonic mean rule and is equal to

$$\lambda_2^{(1)} = \left(p/\kappa_1 + (1-p)/\kappa_3\right)^{-1}. \tag{4.3}$$

2. At the second step we use the idea of imitation. We treat the previously obtained mixture as a new homogeneous material and mix it with the total amount available m_2 of the material κ_2 in the laminates parallel to the axis x_2, see Fig. 3b. We assume that the scale of the second lamination is much larger than the scale of the lamination at the first step.

Let us calculate the properties of the resulting composite. Both components have the same properties κ_2 and $\lambda_1^{(1)} = \kappa_2$ in the direction x_1. Therefore, the conductivity $\lambda_1^{(2)}$ in the direction x_1 (given by the harmonic mean rule) is equal to κ_2, i.e.

$$\lambda_1^{(2)} = \left[\frac{\mu}{(\mu+m_2)\lambda_1^{(1)}} + \frac{m_2}{(\mu+m_2)\kappa_2}\right]^{-1} = \left[\frac{\mu}{(\mu+m_2)} + \frac{m_2}{(\mu+m_2)}\right]^{-1}\kappa_2 = \kappa_2. \tag{4.4}$$

Here μ is the amount of the mixture of the first and third materials prepared at the first step of the process. On the other hand, $\lambda_1^{(2)}$ is equal to the arithmetic mean of the component's conductivities $\lambda_1^{(1)}$ and κ_2 (indeed, the arithmetic and the harmonic means of equal quantities trivially coincide!):

$$\lambda_1^{(2)} = \frac{\mu}{(\mu+m_2)}\lambda_1^{(1)} + \frac{m_2}{(\mu+m_2)}\kappa_2 = \kappa_2. \tag{4.5}$$

The conductivity of the mixture in the other direction x_2 is equal to the arithmetic mean of the component's conductivities $\lambda_2^{(1)}$ and κ_2 and is given by the lamination formula:

$$\lambda_2^{(2)}(\mu) = \frac{\mu}{(\mu + m_2)}\lambda_2^{(1)} + \frac{m_2}{(\mu + m_2)}\kappa_2 \tag{4.6}$$

This step is the key point of the construction. Indeed, we obtain the composite with effective properties in all directions equal to the arithmetic mean of the properties of the component's that enter the process at the second step. We have achieved this by a special choice of the intermediate material prepared at the first step. This material "imitates" the material κ_2 with respect to the conductivity in the direction x_1 and guarantees the *arithmetic* rule averaging (instead of the expected *harmonic* mean averaging) for the conductivity *across* the laminates. We follow here the idea exploited by Schulgasser (1976) for a three-dimensional polycrystal structure. This idea has been used also by Milton (1981c), and by Lurie & Cherkaev (1985) for multiphase isotropic structures. They have considered isotropic mixtures that imitate the intermediate material κ_2 with respect to the properties in all directions.

Remark: Let us comment on the properties of the structure in terms of the applied fields. If one applies an external temperature gradient in the direction x_1, the local field is constant throughout the composite because the properties of both components in this direction are equal to $\lambda_1^{(1)} = \kappa_2$, according to (4.4). Therefore, the conductivity $\lambda_1^{(2)}$ of this structure in the direction x_1 is equal to κ_2. On the other hand, if one applies the external temperature gradient in the direction x_2, the heat flux is not constant and the conductivity of the mixture in that direction is different from the harmonic mean value κ_h. Indeed, the conductivities (in the direction x_2) of the materials that are mixed at the second step differ, i.e. $\lambda_2^{(1)} \neq \kappa_2$.

3. To finish the construction let us laminate the already obtained amount

$$\nu_2 = \mu + m_2 \tag{4.7}$$

of the described composite with the remaining amounts

$$\nu_1 = m_1 - p\mu, \quad \nu_3 = m_3 - (1-p)\mu \tag{4.8}$$

of the first and the third materials, respectively. Now, we orient the lamination along the x_1 axis, see Fig.3c. Again, we assume that the scale of the third rank lamination is much larger than the scale of the lamination at the second step of the process.

Applying the arithmetic and harmonic mean rules we find that the conductivity $\lambda_1^{(3)}$ of this mixture in the direction x_1 is equal to

$$\lambda_1^{(3)} = \nu_1\kappa_1 + \nu_2\lambda_1^{(2)} + \nu_3\kappa_3. \tag{4.9}$$

One can substitute $\lambda_1^{(2)} = \kappa_2$ and the values of the concentrations ν_1, ν_2, ν_3 into the equation (4.9) and check that the resulting conductivity is given by the arithmetic mean of the initial components:

$$\lambda_1^{(3)} = m_1\kappa_1 + m_2\kappa_2 + m_3\kappa_3 \tag{4.10}$$

(see (4.5), (4.7), (4.8)). It is clear because this value is a result of three sequential arithmetic averagings. Physically, the external temperature gradient applied to the described composite along the x_1 axis causes the constant local field. This implies the equality (4.10).

