Phase transformations surfaces and exact energy lower bounds

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Dedicated to Prof. Sergey Kanaun on the occasion of his 70th birthday

Abstract

The paper investigates two-phase microstructures of optimal 3D composites that store minimal elastic energy in a given strain field. The composite is made of two linear isotropic materials which differ in elastic moduli and self-strains. We find optimal microstructures for all values of external strains and volume fractions of components. This study continues research by Cherkaev and Gibiansky [42, 43] and Chenchiah and Bhattacharya [15], where partial results were obtained. In the present paper we demonstrate energy is minimized by that laminates of various ranks. Optimal structures are either simple laminates that are codirected with external eigenstrain directions, or inclined laminates, direct and skew second-rank laminates and third-rank laminates. These results are applied for description of direct and reverse transformations limit surfaces in a strain space for elastic solids undergoing phase transformations of martensite type. The surfaces are computed as the values of external strains at which the optimal volume fraction of one of the

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phases tends to zero. Finally, we compare the transformation surfaces with the envelopes of the nucleation surfaces constructed earlier for nuclei of various geometries (planar layers, elliptical cylinders, ellipsoids). We show the energy equivalence of the cylinders and direct second-rank-laminates, ellipsoids and third-rank laminates. We note that skew second-rank laminates make the nucleation surface convex function of external strain, and they do not correspond to any of the mentioned nuclei.

Keywords: optimal composites design, exact energy bounds, translation energy estimates, stress-induced phase transitions, limit transformation surfaces

1. Introduction

In the present paper, we relate two problems which initially arise from different branches of mechanics of materials: construction of transformation surfaces for strain-induced phase transitions and optimal design of 3D-composites in the sense of minimizing its energy. Both problems are formulated as a variational problem about a structure of two-phase elastic composite of minimal energy, they are solved by the same formalism. The previous paper [42], translated as [43], considered this problem in an asymptotic case when the compliance of one phase is zero, and the paper [15] deals with a similar variational problem and contains a part of results; however, some optimal structures were missed there.

Phase transformations of martensite type are characterized by a priori unknown interfaces which divide a body into domains occupied by different phases; these are accompanied by transformation strains, jumps of elastic moduli and a jump of a chemical energy (see, e.g., [12, 54] and reference therein). The transformation cannot occur until the external strain attains the transformation limit surface.

One of the approaches to the transformation surface construction can be based on a semi-inverse method. According to this approach the new phase nucleus shape can be prescribed (layers, ellipsoids, elliptical cylinders), and external strains at which the boundary of such a nucleus can satisfy the local thermodynamic equilibrium condition (the Maxwell relation) can be found. Then the geometric parameters of the nucleus can be found in dependence on the external strains (see, e.g., [48, 52, 30, 49, 38, 36, 7, 8, 39]). Then some kind of a transformation surface can be constructed as an envelope of the surfaces which correspond to external strains at which the appearance of different types of new phase nuclei becomes possible.

Such an approach allows to specify the shape and orientation of new phase nucleus in dependence on strain state and to study local strains. However, the local equilibrium conditions are only necessary conditions for the energy minimum and an additional stability analysis is needed. It was shown that the instability of such two-phase deformations with respect to various smooth perturbations of the interface was not found if strains at the interfaces corresponded to the external boundaries of so-called phase transitions zones (see, e.g., [41, 26]). The phase transition zone (PTZ) is formed in a strain space by all strains which can satisfy the local equilibrium conditions and allows to describe locally all equilibrium interfaces feasible in a given material. The

concept of the PTZ was offered in [32] and its construction was considered for finite and small strains [33, 62, 35, 40, 37, 38]. The external PTZ-boundaries are the surfaces of the nucleation of new phase plane layers. In the papers [46, 47] it was proved that belonging strains to the external PTZ-boundaries is a necessary stability condition.

But even if these necessary conditions are satisfied by the choice of the geometry of a new phase domain and instability of the solution chosen is not found, one cannot be sure that the solution corresponds to the energy minimizer. We also note that the variational problem in the case of phase transformation has a two-wells nonconvex Lagrangian, therefore, the conventional variational technique is not applicable; the solution is characterized by a microstructure of mixed phases with a generalized boundary between them. Such solutions are investigated by constructing the minimizing sequences and establishing a lower bound for the energy [10, 11].

That is why, accepting that the transformation cannot start if two-phase microstructure appearance do not lead to energy relaxation in comparison with one-phase states, we develop the approach based on the construction of the exact energy lower bounds of two-phase composites. The energy functional for the case of a given external strain and temperature is the Helmholtz free energy. We assume that the phases are linear-elastic and, for simplicity, isotropic.

The transformation surface construction includes several steps. We find the structure of two-phase composites that stores minimal energy at a given external strain, using different constructions for upper and lower bounds of the energy and observe that these bounds coincide. This approach was used in most papers on the subject starting with [55, 10, 57]. In most papers on optimal 3D elastic composites, the minimum of the complementary energy (dual or stress energy) was considered, since it leads to the strongest structures, see e.g. [29, 20, 25, 23, 4]. We, however, consider the minimum of the strain energy (the weakest composites), as it is required by the Gibbs principle.

Both upper and lower bounds require a nontrivial search for optimal parameters of the estimates. We use them simultaneously, finding the hints for values of the parameters of the lower estimate from the upper estimate and vice versa. A similar strategy was exploited starting with [42, 59] (see also [43] and monographs [22, 61]) and has been actively elaborated for the estimations of electric, thermal and elastic properties of composite materials basing on the translation method [58, 60, 28, 67, 45, 43, 9].

We find a two-phase composite of minimal strain energy at given volume fractions of the components. We start with considering the specific microstructures namely laminates of different ranks and we minimize the energy in this class of structures obtaining the upper bound for the minimizing energy. Note that obtaining exact energy estimations with the use of layered microstructures became standard procedure in the analysis of optimal microstructures [43, 15, 3, 9, 59, 51, 17, 1, 21].

Then we construct a lower translation bound for the composite energy (see, e.g., the monographs [22, 61] and reference therein). The translation bound does not depend on microstructure and it may or may not be attained. However, the direct energy calculation shows that the energy of the optimal laminates coincides with the polyconvex energy envelope. The lower bound depends on so-called translation parameters that should be optimally adjusted. The translation method provides optimal strains in the materials, which are utilized when we find optimal microstructures among laminates. This way, translation bound and optimal laminates' energy are coupled and allow for the definition of optimal translation parameters and optimal parameters of laminates. Here we follow the approach developed in [21, 16] for optimal structures of multimaterial mixtures.

Then we further minimize the lower bound constructed with respect to the volume fractions and find all strains at which the minimizer corresponds to the limiting values (zero or one) of the volume fraction of one of the phases. The strains that correspond to these values form the direct and the reverse transformation limit surfaces, respectively. Two-phase structures cannot have lower energy than the energy of one-phase state until the limit surface is reached. Such domains of pure materials and optimal mixtures in the context of structural optimization were described in [18] and [19] for 2D and 3D strongest elastic composites, respectively, and in [14] for 2D three-material strongest elastic composites.

Finally, we compare the limit surfaces constructed with nucleation surfaces for ellipsoidal, cylindrical and planar nuclei. The coincidence of the surfaces indicates the fact that layered microstructures are energetically equivalent to microstructures with smooth interfaces (layers, elliptical cylinders, ellipsoids).

2. Problem statement

In this section, we formulate the problem of minimal Helmholtz free energy for a phase transition between two isotropic elastic phases and introduce notations. The formulation generally follows the variational approach presented in the earlier papers [57, 11, 48]).

Geometry and elasticity. Consider a periodic structure in three-dimensional space $\mathbb{R}^3$. A periodic cell is a unit cube

$$\Omega = \{x : 0 \leq x_i \leq 1, i = \overline{1, 3}\},$$

$\text{meas}(\Omega) = 1$. Assume that Ω is divided into two parts Ω_- and Ω_+ with volumes $\text{meas}(\Omega_-) = m_-$ and $\text{meas}(\Omega_+) = m_+$; obviously, $m_- + m_+ = 1$. We denote the interface between subregions as Γ and introduce the characteristic function $H(\mathbf{x})$ of the subregion Ω_+

$$H(\mathbf{x}) = \begin{cases} 1, & \mathbf{x} \in \Omega_+, \\ 0, & \mathbf{x} \in \Omega_-. \end{cases}$$

Assume that these parts are occupied by linear elastic phases with the elasticity tensors $\mathbf{C}_-$, and $\mathbf{C}_+$, respectively. The constitutive equations are written as

$$\boldsymbol{\sigma}(\boldsymbol{\varepsilon}, \mathbf{x}) = (1 - H(\mathbf{x}))\mathbf{C}_- : (\boldsymbol{\varepsilon}(\mathbf{x}) - \boldsymbol{\varepsilon}_-^p) + H(\mathbf{x})\mathbf{C}_+ : (\boldsymbol{\varepsilon}(\mathbf{x}) - \boldsymbol{\varepsilon}_+^p) \quad (1)$$

where $\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon} = (\nabla \mathbf{u})^s$ are the stress and strain tensors, respectively, $\mathbf{u}$ is the displacement, $\boldsymbol{\varepsilon}_\pm^p$ are the strains in stress-free states that characterize phases plus and minus.

We use the following notation for products of vectors and tensors: $(\mathbf{q} \cdot \mathbf{k})_i = q_{ij}k_j$, $(\mathbf{q} \cdot \mathbf{m})_{ij} = q_{ik}m_{kj}$, $\mathbf{q} : \mathbf{m} = q_{ij}m_{ij}$, $(\mathbf{m} \otimes \mathbf{q})_{ijkl} = m_{ij}q_{kl}$, $(\mathbf{A} \cdot \mathbf{q})_{ijkl} = A_{ijkm}q_{ml}$, $(\mathbf{A} : \mathbf{q})_{ij} = A_{ijkl}q_{kl}$, $(\mathbf{A} : \mathbf{B})_{ijmn} = A_{ijkl}B_{klmn}$ where $\mathbf{k}$ is a vector, $\mathbf{q}$, $\mathbf{m}$ are second rank tensors, and $\mathbf{A}$, $\mathbf{B}$ are forth rank tensors, a summation rule by repeating indices is implied.

Assume that the medium is deformed by a homogeneous external strain $\boldsymbol{\varepsilon}_0$. The equilibrium equations, traction and displacement continuity conditions at the interfaces Γ and boundary conditions in the case of zero body forces are

$$\begin{aligned} \mathbf{x} \in \Omega_- \cup \Omega_+ : \quad \nabla \cdot \boldsymbol{\sigma} &= 0, \\ \mathbf{x} \in \Gamma : \quad \llbracket \boldsymbol{\sigma} \rrbracket \cdot \mathbf{n} &= 0, \quad \llbracket \mathbf{u} \rrbracket = 0, \\ \mathbf{x} \in \partial\Omega : \quad \mathbf{u} &= \boldsymbol{\varepsilon}_0 \cdot \mathbf{x}. \end{aligned} \quad (2)$$

Here, we denote a jump across the interface by square brackets: $[[\cdot]] = (\cdot)_+ - (\cdot)_-$. The above condition states also that at the interphase Γ , the tangent components of the strain are continuous, and the average strain in Ω is $\boldsymbol{\varepsilon}_0$:

$$\boldsymbol{\varepsilon}_0 = \int_{\Omega} \boldsymbol{\varepsilon}(\mathbf{x}) d\Omega.$$

Variational problem. We consider the minimization problem for the energy of the cell, that is we are looking for such microstructure (characteristic function $H(\mathbf{x})$) and strains which correspond to minimum of the Helmholtz free energy F of the cell. Strictly speaking, this problem does not have a solution, only minimizing sequences [10], which we show below. Correspondingly, the Helmholtz free energy tends to its infimum rather than reaches the minimum. However, below we use both terms.

By (1), the Helmholtz free energy density is written as

$$f_H(\mathbf{x}, \boldsymbol{\varepsilon}) = (1 - H(\mathbf{x}))f_-(\boldsymbol{\varepsilon}) + H(\mathbf{x})f_+(\boldsymbol{\varepsilon})$$

where

$$f_{\pm}(\boldsymbol{\varepsilon}) = f_{\pm}^0 + w_{\pm}(\boldsymbol{\varepsilon}), \quad w_{\pm}(\boldsymbol{\varepsilon}) = \frac{1}{2}(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_{\pm}^p) : \mathbf{C}_{\pm} : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_{\pm}^p), \quad (3)$$

$w_{\pm}$ are the strain energy densities of a material in phase states “ $\pm$ ”, $f_{\pm}^0$ are the free energy densities of the phases in stress-free states (so called chemical energies).

Given average strain $\boldsymbol{\varepsilon}_0$, the optimal structure minimizes the Helmholtz free energy over all possible microstructures and volume fractions of the phases in the phase transformation. This yields to the variational problem for the minimizers m_+ , H and $\boldsymbol{\varepsilon}$:

$$\mathcal{J}_f = \inf_{0 \leq m_+ \leq 1} \inf_{\int_{\Omega} H d\Omega = m_+} \inf_{\boldsymbol{\varepsilon} \in \mathcal{E}_0} \int_{\Omega} f_H(\mathbf{x}, \boldsymbol{\varepsilon}) d\Omega \quad (4)$$

where $\mathcal{E}_0$ is the set of strain fields with an average $\boldsymbol{\varepsilon}_0$.

We perform the minimization over $f_H(\mathbf{x}, \boldsymbol{\varepsilon})$ first. Since H takes only two values, zero and one, the minimum corresponds to a two-well function $f(\boldsymbol{\varepsilon})$ as follows:

$$\inf_H f_H(\mathbf{x}, \boldsymbol{\varepsilon}) = f(\boldsymbol{\varepsilon}), \quad f(\boldsymbol{\varepsilon}) = \min_{+,-} \{f_-(\boldsymbol{\varepsilon}), f_+(\boldsymbol{\varepsilon})\}.$$

Minimization method of a two-well energy. Next, we minimize (4) assuming that external strains $\boldsymbol{\varepsilon}_0$ and volume fraction m_+ are given. Since the chemical energies $f_0^\pm$ do not make any impact onto the minimization problem at this step, we focus on finding the minimum of the strain energy

$$\mathcal{J}_{wm}(m_+, \boldsymbol{\varepsilon}_0) = \inf_{\substack{\int_{\Omega} H d\Omega = m_+}} \inf_{\boldsymbol{\varepsilon} \in \mathcal{E}_0} \int_{\Omega} ((1 - H(\mathbf{x}))w_-(\boldsymbol{\varepsilon}) + H(\mathbf{x})w_+(\boldsymbol{\varepsilon})) d\Omega \quad (5)$$

This is a problem of optimal composite microstructure.

Finally, the obtained can be additionally minimized over m_+ . This leads to the energy $\mathcal{J}_f(\boldsymbol{\varepsilon}_0)$ of the deformable solid under the phase transition,

$$\mathcal{J}_f(\boldsymbol{\varepsilon}_0) = \inf_{0 \leq m_+ \leq 1} \{f_0^- + m_+\gamma + \mathcal{J}_{wm}(m_+, \boldsymbol{\varepsilon}_0)\} \quad (6)$$

where $\gamma = \llbracket f_0 \rrbracket$. Obviously, only the difference γ of the chemical energies affects the problem, f_0^- gives just a reference level for the energy calculation. In phase transition problems the parameter γ depends on the temperature and can be treated as an “energetic temperature”.

Notice that the minimization of a two-well Lagrangian (5) leads to optimal solutions with infinitely often oscillating minimizers (strains) that physically corresponds to a microstructured material. The cost $\mathcal{J}_{wm}(m_+, \boldsymbol{\varepsilon}_0)$, the infimum over all possible oscillating sequences, is called the relaxed two-well Lagrangian or the quasiconvex envelope of the Lagrangian. The variational problem for $\mathcal{J}_{wm}(m_+, \boldsymbol{\varepsilon}_0)$ possess a smooth solution that can be found by solving the Euler-Lagrange equation.