The other principal conductivity equal to

$$\lambda_2^{(3)} = \left[\frac{\nu_1}{\kappa_1} + \frac{\nu_2}{\lambda_2^{(2)}} + \frac{\nu_3}{\kappa_3}\right]^{-1} = \lambda_2^{(3)}(\mu). \tag{4.11}$$

This value equal to the harmonic mean κ_h only if $\mu = 0$, otherwise it lies between κ_h and κ_a. Therefore, we obtain the composite that corresponds to some point of the side of the AHM square but not to its corners.

The effective conductivity of the obtained mixture depends on the amount μ of the material involved at the first step of the process. More exactly, the eigenvalue $\lambda_1^{(3)} = \kappa_a$ of the conductivity tensor is independent of μ but the other eigenvalue $\lambda_2^{(3)}$ depends on it. One can check, that $\lambda_2^{(3)}(\mu)$ monotonically increases as μ increases. By changing μ one obtains an interval of the attainable points on the side of the AHM square. The value $\mu = 0$ corresponds to the simple laminate composite, i.e. to the corner points $B = (\kappa_h, \kappa_a)$ or $D = (\kappa_a, \kappa_h)$ of the AHM square. The maximal value $\mu_{\max}$ corresponds to the other end of the interval.

The maximum amount μ allowed by this construction is equal to

$$\mu_{\max} = \min\left\{\frac{m_1}{p}, \frac{m_3}{(1-p)}\right\} = \min\left\{m_1\frac{\kappa_1 - \kappa_3}{\kappa_2 - \kappa_3}, m_3\frac{\kappa_1 - \kappa_3}{\kappa_1 - \kappa_2}\right\}, \tag{4.12}$$

(see (4.8)). Indeed, if

$$m_1/p \le m_3/(1-p), \tag{4.13}$$

or, equivalently,

$$m_1(\kappa_2 - \kappa_1) - m_3(\kappa_3 - \kappa_2) \le 0, \tag{4.14}$$

then μ is restricted by the available amount m_1 of the first phase. If, on the contrary,

$$m_1(\kappa_2 - \kappa_1) - m_3(\kappa_3 - \kappa_2) \ge 0, \tag{4.15}$$

then the value μ is restricted by the available amount m_3 of the third phase.

The structures corresponding to these two different limiting cases

$$\mu_{max} = \mu' = m_1/p \tag{4.16}$$

and

$$\mu_{max} = \mu'' = m_3/(1-p) \tag{4.17}$$

are shown schematically on Fig. 4a and Fig. 4b, respectively. The maximum value of the effective conductivity $\lambda_2^{(3)}$ is equal to

$$\lambda_{max} = \lambda_2^{(3)}(\mu_{max}) = \begin{cases} \lambda_2^{(3)}(\mu') & \text{if} \quad (4.14) \quad \text{holds}, \\ \lambda_2^{(3)}(\mu'') & \text{if} \quad (4.15) \quad \text{holds}. \end{cases} \tag{4.18}$$

In summary, we have found the composites corresponding to any point of the intervals

$$\lambda_1 = \kappa_a, \quad \lambda_2 \in [\kappa_h, \lambda_{max}]; \qquad \lambda_2 = \kappa_a, \quad \lambda_1 \in [\kappa_h, \lambda_{max}], \tag{4.19}$$

on the boundary of the AHM square.

4.2 Structures that support constant heat flux

In this section we describe the composites with the principal heat conductivity in the direction x_2 equal to the harmonic mean κ_h: $\lambda_2 = \kappa_h$.

Consider the same three-steps lamination procedure. At the first step we laminate the first and the third materials. We choose the fraction $\hat{p}$ so that the conductivity $\hat{\lambda}_2^{(1)}$ *across* the layers is equal to κ_2, i.e.

$$\hat{\lambda}_2^{(1)} = \left[\frac{\hat{p}}{\kappa_1} + \frac{1-\hat{p}}{\kappa_3}\right]^{-1} = \kappa_2, \tag{4.20}$$

(compare with (4.1)). This proportion is equal to:

$$\hat{p} = (\kappa_2^{-1} - \kappa_3^{-1})/(\kappa_1^{-1} - \kappa_3^{-1}), \quad \text{where} \quad \hat{p} \in [0,1] \tag{4.21}$$

(compare with (4.2)). The other principal conductivity $\hat{\lambda}_1^{(1)}$ is given by the arithmetic mean rule

$$\hat{\lambda}_1^{(1)} = \hat{p}\kappa_1 + (1-\hat{p})\kappa_3. \tag{4.22}$$

Now at the second step both components possess the same properties κ_2 and $\hat{\lambda}_2^{(1)} = \kappa_2$ in the direction x_2. Therefore, the conductivity $\hat{\lambda}_2^{(2)}$ in this direction equals to κ_2. Again, the arithmetic and harmonic means of the equal quantities $\hat{\lambda}_2^{(1)} = \kappa_2$ and κ_2 trivially coincide. The conductivity of the mixture in the other direction x_1 is equal to the harmonic mean of the component's conductivities $\hat{\lambda}_1^{(1)}$ and κ_2 given by the lamination formula:

$$\hat{\lambda}_1^{(2)}(\hat{\mu}) = \left[\frac{\hat{\mu}}{(\hat{\mu}+m_2)\hat{\lambda}_1^{(1)}} + \frac{m_2}{(\hat{\mu}+m_2)\kappa_2}\right]^{-1}. \tag{4.23}$$