The relaxation in (5) is performed by constructing upper and lower bounds for $\mathcal{J}_{wm}(m_+, \boldsymbol{\varepsilon}_0)$,

$$\mathcal{PW}(m_+, \boldsymbol{\varepsilon}_0) \leq \mathcal{J}_{wm}(m_+, \boldsymbol{\varepsilon}_0) \leq \mathcal{LW}(m_+, \boldsymbol{\varepsilon}_0)$$

The upper bound $\mathcal{LW}$ is the minimum of the energy of any microstructure from an a priori chosen class of structures. It is constructed in Section 3. The lower bound $\mathcal{PW}(m_+, \boldsymbol{\varepsilon}_0)$ used here is the so-called translation bound [60, 22, 61] that exploits the idea of the polyconvex envelope, see [24]. The bound is being constructed in Section 4 without direct referring to any specific microstructure and is a structure-independent lower bound for the energy. Then we demonstrate that the bounds is exact by showing that

$$\mathcal{PW}(m_+, \boldsymbol{\varepsilon}_0) = \mathcal{LW}(m_+, \boldsymbol{\varepsilon}_0) \quad \forall m_+, \boldsymbol{\varepsilon}_0. \quad (7)$$

Thus, we also determine the minimal energy of the composite $\mathcal{J}_{wm} = \mathcal{LW} = \mathcal{PW}$, solving problem (5). In other terms, we describe the quasiconvex envelope of the two-well Lagrangian, see for example [22]. In Section 5, we analyze problem (6) and find the boundaries of the composite zones and construct a transformation surface.

3. Laminates with minimal stored energy

In this section, we calculate the energy $\mathcal{LW}(m_+, \epsilon_0)$ of simple and higher rank laminates that turn out to be optimal for the considered problem. We minimize the energy at this class of structures at given external strains by choosing microstructure parameters and we derive necessary conditions of optimality in terms of the fields inside the laminates.

3.1. Lamination formulae

Laminates construction. The rank- n laminate construction [56, 59] is a multistep process. At the first step, one takes a simple laminate that consists of alternating planar layers occupied by homogeneous phases “−” and “+”. We call this a simple (or rank-1) laminate. A second-rank laminate consists of alternating layers of the phase “−” and layers which are themselves simple laminates. The third-rank laminate consists of the layers of the phase “−” and layers which are second-rank laminates (Fig. 1). The rank- n laminate consists of alternating layers of the phase “−” and rank- $(n - 1)$ layers.

In our model, the characteristic size of simple layers is much less than the size of the second rank layers that in turn is much less than the characteristic size of the third rank layers, etc. The strains in such layered material tend to piece-wise constant function when the scale separation increases, as it is shown in [13]. We will show that the fields in the “+” phase (inclusion) in an optimal laminate belong to the above mentioned PTZ-boundary.

We use subscripts 1, 2 to identify the “macroscopic” layers in laminates. Subscript 1 refers to the layer occupied by phase “−”. Subscript 2 refers to another layer that is itself a layer of the rank $(k - 1)$ in the case of a rank- k laminate. The superscripts (1), (2)... in parentheses denote the rank of the laminate. The normals to the layers at various scale levels are $\mathbf{n}^1, \mathbf{n}^2...$ (see. Fig. 2).

We denote volume fractions of the phase “−” within the laminate of the rank k as $m_1^{(k)}$, and $m_2^{(k)}$ is the volume fraction of homogenized rank- $(k - 1)$ layers, $m_1^{(k)} + m_2^{(k)} = 1$. Let $\epsilon_1^{(k)}$ be a strain in a phase “−” layer inside the

rank- k layer. Then $\boldsymbol{\varepsilon}_2^{(k)}$ is a strain averaged within the rank- $(n-1)$ layer. The strains $\boldsymbol{\varepsilon}_{1,2}^{(k)}$ and stresses $\boldsymbol{\sigma}_{1,2}^{(k)}$ in each subdomain are uniform, and the following relations are fulfilled for the volume fractions, strains and stresses defined at different scales in the case of the rank- n laminate:

$$\begin{aligned}
m_1^{(1)} \boldsymbol{\varepsilon}_1^{(1)} + m_2^{(1)} \boldsymbol{\varepsilon}_2^{(1)} &= \boldsymbol{\varepsilon}_2^{(2)}, & m_1^{(1)} \boldsymbol{\sigma}_1^{(1)} + m_2^{(1)} \boldsymbol{\sigma}_2^{(1)} &= \boldsymbol{\sigma}_2^{(2)}, \\
m_1^{(2)} \boldsymbol{\varepsilon}_1^{(2)} + m_2^{(2)} \boldsymbol{\varepsilon}_2^{(2)} &= \boldsymbol{\varepsilon}_2^{(3)}, & m_1^{(2)} \boldsymbol{\sigma}_1^{(2)} + m_2^{(2)} \boldsymbol{\sigma}_2^{(2)} &= \boldsymbol{\sigma}_2^{(3)}, \\
&\dots\dots\dots \\
m_1^{(n)} \boldsymbol{\varepsilon}_1^{(n)} + m_2^{(n)} \boldsymbol{\varepsilon}_2^{(n)} &= \boldsymbol{\varepsilon}_2^{(n+1)} \equiv \boldsymbol{\varepsilon}_0, & m_1^{(n)} \boldsymbol{\sigma}_1^{(n)} + m_2^{(n)} \boldsymbol{\sigma}_2^{(n)} &= \boldsymbol{\sigma}_2^{(n+1)} \equiv \boldsymbol{\sigma}_0, \\
m_1^{(k)} + m_2^{(k)} &= 1, \quad k = 1, 2 \dots n, & \prod_{i=1}^n m_2^{(i)} &= m_+ \\
\boldsymbol{\sigma}_1^{(k)} &= \mathbf{C}_- : (\boldsymbol{\varepsilon}_1^{(k)} - \boldsymbol{\varepsilon}_-^p), & \boldsymbol{\sigma}_2^{(k)} &= \mathbf{C}_2^{(k)} : (\boldsymbol{\varepsilon}_2^{(k)} - \boldsymbol{\varepsilon}_2^{p(k)})
\end{aligned}$$

where $\mathbf{C}_2^{(k)}$ is the effective elasticity tensor that relates the average stress and strain within the rank- $(k-1)$ sublayer of the rank- k laminate, $\boldsymbol{\varepsilon}_2^{p(k)}$ is the effective transformation strain produced by the rank- $(k-1)$ sublayer, $\mathbf{C}_2^{(n+1)} \equiv \mathbf{C}_0$ and $\boldsymbol{\varepsilon}_2^{p(n+1)} \equiv \boldsymbol{\varepsilon}_0^p$ are effective elasticity tensor and effective transformation strain of the composite presented by the rank- n laminate.

To avoid misunderstanding, note that the layer 1 is always the layer of the phase “-”, according to the accepted super and subscripts notation

Figure 1: Laminated microstructures : (a) simple rank laminate, (b) second-rank laminate, (c) third-rank laminate.

$\mathbf{C}_1^{(k)} = \mathbf{C}_-$, $\boldsymbol{\varepsilon}_1^{p(k)} = \boldsymbol{\varepsilon}_-^p$ ($k = 1, 2 \dots n$). The strain $\boldsymbol{\varepsilon}_2^{(1)}$ is always a strain inside the domain Ω_+ , $\boldsymbol{\varepsilon}_2^{(1)} = \boldsymbol{\varepsilon}_+$. Further, for the case of the rank- n laminate we express $\boldsymbol{\varepsilon}_2^{(1)} = \boldsymbol{\varepsilon}_+$ through $\boldsymbol{\varepsilon}_2^{(2)}$, $\boldsymbol{\varepsilon}_2^{(2)}$ through $\boldsymbol{\varepsilon}_2^{(3)}$, ... $\boldsymbol{\varepsilon}_2^{(n)}$ through $\boldsymbol{\varepsilon}_0$ and finally derive the dependence of $\boldsymbol{\varepsilon}_+$ on average strain $\boldsymbol{\varepsilon}_0$ and microstructure parameters $\mathbf{n}^k$ and $m_1^{(k)}$ ($k = 1, 2 \dots n$).

Interaction energy. The Helmholtz free energy

$$F = \int_{\Omega} f_H(\mathbf{x}, \boldsymbol{\varepsilon}) d\Omega$$

of a two-phase body $\Omega = \Omega_- \cup \Omega_+$ at prescribed displacements at the boundary $\partial\Omega$ can be presented as a sum of the free energy

$$F_0 = \int_{\Omega} f_-(\boldsymbol{\varepsilon}) d\Omega$$

of a homogeneous body in a phase state “−” calculated at the same boundary conditions and the interaction energy E :

$$E = F - F_0.$$

The advantage of such a representation is that F_0 does not depend on microstructure, and the interaction energy is expressed in a form of an integral over the closed domains Ω_+ occupied by the phase “+” [27, 63]. Moreover, as it was mentioned above, the strain is uniform inside Ω_+ in the case of the laminates. This will additionally simplify the consideration.

If the free energy densities of the phases are given by (3) then (see, e.g., [36])

$$E = \int_{\Omega_+} \left(\gamma + \frac{1}{2} \llbracket \boldsymbol{\varepsilon}^p : \mathbf{C} : \boldsymbol{\varepsilon}^p \rrbracket + \frac{1}{2} (\boldsymbol{\varepsilon}_+ : \llbracket \mathbf{C} \rrbracket : \boldsymbol{\varepsilon}_0 - (\boldsymbol{\varepsilon}_+ + \boldsymbol{\varepsilon}_0) : \llbracket \mathbf{C} : \boldsymbol{\varepsilon}^p \rrbracket) \right) d\Omega,$$

where $\gamma = \llbracket f^0 \rrbracket$.

Further we will assume that the inverse $\llbracket \mathbf{C} \rrbracket^{-1}$ exists. Then the expression of the interaction energy can be rewritten in a form [52, 36]

$$E = \int_{\Omega_+} \left(\gamma_* + \frac{1}{2} \mathbf{e}_0(\mathbf{x}) : \mathbf{q}_+(\mathbf{x}) \right) d\Omega$$

where

$$\mathbf{e}_0 = \boldsymbol{\varepsilon}_0 - \llbracket \mathbf{C} \rrbracket^{-1} : \llbracket \mathbf{C} : \boldsymbol{\varepsilon}^p \rrbracket, \quad (8)$$

$$\mathbf{q}_+(\mathbf{x}) = \llbracket \mathbf{C} \rrbracket : \boldsymbol{\varepsilon}_+(\mathbf{x}) - \llbracket \mathbf{C} : \boldsymbol{\varepsilon}^p \rrbracket, \quad (9)$$

$$\gamma_* = \gamma + \frac{1}{2} \llbracket \boldsymbol{\varepsilon}^p \rrbracket : \llbracket \mathbf{C}^{-1} \rrbracket^{-1} : \llbracket \boldsymbol{\varepsilon}^p \rrbracket,$$

$\boldsymbol{\varepsilon}_0(\mathbf{x})$ is the strain that would be in the domain Ω_+ in the case of a homogeneous body in the phase state “–”, $\boldsymbol{\varepsilon}_+(x)$ is the strain inside Ω_+ in the case of the two-phase body.

In the optimal composite problem the volume fractions m_+ or $m_- = 1 - m_+$ of the phases are fixed, and therefore we will temporary exclude from consideration the chemical energies f_-^0 and f_+^0 and focus on the minimization of the strain energy, i.e. on the calculation and minimization of

$$E_q = \frac{1}{2} \int_{\Omega_+} \mathbf{e}_0 : \mathbf{q}_+ d\Omega$$

for laminates of various ranks.

Strain energy of laminates. The inhomogeneities affect stress-strain state of a body only through the tensor $\mathbf{q}_+$ [53, 50], and we will further use a formula that follows from the displacement and traction continuity conditions (2) at the interfaces and relates the jump in strain across the interface with the tensor $\mathbf{q}_+$ and, thus, with the strain $\boldsymbol{\varepsilon}_+$ [53] (see also [50, 31]). If $\boldsymbol{\varepsilon}_\pm$ are the strains at the interface then in a point with a normal $\mathbf{n}$

$$\llbracket \boldsymbol{\varepsilon} \rrbracket = -\mathbf{K}_-(\mathbf{n}) : \mathbf{q}_+ \quad (10)$$

where $\mathbf{K}_-(\mathbf{n}) = (\mathbf{n} \otimes \mathbf{G}_-(\mathbf{n}) \otimes \mathbf{n})^s$, $\mathbf{G}_-(\mathbf{n}) = (\mathbf{n} \cdot \mathbf{C}_- \cdot \mathbf{n})^{-1}$, superscript s means symmetrization:

$$K_{ijkl} = n_{(i} G_{j)(k} n_{l)}.$$

Since the tensor $\mathbf{q}_+$ is uniform inside Ω_+ ,

$$E_q = \frac{1}{2} m_+ \mathbf{e}_0 : \mathbf{q}_+ \quad (11)$$

Thus, to calculate E_q in a case of the rank- n laminate one have to express $\mathbf{q}_+$ through $\mathbf{e}_0$. Obviously, $\mathbf{q}_+$ is a linear function of $\mathbf{e}_0$. It can be derived

(see Appendix A) that the use of shifted strain $\mathbf{e}_0$ instead of $\boldsymbol{\varepsilon}_0$ results in the simplest transmitting formula. For the rank- n laminate

$$\mathbf{q}_+ = \mathbf{M}_-^{(n)} : \mathbf{e}_0 \quad (12)$$

where $\mathbf{e}_0$ and $\mathbf{q}_+$ are defined by (8) and (9), the transmitting tensor

$$\mathbf{M}_-^{(n)} = \left(\llbracket \mathbf{C} \rrbracket^{-1} + m_- \sum_{i=1}^n \beta^{(i)} \mathbf{K}_-(\mathbf{n}^{(i)}) \right)^{-1}, \quad (13)$$

microstructure parameters

$$\beta^{(i)} = \frac{m_1^{(i)}}{m_- m_2^{(i)}} \prod_{j=1}^i m_2^{(j)} \quad (i = 1, 2 \dots n) \quad (14)$$

satisfy the restriction

$$\sum_1^n \beta^{(i)} = 1. \quad (15)$$

Tensors

$$\mathbf{q}_2^{(i)} = \left(\mathbf{C}_2^{(i)} - \mathbf{C}_- \right) : \boldsymbol{\varepsilon}_2^{(i)} - \left(\mathbf{C}_2^{(i)} : \boldsymbol{\varepsilon}_2^{p(i)} - \mathbf{C}_- : \boldsymbol{\varepsilon}_-^p \right), \quad i = 1, 2 \dots n$$

are related with $\mathbf{q}_+$ as

$$\mathbf{q}_2^{(i)} = \left(\prod_{i=1}^{i-1} m_2^{(i)} \right) \mathbf{q}_+, \quad \mathbf{q}_2^{(n)} = \prod_{i=1}^{n-1} m_2^{(i)} \mathbf{q}_+ = \frac{m_+}{m_2^{(n)}} \mathbf{q}_+ \quad (16)$$

Average stress and strain within the rank- i sublayer of the rank- k laminate

$$\boldsymbol{\sigma}_2^{(i+1)} = \mathbf{C}_2^{(i+1)} : \left(\boldsymbol{\varepsilon}_2^{(i+1)} - \boldsymbol{\varepsilon}_2^{p(i+1)} \right)$$

where the effective elasticity tensors of the sublayer and effective transformation strain

$$\begin{aligned} \mathbf{C}_2^{(i+1)} &= \mathbf{C}_- + m_+ \mathbf{M}_-^{(i)}, \\ \boldsymbol{\varepsilon}_2^{p(i+1)} &= \boldsymbol{\varepsilon}_-^p + m_+ \left(\mathbf{C}_2^{(i+1)} \right)^{-1} : \mathbf{M}_-^{(i)} : \llbracket \mathbf{C} \rrbracket^{-1} : \mathbf{C}_+ : \llbracket \boldsymbol{\varepsilon}^p \rrbracket \end{aligned}$$