Here $\hat{\mu}$ is the amount of the mixture of the first and the third materials prepared at the first step of the process. As we see, at the second step of this procedure we obtain a composite with effective properties in all directions equal to the *harmonic* mean of the conductivities of the components that enter the process at the second step. The intermediate material prepared at the first step "imitates" the material κ_2 with respect to the conductivity in the direction x_2.

To finish the construction we laminate the obtained amount $\hat{\nu}_2 = \hat{\mu} + m_2$ of the described composite with the remaining amounts $\hat{\nu}_1 = m_1 - \hat{p}\hat{\mu}$, and $\hat{\nu}_3 = m_3 - (1-\hat{p})\hat{\mu}$ of the first and the third materials, respectively. Applying the harmonic mean rule we obtain the conductivity $\hat{\lambda}_2^{(3)}$ of this mixture in the direction x_2 as

$$\hat{\lambda}_2^{(3)} = \left[\frac{\hat{\nu}_1}{\kappa_1} + \frac{\hat{\nu}_2}{\kappa_2} + \frac{\hat{\nu}_3}{\kappa_3}\right]^{-1} = \left[\frac{m_1}{\kappa_1} + \frac{m_2}{\kappa_2} + \frac{m_3}{\kappa_3}\right]^{-1}. \tag{4.24}$$

The other principal conductivity is equal to

$$\hat{\lambda}_1^{(3)}(\hat{\mu}) = \hat{\nu}_1\kappa_1 + \hat{\nu}_2\hat{\lambda}_1^{(2)} + \hat{\nu}_3\kappa_3. \tag{4.25}$$

This value is generally less than the arithmetic mean κ_a (they coincide only if $\hat{\mu} = 0$). Therefore, we have constructed composite that corresponds to the point on the other side of the boundary of the AHM square.

Again, the effective heat conductivity $\hat{\lambda}_1^{(3)}$ depends on the amount $\hat{\mu}$ of the material prepared at the first step of the process. One can check, that $\hat{\lambda}_1^{(3)}(\hat{\mu})$ monotonically decreases as $\hat{\mu}$ increases. The value $\hat{\mu} = 0$ corresponds to the simple laminate composite, i.e. to the corner point $B = (\kappa_h, \kappa_a)$ or $B = (\kappa_a, \kappa_h)$ of the AHM square. As in the previous Section one can check that the maximum amount $\hat{\mu}$ allowed by the available resources is equal to

$$\hat{\mu}_{\max} = \min\left\{\frac{m_1}{\hat{p}}, \frac{m_3}{(1-\hat{p})}\right\} = \min\left\{m_1\frac{\kappa_1^{-1}-\kappa_3^{-1}}{\kappa_2^{-1}-\kappa_3^{-1}}, m_3\frac{\kappa_1^{-1}-\kappa_3^{-1}}{\kappa_1^{-1}-\kappa_2^{-1}}\right\}, \tag{4.26}$$

(compare with (4.12)). The minimum value of the effective conductivity $\hat{\lambda}_1^{(3)}$ is equal to

$$\hat{\lambda}_{min} = \hat{\lambda}_1^{(3)}(\hat{\mu}_{max}) \tag{4.27}$$

In summary, we have found the composites corresponding to any point of the intervals

$$\hat{\lambda}_1 \in [\hat{\lambda}_{min}, \kappa_a], \quad \hat{\lambda}_2 = \kappa_h; \qquad \hat{\lambda}_2 \in [\hat{\lambda}_{min}, \kappa_a], \quad \hat{\lambda}_1 = \kappa_h \tag{4.28}$$

on the sides of the AHM square.

5 Discussion

- The composites obtained may cover significant part of the boundary of the AHM square. For example, consider the case when κ_3 is infinitely large (superconducting phase). Then $\kappa_a = \infty$ and this square also becomes infinitely large:

$$\lambda_1, \ \lambda_2 \ \in \ \left[(\frac{m_1}{\kappa_1} + \frac{m_2}{\kappa_2})^{-1}, \ \ \infty \right]. \tag{5.1}$$

  The obtained structures cover semi-infinite intervals (4.28) on the sides of the AHM square if, in addition, $\hat{\lambda}_{\min} \leq \infty$ or, equivalently,

$$m_1 \kappa_2 \geq (m_1 + m_3)\kappa_1. \tag{5.2}$$

  Indeed, one can check that in this case the extremal structure with the eigenvalues $\lambda_1 = \kappa_a$, $\lambda_2 = \hat{\lambda}_{\min}$ that we have found possesses finite conductivities in both directions; the intervals (4.28) are semi-infinite.

- We calculate the heat conductivities of the extremal composites for the parameters given by (3.9) and mark them on Figure 2. In the scale of Figure 2 the points corresponding to the optimal microstructures virtually coincide with the points E, F, G, and H of the trace bounds. It is not always so. Figure 5 illustrates the different situation when

$$\kappa_1 = 1, \quad \kappa_2 = 5, \quad \kappa_3 = 25, \quad m_1 = 0.004, \quad m_2 = 0.4, \quad m_3 = 0.596. \tag{5.3}$$

  For these parameters the attainability conditions (3.8) are satisfied for the most part of the upper bound (bold line on Fig.5), the microstructures that we found lie very close to the trace upper bound. The attainability conditions (3.7) failed in all the points of the lower bound. The distance between our structures (points Q and R) and the lower bound (points E and H) is very large. It is not surprising because the lower bound is expected to be crude for this choice of parameters (which come close to realizing the condition of the test (3.10)).

  From numerical experiments we have evidence that if the condition $\kappa^L \leq \kappa_2$ of attainability of the isotropic point of the Hashin-Shtrikman lower bound holds, our extremal structures lie close to the intersection of the lower bounds (3.5) with the boundary of the AHM square. The same is true for the upper bound (3.6) provided the inequality $\kappa^U \geq \kappa_2$ holds. Figure 2 shows that our structures can lie close to the trace bound even when this condition is not met.

- We have described here some components of the boundary of the G_m-closure. The remaining components are still unknown. The G_m-closure is, however, bounded from outside by the inequalities (3.5)-(3.6) mentioned above. On the other hand, following an approach similar to that discussed here, one can consider other special laminate composites and, at least, bound the G_m-closure from inside. We will not guess here what the extremal structures are, but clearly the boundary of the set of pairs of their eigenvalues connects the obtained points, as schematically shown on Fig.5 by the dashed line. This line represents the heat conductivity of the polycrystals made of the extremal composite corresponding to the point Q. (The effective conductivity of any two-dimensional polycrystal has the fixed value of the product of eigenvalues, see Lurie & Cherkaev (1981).) Note that these structures are used here because they are simple, not because they are extremal. The optimal structures for this component are still unknown.

- At this point we have not proved that there are no any microgeometries corresponding to the points in the intervals PQ and PM. This possibility cannot be ruled out based on our analyses.

- The obtained results can be easily generalized for the three-dimensional composite assembled of more than two phases. Indeed, the same construction (which exploits the idea of imitation) is directly applicable to the three-dimensional problem. Following the described scheme, one can obtain an anisotropic structures which possess the harmonic mean conductivity in x_1 direction, the arithmetic mean conductivity in an orthogonal direction x_2, and a conductivity in the third direction x_3 which is less than the arithmetic mean but belongs to the interval (4.28). These structures correspond to a cylindrical geometries with the cross-section (along (x_1, x_3) plane which is identical to the described above two-dimensional structures (Fig. 1-2). Similarly, one can find structures which possess arithmetic mean heat conductivity in two orthogonal directions, but with the conductivity in the third direction which belongs to the interval (4.19). In other words, we are able to show the attainability of all points of the AHM cube in a neighborhood of the corner points $(\lambda_a, \lambda_a, \lambda_h)$, $(\lambda_a, \lambda_h, \lambda_a)$, and $(\lambda_h, \lambda_a, \lambda_a)$.