Average stress and strain for the rank- n laminate are related as

$$\boldsymbol{\sigma}_0 = \mathbf{C}_0 : (\boldsymbol{\varepsilon}_0 - \boldsymbol{\varepsilon}_0^p), \quad (17)$$

where effective elasticity tensor and effective transformation strain are, respectively,

$$\mathbf{C}_0 = \mathbf{C}_- + m_+ \mathbf{M}_-(n), \quad \boldsymbol{\varepsilon}_0^p = \boldsymbol{\varepsilon}_-^p + m_+ (\mathbf{C}_0)^{-1} : \mathbf{M}_-^{(n)} : \llbracket \mathbf{C} \rrbracket^{-1} : \mathbf{C}_+ : \llbracket \boldsymbol{\varepsilon}^p \rrbracket. \quad (18)$$

Finally, substituting (12) into (11) we obtain the formula for the strain energy of the rank- n laminate:

$$\begin{aligned} W^{(n)} = & \frac{1}{2} (\boldsymbol{\varepsilon}_0 - \boldsymbol{\varepsilon}_-^p) : \mathbf{C}_- : (\boldsymbol{\varepsilon}_0 - \boldsymbol{\varepsilon}_-^p) \\ & + \frac{1}{2} m_+ \llbracket \boldsymbol{\varepsilon}^p \rrbracket : \llbracket \mathbf{C}^{-1} \rrbracket^{-1} : \llbracket \boldsymbol{\varepsilon}^p \rrbracket + \frac{1}{2} m_+ \mathbf{e}_0 : \mathbf{M}_-^{(n)} : \mathbf{e}_0. \end{aligned} \quad (19)$$

Of course, by (17) and (18),

$$W^{(n)} = \frac{1}{2} (\boldsymbol{\varepsilon}_0 - \boldsymbol{\varepsilon}_0^p) : \mathbf{C}_0 : (\boldsymbol{\varepsilon}_0 - \boldsymbol{\varepsilon}_0^p),$$

but the representation (19) demonstrate explicitly the input of the second phase into the strain energy of the composite in comparison with an one-phase state.

Expressions similar to (19) for the energy of rank- n laminates were earlier derived in matrix form at zero transformation strains [43, 22], see also [2] and reference therein. The form (19) takes into account the transformation strains and shows that it is natural to use a shifted strain $\mathbf{e}_0$ instead of $\boldsymbol{\varepsilon}_0$ in this case. Laminated microstructures have also been considered in applications to phase transformations (see e.g. [66, 57, 44, 68] and reference therein). In the Appendix A, the lamination formulae (16)–(19) are derived in terms of the notation accepted in the present paper.

The following Proposition relates the sign of the tensor $\mathbf{M}_-^{(n)}$ with the sign of the jumps $\llbracket \mathbf{C} \rrbracket$ (see the proof in Appendix A).

Proposition 1. *If the jump $\llbracket \mathbf{C} \rrbracket$ of the elasticity tensor is a sign-definite tensor then the transmitting tensor $\mathbf{M}_-^{(n)}$ is of the same sign-definiteness.*

The proof also shows the existence of $\mathbf{M}_-^{(n)}$. Additional analysis is needed if the jump $\llbracket \mathbf{C} \rrbracket$ is not sign-definite. To confirm the consistence of the results note that, by (19), if the transformation strain is zero, i.e. $\llbracket \boldsymbol{\varepsilon}^p \rrbracket = 0$, then the strain energy decreases if $\llbracket \mathbf{C}^{-1} \rrbracket < 0$ and increases if $\llbracket \mathbf{C}^{-1} \rrbracket > 0$, as it is to be.

Relations between strains averaged over the phases. Microstructure parameters β_i are positive and satisfy the restriction (15). The sense of $\beta^{(i)}$ is clarified by the formula for the difference of strains averaged within the phases. Let

$$\bar{\epsilon}_{\pm} = \frac{1}{m_{\pm}} \int_{\Omega_{\pm}} \epsilon(\mathbf{x}) d\Omega. \quad (20)$$

Then from the fact that (12) is equivalent to the equation

$$\epsilon_+ + m_- \sum_{i=1}^n \beta^{(i)} \mathbf{K}_-(\mathbf{n}^{(i)}) : \mathbf{q}_+ = \epsilon_0$$

and from the equalities

$$m_- \bar{\epsilon}_- + m_+ \bar{\epsilon}_+ = \bar{\epsilon}_+ - m_- (\bar{\epsilon}_+ - \bar{\epsilon}_-) = \epsilon_0, \quad \bar{\epsilon}_+ = \epsilon_+ \quad (21)$$

it follows that

$$\bar{\epsilon}_+ - \bar{\epsilon}_- = - \sum_{i=1}^n \beta^{(i)} \mathbf{K}_-(\mathbf{n}^{(i)}) : \mathbf{q}_+. \quad (22)$$

Formula (22) allows to formulate strain compatibility conditions in terms of strains averaged over the phases. Displacement continuity across the interface corresponds to the fulfilling the identity

$$\mathbf{K}(\mathbf{n}) : \boldsymbol{\tau} \otimes \boldsymbol{\tau}' \equiv 0 \quad \forall \boldsymbol{\tau}, \boldsymbol{\tau}' \perp \mathbf{n}.$$

Figure 2: Second-rank laminate

In the case of a simple laminate $\bar{\epsilon}_{\pm} = \epsilon_{\pm}$, strain compatibility at the interface means that

$$(\bar{\epsilon}_+ - \bar{\epsilon}_-) : \boldsymbol{\tau} \otimes \boldsymbol{\tau}' = 0 \quad \forall \boldsymbol{\tau}, \boldsymbol{\tau}' \perp \mathbf{n}^{(1)}. \quad (23)$$

In the less obvious case of the second-rank laminate such that $\mathbf{K}_-(\mathbf{n}^{(1)}) : \mathbf{q}_+ \neq \mathbf{K}_-(\mathbf{n}^{(2)}) : \mathbf{q}_+$ from (22) it follows that

$$(\bar{\epsilon}_+ - \bar{\epsilon}_-) : \boldsymbol{\tau} \otimes \boldsymbol{\tau} = 0 \quad \forall \boldsymbol{\tau} \parallel \mathbf{n}^{(1)} \times \mathbf{n}^{(2)} \quad (24)$$

The case $\mathbf{K}_-(\mathbf{n}^{(1)}) : \mathbf{q}_+ = \mathbf{K}_-(\mathbf{n}^{(2)}) : \mathbf{q}_+$ is not of interest for the minimization problem since can be reduced to the consideration of the simple laminate, as it is shown below. Of course, (23), (24) can be directly derived from strain jumps representations in diadic forms

$$\epsilon_2^{(1)} - \epsilon_1^{(1)} = (\mathbf{n}^{(1)} \otimes \mathbf{a}^{(1)})^s \quad \text{and} \quad \epsilon_2^{(2)} - \epsilon_1^{(2)} = (\mathbf{n}^{(2)} \otimes \mathbf{a}^{(2)})^s,$$

where $\mathbf{a}^{(1)}$ and $\mathbf{a}^{(2)}$ are amplitudes of jumps. The compatibility conditions (23), (24) will be used in Section 4 as a hint for the choice of the translator parameters.

3.2. Minimization of the strain energy of laminates

The energy of the laminates can be minimized over the normals $\mathbf{n}_i$, structural parameters β_i , and the rank n :

$$\mathcal{LW} = \min_{(n)} \min_{\mathbf{n}^{(i)}} \min_{\beta^{(i)} : \beta^{(i)} > 0, \sum_{i=1}^n \beta^{(i)} = 1} W^{(n)}.$$

First of all we are searching the normals $\mathbf{n}^{(i)}$ and structural parameters $\beta^{(i)}$ satisfying the conditions

$$\frac{\partial \left(W^{(n)} - \zeta \left(\sum_{i=1}^n \beta^{(i)} - 1 \right) \right)}{\partial \beta^{(i)}} = 0, \quad (25)$$

$$\frac{\partial \left(W^{(n)} - \sum_{i=1}^n \kappa^{(i)} (\mathbf{n}^{(i)} \cdot \mathbf{n}^{(i)} - 1) \right)}{\partial \mathbf{n}^{(i)}} = 0 \quad (26)$$

where $\kappa^{(i)}$ and ζ are the Lagrange multipliers.