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FIGURE CAPTIONS

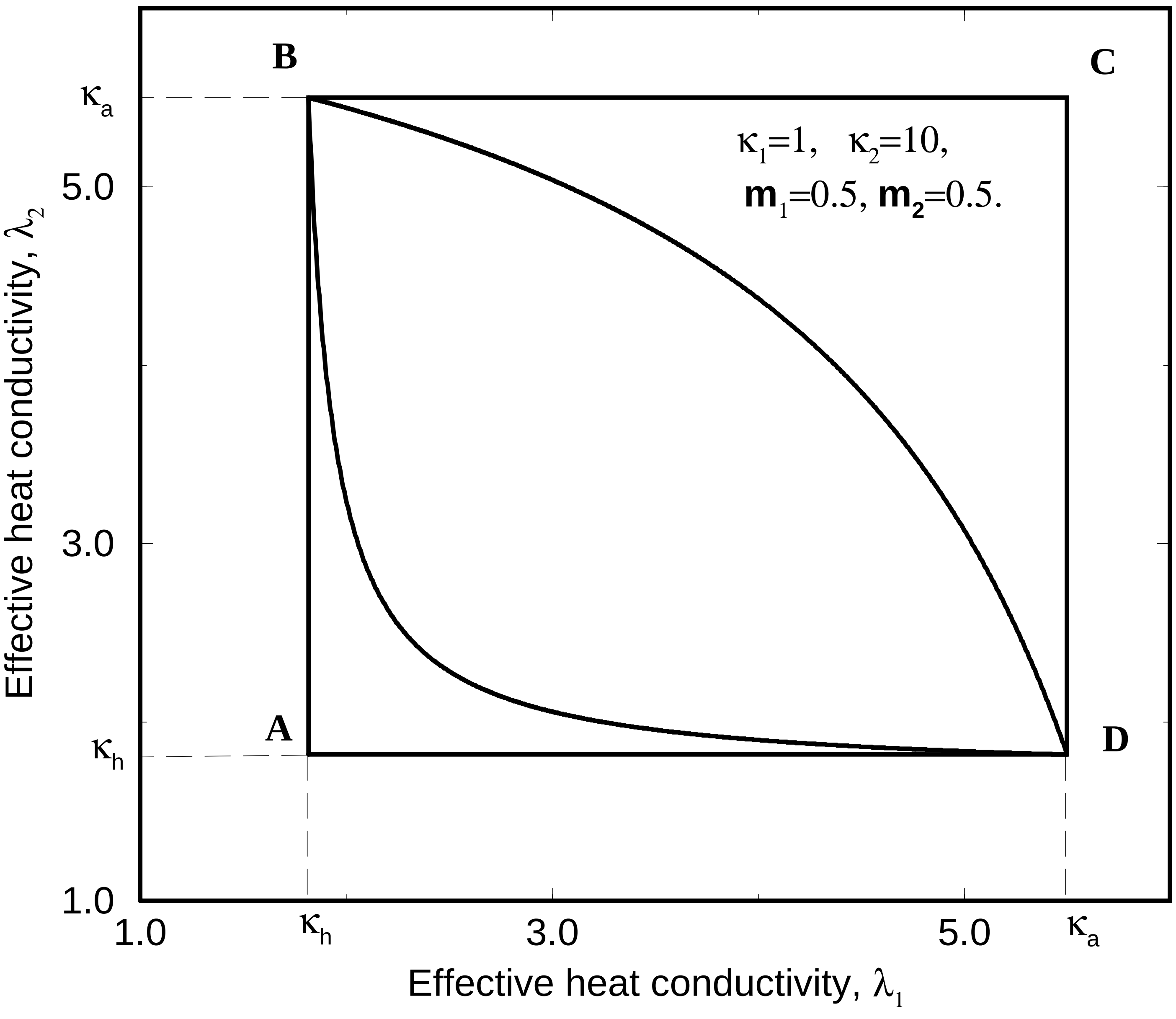
Figure 1: G_m-closure set for the two-phase two-dimensional problem. Square $ABCD$ corresponds to the AHM bounds.

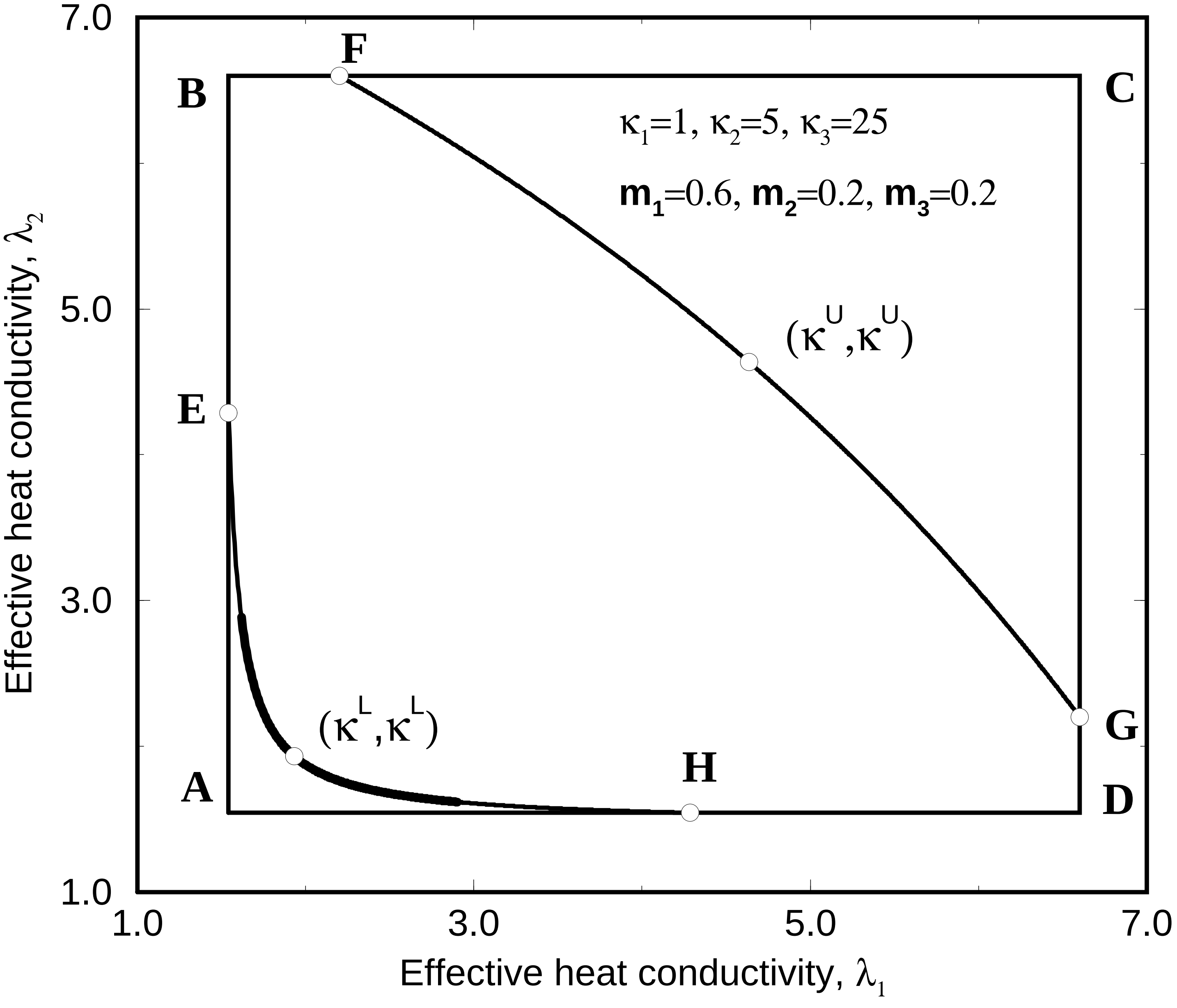
Figure 2: Bounds on the G_m-closure set for the three-phase two-dimensional problem. The bold part of the lower bound EH is known to be attainable. In the scale of the Figure, the points E, F, G, H (that mark the intersections of the bounds (3.5), (3.6) with the boundary of the AHM square $ABCD$) are indistinguishable from the points that correspond to the structures that we found.