Since $\delta_{\beta^{(i)}} \mathbf{M}_-^{(n)} = -m_- \mathbf{M}_-^{(n)} : \mathbf{K}_-(\mathbf{n}^{(i)}) : \mathbf{M}_-^{(n)} \delta \beta^{(i)}$, the condition (25) takes the form

$$m_- m_+ \mathbf{q}_+ : \mathbf{K}_-(\mathbf{n}^{(i)}) : \mathbf{q}_+ + 2\zeta = 0, \quad i = 1, 2 \dots n \quad (27)$$

from where it follows that, in the case of the rank- n laminate ($n \geq 2$), the tensor $\mathbf{q}_+$ and the normals are to be such that the quadratic form has the same values for all $\mathbf{n}^{(i)}$ ($i = 1, 2 \dots n$).

Since $\delta_{\mathbf{n}^{(i)}} \mathbf{M}_-^{(n)} = -\beta^{(i)} m_- \mathbf{M}_-^{(n)} : \delta_{\mathbf{n}^{(i)}} \mathbf{K}_-(\mathbf{n}^{(i)}) : \mathbf{M}_-^{(n)}$, the condition (26) can be rewritten as

$$\frac{1}{2} m_- m_+ \beta^{(i)} \mathbf{q}_+ : \delta \mathbf{K}_-(\mathbf{n}^{(i)}) : \mathbf{q}_+ + \kappa^{(i)} \delta \mathbf{n}^{(i)} \cdot \mathbf{n}^{(i)} = 0 \quad (28)$$

where (12) is accounted for.

The equations (28) look like the extremum conditions of the quadratic forms

$$\mathcal{K}_-(\mathbf{n}^{(i)} | \mathbf{q}_+) = \mathbf{q}_+ : \mathbf{K}_-(\mathbf{n}^{(i)}) : \mathbf{q}_+, \quad \mathbf{n}^{(i)} \cdot \mathbf{n}^{(i)} = 1$$

at given $\mathbf{q}_+$, and the maximum of $\mathcal{K}_-$ corresponds to minimum of $W^{(n)}$. Maximal and minimal values of $\mathcal{K}(\mathbf{n})$ have been found in [62, 35] in the context of the PTZ construction. The maximal value corresponds to external PTZ boundary related, as it was mentioned above, with locally stable interfaces. The maximal value also corresponds to the minimal energy of the simple laminates [38].

If the phase “-” is isotropic then

$$\begin{aligned} \mathbf{C}_- &= \lambda_- \mathbf{E} \otimes \mathbf{E} + 2\mu_- \mathbf{I}, \\ \mathbf{K}_-(\mathbf{n}) &= \frac{1}{\mu_-} \left((\mathbf{n} \otimes \mathbf{E} \otimes \mathbf{n})^s - \frac{1}{2(1 - \nu_-)} \mathbf{n} \otimes \mathbf{n} \otimes \mathbf{n} \otimes \mathbf{n} \right) \end{aligned}$$

and therefore

$$\mathbf{K}_-(\mathbf{n}) : \mathbf{q} = \frac{1}{2\mu_-} \left(\mathbf{q}_n \otimes \mathbf{n} + \mathbf{n} \otimes \mathbf{q}_n - \frac{q_{nn}}{1 - \nu_-} \mathbf{n} \otimes \mathbf{n} \right), \quad (29)$$

$$\mathcal{K}_-(\mathbf{n}, \mathbf{q}) = \frac{1}{\mu_-} (N_2 - \kappa_- N_1^2), \quad \kappa_- = \frac{1}{2(1 - \nu_-)} \quad (30)$$

Here $\mathbf{E}$ and $\mathbf{I}$ are the second and forth rank unit tensors, in Cartesian coordinates $E_{ij} = \delta_{ij}$, $I_{ijkl} = \frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$, δ_{ij} is Kroneker's delta, $\lambda_{\pm}$ and $\mu_{\pm}$

are the Lamé coefficients, ν_- is Poisson's ratio, $\mathbf{q}_n = \mathbf{q} \cdot \mathbf{n}$, $N_1 = q_{nn} = \mathbf{n} \cdot \mathbf{q} \cdot \mathbf{n}$ and $N_2 = \mathbf{n} \cdot \mathbf{q}^2 \cdot \mathbf{n}$ are so-called orientation invariants [62, 35], q_i ($i = 1, 2, 3$) are the eigenvalues of $\mathbf{q}$.

It was shown [62, 35] that the direction of the normal providing the maximum

$$\mathcal{K}_-^{max} = \max_{\mathbf{n}: |\mathbf{n}|=1} \mathcal{K}_-(\mathbf{n} | \mathbf{q}_+)$$

depends on the relationships between eigenvalues of $\mathbf{q}_+$ as follows.

Assume that the tensor $\mathbf{q}_+$ is given and has different eigenvalues, and $q_{\min}$, $q_{\max}$ and q_{mid} , and $\mathbf{e}_{\max}$, $\mathbf{e}_{\min}$, $\mathbf{e}_{\text{mid}}$ are the minimal, maximal and intermediate eigenvalues and corresponding eigenvectors of $\mathbf{q}_+$, $n_{\min}$, $n_{\max}$ and n_{mid} are components of the maximizing normal $\mathbf{n}^*$ in the basis of eigenvectors of $\mathbf{q}_+$, $|q|_{\max}$ is the maximal absolute eigenvalue and $\mathbf{e}_{|q|_{\max}}$ is the corresponding eigenvector of $\mathbf{q}_+$, $|q|_{\min}$ is the minimal absolute eigenvalue of $\mathbf{q}_+$. Then if

$$q_{\min}q_{\max} < 0 \quad \text{or} \quad \begin{cases} q_{\min}q_{\max} > 0 \\ (1 - \nu_-)|q|_{\min} < \nu_-|q|_{\max} \end{cases} \quad (31)$$

then the normal lies in the plane of maximal and minimal eigenvalues of the tensor $\mathbf{q}_+$, $n_{\text{mid}} = 0$, and the components are

$$n_{\max}^2 = \frac{(1 - \nu_-)q_{\max} - \nu_-q_{\min}}{q_{\max} - q_{\min}}, \quad n_{\min}^2 = \frac{\nu_-q_{\max} - (1 - \nu_-)q_{\min}}{q_{\max} - q_{\min}}. \quad (32)$$

In this case, by (29) and (30),

$$\mathbf{K}_-(\mathbf{n}^*) : \mathbf{q}_+ = \frac{q_{\max} - q_{\min}}{2\mu_-} (n_{\max}^2 \mathbf{e}_{\max} \otimes \mathbf{e}_{\max} - n_{\min}^2 \mathbf{e}_{\min} \otimes \mathbf{e}_{\min}), \quad (33)$$

$$\begin{aligned} \mathcal{K}_-^{max} &= \frac{q_{\max} - q_{\min}}{2\mu_-} (n_{\max}^2 q_{\max} - n_{\min}^2 q_{\min}) \\ &= \frac{1 - \nu_-}{2\mu_-} (q_{\max}^2 + q_{\min}^2) - \frac{\nu_-}{\mu_-} q_{\max} q_{\min}. \end{aligned} \quad (34)$$

Otherwise

$$\mathbf{n}^* = \mathbf{e}_{|q|_{\max}}, \quad (35)$$

$$\mathbf{K}_-(\mathbf{n}^*) : \mathbf{q}_+ = \frac{1 - 2\nu_-}{2\mu_-(1 - \nu_-)} |q|_{\max} \mathbf{e}_{|q|_{\max}} \otimes \mathbf{e}_{|q|_{\max}}, \quad (36)$$

$$\mathcal{K}_-^{max} = \frac{1 - 2\nu_-}{2\mu_-(1 - \nu_-)} |q|_{\max}^2. \quad (37)$$