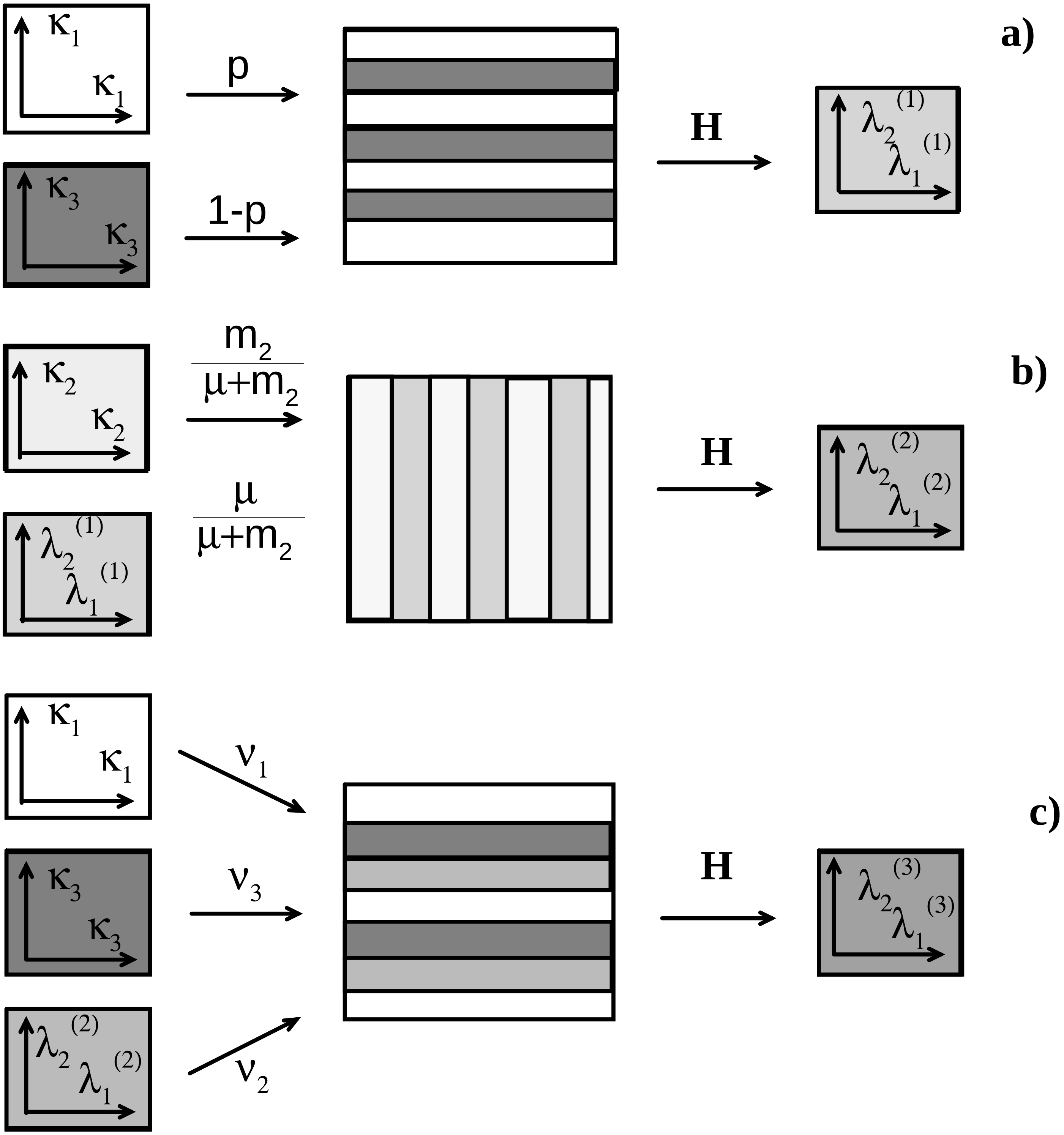
Figure 3: Schematic picture of our three-step process for creating optimal microstructures.