Let $\mathbf{q}_+$ be axisymmetric: $\mathbf{q}_+ = q(\mathbf{E} - \mathbf{k} \otimes \mathbf{k}) + q_k \mathbf{k} \otimes \mathbf{k}$. If

$$\begin{aligned} q_k q < 0 \quad \text{or} \quad \begin{cases} q_k q > 0 \\ (1 - \nu_-)|q|_{\min} < \nu_-|q|_{\max} \end{cases} \quad (38) \\ |q|_{\min} = \min\{|q_k|, |q|\}, \quad |q|_{\max} = \max\{|q_k|, |q|\} \end{aligned}$$

then maximum of $\mathcal{K}_-$ is reached at any normal with the projection onto the axe $\mathbf{k}$

$$n_k^2 = \frac{(1 - \nu_-)q_k - \nu_-q}{q_k - q}. \quad (39)$$

Then

$$\mathbf{K}_-(\mathbf{n}^*) : \mathbf{q}_+ = \frac{q_k - q}{2\mu_-} (n_k^2 \mathbf{k} \otimes \mathbf{k} - (1 - n_k^2) \mathbf{e} \otimes \mathbf{e}), \quad (40)$$

$$\mathcal{K}_-^{\max} = \frac{q_k - q}{2\mu_-} (q_k n_k^2 - q(1 - n_k^2)) = \frac{1 - \nu_-}{2\mu_-} (q_k^2 + q^2) - \frac{\nu_-}{\mu_-} q_k q, \quad (41)$$

where $\mathbf{e} = \mathbf{k} \times \frac{\mathbf{k} \times \mathbf{n}^*}{|\mathbf{k} \times \mathbf{n}^*|}$ is the eigenvector of $\mathbf{K}_-(\mathbf{n}^*) : \mathbf{q}_+$ lying in the plane containing the vectors $\mathbf{k}$ and $\mathbf{n}^*$.

Otherwise

$$\mathbf{n}^* = \mathbf{k} \text{ if } |q_k| > |q|, \quad (42)$$

$$\mathbf{n}^* \perp \mathbf{k} \text{ if } |q_k| < |q|, \quad (43)$$

$$\mathbf{K}_-(\mathbf{n}^*) : \mathbf{q}_+ = \frac{1 - 2\nu_-}{2\mu_-(1 - \nu_-)} \max\{|q_k|, |q|\} \mathbf{n}^* \otimes \mathbf{n}^*, \quad (44)$$

$$\mathcal{K}_-^{\max} = \frac{1 - 2\nu_-}{2\mu_-(1 - \nu_-)} (\max\{|q_k|, |q|\})^2. \quad (45)$$

If $\mathbf{q}_+ = q\mathbf{E}$ then

$$\mathbf{K}_-(\mathbf{n}) : \mathbf{q}_+ = cq\mathbf{n} \otimes \mathbf{n}, \quad (46)$$

$\mathcal{K}_-$ does not depend on $\mathbf{n}$,

$$\mathbf{q}_+ : \mathbf{K}_-(\mathbf{n}) : \mathbf{q}_+ = cq^2, \quad c = \frac{1 - 2\nu_-}{2\mu_-(1 - \nu_-)} = \left(k_- + \frac{4}{3}\mu_-\right)^{-1}, \quad (47)$$

k_- is the bulk modulus.

If the normal $\mathbf{n}^*$ corresponds to the maximum of $\mathcal{K}_-(\mathbf{n}, \mathbf{q}_+)$ then the jump of strains has the same eigenvectors as the tensor $\mathbf{q}_+$. Thus, since the both phases are isotropic and strains $\boldsymbol{\varepsilon}_\pm^p$ are spherical, and the strain tensors $\boldsymbol{\varepsilon}_+$ and $\boldsymbol{\varepsilon}_-$ at the interfaces satisfying the relationships (31), (32) or (35) or (38)–(43) have the same eigenvalues [62]. Note that from (29) one can see that $\mathbf{q}_+ = \sum q_i \mathbf{e}_i \otimes \mathbf{e}_i$ and $\mathbf{K}_-(\mathbf{n}) : \mathbf{q}_+$ have the same eigenvectors $\mathbf{e}_i$ ($i = 1, 2, 3$) if and only if

$$\mathbf{e}_i \cdot (\mathbf{K}_-(\mathbf{n}) : \mathbf{q}_+) \cdot \mathbf{e}_j = \frac{1}{2\mu_-} \left(q_i + q_j - \frac{q_{nn}}{1 - \nu_-} \right) n_i n_j = \begin{cases} 0 & \text{if } i \neq j \\ K_i & \text{if } i = j \end{cases} \quad (48)$$

where K_i are the eigenvalues of $\mathbf{K}_-(\mathbf{n}) : \mathbf{q}_+$. All the cases listed above are particular cases of (48).

Taking into account relationships (30)–(47), we can *a priory* characterize the strains in the phase “+” and the directions of the normals in the laminates of various ranks which can satisfy both conditions (28) and (27). To distinguish different cases of interest we will use the following properties of strains in laminates (see derivations and proofs in Appendix B):

1. Strains at different scales are related by a transmitting formula

$$\boldsymbol{\varepsilon}_1^{(i)} - \boldsymbol{\varepsilon}_1^{(i-1)} = \left(\prod_{j=1}^{i-1} m_2^{(j)} \right) (\mathbf{K}_-(\mathbf{n}^{(i)}) - \mathbf{K}_-(\mathbf{n}^{(i-1)})) : \mathbf{q}_+ \quad (49)$$

2. We formulate another feature as

Proposition 2. *Let two rank- n laminates A and B differ by the permutation of adjacent normals $\mathbf{n}^{(k)}$ and $\mathbf{n}^{(k+1)}$ ($1 \leq k \leq n-1$) such that*

$$\begin{aligned} \mathbf{n}_B^{(i)} &= \mathbf{n}_A^{(i)} & \text{if } 1 \leq i < k-1 & \text{ and } k+1 < i \leq n \\ \mathbf{n}_B^{(k)} &= \mathbf{n}_A^{(k+1)}, & \mathbf{n}_B^{(k+1)} &= \mathbf{n}_A^{(k)} \end{aligned}$$

and the volume fractions $m_{1A,B}^{(k)}$, $m_{1A,B}^{(k+1)}$ and $m_{2A,B}^{(k)}$ obey the relationships

$$m_{1A}^{(k)} = m_{1B}^{(k+1)} m_{2B}^{(k)}, \quad m_{1B}^{(k)} = m_{1A}^{(k+1)} m_{2A}^{(k)} \quad (50)$$

Then, given average strain $\boldsymbol{\varepsilon}_0$, the laminates have the same strain energy.

The above statements are used in the proof of the following proposition that allows to reduce the rank of the energy minimizing laminate without changing its energy.

Proposition 3. *If two normals in a laminate satisfy the equality*

$$\mathbf{K}(\mathbf{n}^{(i)}) : \mathbf{q}_+ = \mathbf{K}(\mathbf{n}^{(j)}) : \mathbf{q}_+ \quad (51)$$

then the rank of the laminate can be lowered by a unit without changing the strain energy.

Further, for various combinations of eigenvalues of $\mathbf{q}_+$, we will choose the optimal laminates of the lowest rank among energy equivalent laminates of the first, second and third rank. It can be proved that there are only four cases which represent all energy nonequivalent laminates which satisfy the conditions (26) and (25) (see Appendix C). These cases are:

I. *Simple (first-rank) laminates.* The laminate provides the maximum of $\mathcal{K}_-(\mathbf{n}, \mathbf{q}_+)$ and has the normal determined by (32) either (35), depending on the eigenvalues of $\mathbf{q}_+$.

II. *Second-rank laminates.* The tensor $\mathbf{q}_+$ is axisymmetric,

$$\mathbf{q}_+ = q(\mathbf{E} - \mathbf{k} \otimes \mathbf{k}) + q_k \mathbf{k} \otimes \mathbf{k}$$

- (a) The eigenvalues q and q_k satisfy (38). Then any two different normals with the same square of the projection onto the axe $\mathbf{k}$ equal to (39) and noncoplanar with $\mathbf{k}$ can be taken as $\mathbf{n}^{(1)}$ and $\mathbf{n}^{(2)}$.
- (b) The eigenvalues q and q_k do not satisfy (38) and $|q_k| < |q|$. Then two different normals $\mathbf{n}^{(1)}$ and $\mathbf{n}^{(2)}$ lie in a plane perpendicular to the axe $\mathbf{k}$.

III. *Third-Rank laminates.* The tensor $\mathbf{q}_+$ is spherical, any three non-coplanar unit vectors can be the normals.

It can be also proved that optimal laminates of the ranks higher than three are energy equivalent to one of the above-mentioned optimal laminates of rank-1,2 or 3 (see Appendix C).