Figure 4: Schematic picture of the extremal microstructures corresponding to the points E, F, G, or H. Figure 4a (4b) corresponds to the higher (lower) volume fraction of the third phase.

Figure 5: Bounds on the G_m-closure set for the three-phase two-dimensional problem. The bold part of the upper bound FG is known to be attainable. In the scale of the Figure, the points F and G (that mark the intersections of the upper bound (3.6) with the boundary of the ANM square $ABCD$) are virtually indistinguishable from the points that correspond to the structures that we found. The points Q and R correspond to the extremal microstructures described in the text. Dashed line corresponds to the curve $\lambda_1\lambda_2 = \lambda_{1Q}\lambda_{2Q}$ where λ_{1Q} and λ_{2Q} are hte moduli of the point Q. This corresponds to a polycrystal comprised of grains of material Q.

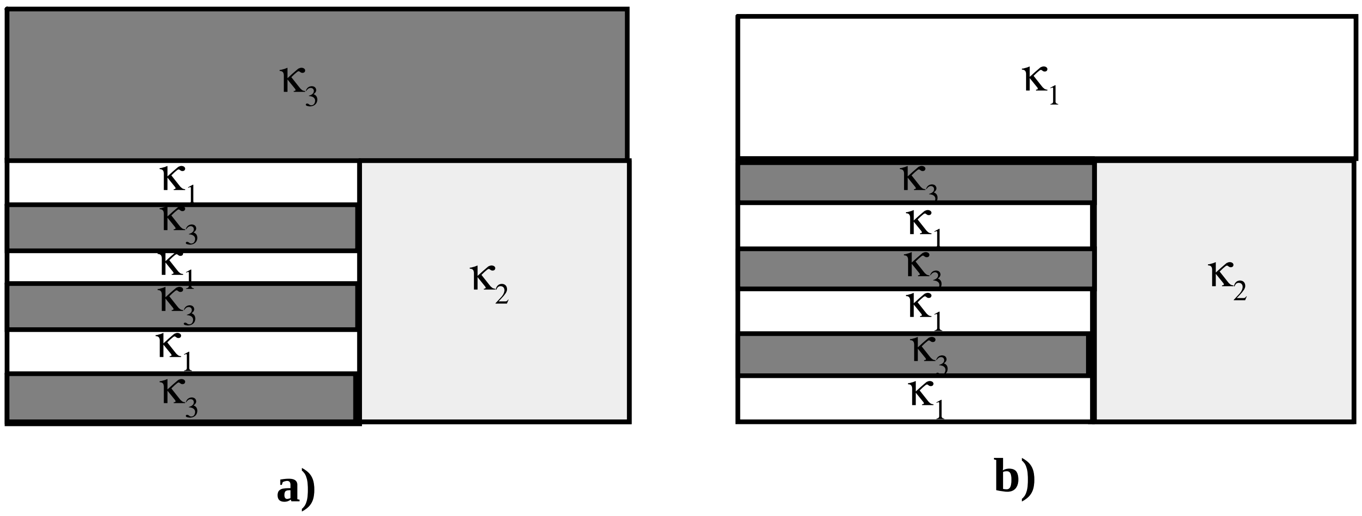

B
C
A
D
κ_a
κ_h
5.0
3.0
1.0
κ_1=1, κ_2=10,
$\mathbf{m}_1$=0.5, $\mathbf{m_2}$=0.5.
1.0
κ_h
3.0
5.0
κ_a
Effective heat conductivity, λ_1
Effective heat conductivity, λ_2

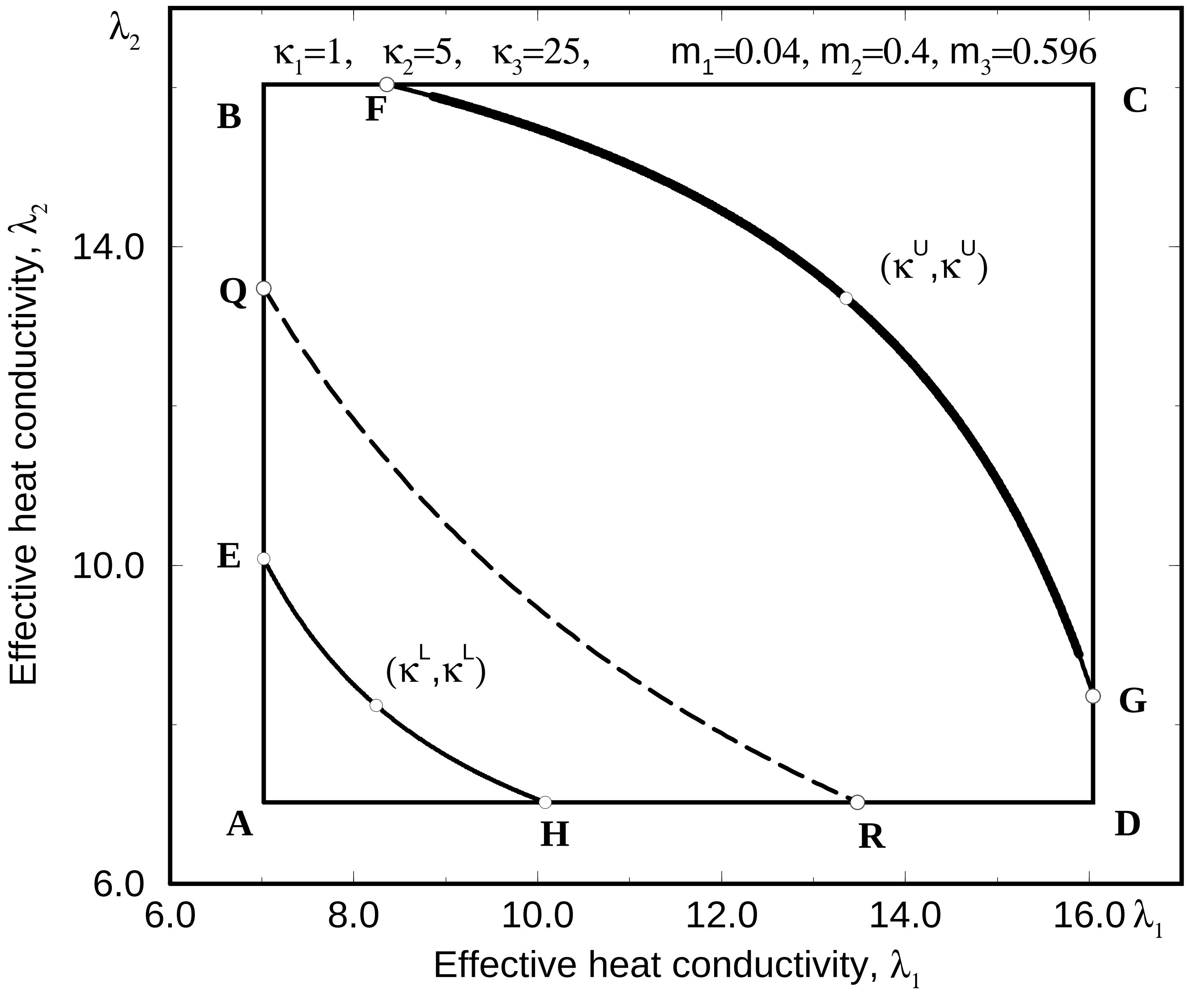

7.0
5.0
3.0
1.0
1.0
3.0
5.0
7.0
Effective heat conductivity, λ_2
Effective heat conductivity, λ_1
F
B
C
κ_1=1, κ_2=5, κ_3=25
m_1=0.6, m_2=0.2, m_3=0.2
(κ^U,κ^U)
E
(κ^L,κ^L)
G
H
A
D



a)
κ_1
κ_1
p
κ_3
κ_3
1-p
H
$\lambda_2^{(1)}$
$\lambda_1^{(1)}$
b)
κ_2
κ_2
$\frac{m_2}{\mu+m_2}$
$\lambda_2^{(1)}$
$\lambda_1^{(1)}$
$\frac{\mu}{\mu+m_2}$
H
$\lambda_2^{(2)}$
$\lambda_1^{(2)}$
c)
κ_1
κ_1
ν_1
κ_3
κ_3
ν_3
$\lambda_2^{(2)}$
$\lambda_1^{(2)}$
ν_2
H
$\lambda_2^{(3)}$
$\lambda_1^{(3)}$

Fig. 4, A.V. Cherkaev and L.V. Gibiansky





λ_2
κ_1=1, κ_2=5, κ_3=25, m_1=0.04, m_2=0.4, m_3=0.596
B
F
C
14.0
Q
(κ^U,κ^U)
E
10.0
(κ^L,κ^L)
G
A
H
R
D
6.0
6.0
8.0
10.0
12.0
14.0
16.0
λ_1
Effective heat conductivity, λ_1
Effective heat conductivity, λ_2