Note that the second-rank laminates are of interest only with axisymmetric tensor $\mathbf{q}_+$, and the third-rank laminates only with a spherical $\mathbf{q}_+$. The cases with other $\mathbf{q}_+$ are reduced to lower rank laminates. Note also that in the case II(a) the normals $\mathbf{n}^{(1)}$ and $\mathbf{n}^{(2)}$ do not lie in the same eigenplane of the tensor $\mathbf{q}_+$, as opposed to II(b).

4. Translation bound for strain energy

4.1. Translated energy

Translator. We construct the lower bound of the optimal energy using the translation method [22, 43, 55, 60, 61] that is based on the polyconvexity [24]. The construction follows [22, 43] (see also [15]).

According to the translation method, we replace differential properties of a strain $\boldsymbol{\varepsilon} = (\nabla \mathbf{u})^s$ with weaker integral corollaries [22, 43] of quasiconvexity: any subdeterminant of Jacobian $\nabla \mathbf{u}$ is quasifine: $\langle \text{subdet}(\nabla \mathbf{u}) \rangle = \text{subdet} \langle \nabla \mathbf{u} \rangle$ where $\langle \cdot \rangle$ denotes averaging over Ω (see, e.g., [65]).

The nonconvex function $\theta_1 = \varepsilon_{23}^2 - \varepsilon_{22}\varepsilon_{33}$ can be presented as

$$\theta_1 = \left(\frac{\partial u_2}{\partial x_3} \frac{\partial u_3}{\partial x_2} - \frac{\partial u_2}{\partial x_2} \frac{\partial u_3}{\partial x_3} \right) + \frac{1}{4} \left(\frac{\partial u_2}{\partial x_3} - \frac{\partial u_3}{\partial x_2} \right)^2,$$

the sum of such subdeterminant and a convex function, where u_i are the components of the displacement vector $\mathbf{u}$. Therefore, Jensen's inequality is satisfied

$$\theta_i(\boldsymbol{\varepsilon}_0) \leq \int_{\Omega} \theta_i(\boldsymbol{\varepsilon}) d\Omega, \quad i = 1, 2, 3, \quad \boldsymbol{\varepsilon}_0 = \int_{\Omega} \boldsymbol{\varepsilon}(\mathbf{x}) d\Omega$$

where the functions θ_2 and θ_3 are obtained from θ_1 by permutation. Multiplying them by three nonnegative numbers t_1, t_2, t_3 and adding the left- and righthand sides, we obtain the inequality of a translator:

$$\varphi(\mathbf{t}, \boldsymbol{\varepsilon}_0) \leq \int_{\Omega} \varphi(\mathbf{t}, \boldsymbol{\varepsilon}) d\Omega \quad \forall t_i \geq 0, \quad i = 1, 2, 3 \quad (52)$$

where translator $\varphi(\mathbf{t}, \boldsymbol{\varepsilon})$ (see [43])

$$\varphi(\boldsymbol{\varepsilon}, t_1, t_2, t_3) = t_3(\varepsilon_{12}^2 - \varepsilon_{11}\varepsilon_{22}) + t_2(\varepsilon_{13}^2 - \varepsilon_{11}\varepsilon_{33}) + t_1(\varepsilon_{23}^2 - \varepsilon_{22}\varepsilon_{33}) \quad (53)$$

is a function dependent of three nonnegative parameters t_1, t_2 and t_3 .

The quadratic form of the translator can be written in tensorial form $\varphi(\mathbf{t}, \boldsymbol{\varepsilon}) = \frac{1}{2} \boldsymbol{\varepsilon} : \mathbf{T} : \boldsymbol{\varepsilon}$, where

$$\mathbf{T} = (\mathbf{t} \otimes \mathbf{E} + \mathbf{E} \otimes \mathbf{t}) + (\text{tr } \mathbf{t})(\mathbf{I} - \mathbf{E} \otimes \mathbf{E}) - (\mathbf{I} \cdot \mathbf{t} + \mathbf{t} \cdot \mathbf{I}). \quad (54)$$

is the corresponding fourth-rank tensor that possesses all symmetries with respect to indices permutations as the elasticity tensor, where tensor $\mathbf{t}$ is the second-rank tensor with the eigenvalues t_1, t_2 and t_3 (see Appendix D for derivation of (54)). Tensorial form is used for the further analysis.

Translation bound. The energy of the composite cell

$$w_0(\boldsymbol{\varepsilon}_0) = \frac{1}{2}(\boldsymbol{\varepsilon}_0 - \boldsymbol{\varepsilon}_0^p) : \mathbf{C}_0 : (\boldsymbol{\varepsilon}_0 - \boldsymbol{\varepsilon}_0^p),$$

where $\mathbf{C}_0$ and $\boldsymbol{\varepsilon}_0^p$ are the effective elasticity tensor and the effective transformation strains, satisfies the variational condition

$$w_0(\boldsymbol{\varepsilon}_0) = \frac{1}{2} \min_{\substack{\boldsymbol{\varepsilon} : \langle \boldsymbol{\varepsilon} \rangle = \boldsymbol{\varepsilon}_0 \\ \boldsymbol{\varepsilon} = (\nabla \mathbf{u})^s}} \int_{\Omega} (\boldsymbol{\varepsilon}(\mathbf{x}) - \boldsymbol{\varepsilon}^p(\mathbf{x})) : \mathbf{C}(\mathbf{x}) : (\boldsymbol{\varepsilon}(\mathbf{x}) - \boldsymbol{\varepsilon}^p(\mathbf{x})) d\Omega.$$

Subtracting (52) from both parts of this equality we obtain an inequality

$$w_0(\boldsymbol{\varepsilon}_0) - \varphi(\boldsymbol{\varepsilon}_0, \mathbf{t}) \geq \min_{\substack{\boldsymbol{\varepsilon} : \langle \boldsymbol{\varepsilon} \rangle = \boldsymbol{\varepsilon}_0 \\ \boldsymbol{\varepsilon} = (\nabla \mathbf{u})^s}} \int_{\Omega} ((1 - H(\mathbf{x}))w_-^t(\boldsymbol{\varepsilon}, \mathbf{t}) + H(\mathbf{x})w_+^t(\boldsymbol{\varepsilon}, \mathbf{t})) d\Omega, \quad \forall \mathbf{t} \quad (55)$$

where

$$w_{\pm}^t(\mathbf{t}, \boldsymbol{\varepsilon}) = \frac{1}{2}(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_{\pm}^p) : \mathbf{C}_{\pm} : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_{\pm}^p) - \frac{1}{2}\boldsymbol{\varepsilon} : \mathbf{T} : \boldsymbol{\varepsilon} \quad (56)$$

are the translated strain energy densities.

Assume that $\mathbf{T}$ is so chosen, that $w_{\pm}^t(\mathbf{t}, \boldsymbol{\varepsilon})$ is a convex function of $\boldsymbol{\varepsilon}$:

$$\boldsymbol{\varepsilon} : (\mathbf{C}_{\pm} - \mathbf{T}) : \boldsymbol{\varepsilon} \geq 0, \quad \forall \boldsymbol{\varepsilon}.$$

The inequality (55) becomes stronger if we increase the set of minimizers $\boldsymbol{\varepsilon}(x)$ by neglecting differential property $\boldsymbol{\varepsilon}(x) = (\nabla \mathbf{u})^s$. Due to convexity of $w_{\pm}^t(\mathbf{t}, \boldsymbol{\varepsilon})$, we can replace $\boldsymbol{\varepsilon}(x)$ in each phase by its average $\bar{\boldsymbol{\varepsilon}}_{\pm}$, respectively.

$$w_0(\boldsymbol{\varepsilon}_0) - \varphi(\boldsymbol{\varepsilon}_0, \mathbf{t}) \geq \min_{m_- \bar{\boldsymbol{\varepsilon}}_- + m_+ \bar{\boldsymbol{\varepsilon}}_+ = \boldsymbol{\varepsilon}_0} (m_- w_-^t(\mathbf{t}, \bar{\boldsymbol{\varepsilon}}_-) + m_+ w_+^t(\mathbf{t}, \bar{\boldsymbol{\varepsilon}}_+)) \quad \forall \mathbf{t} \quad (57)$$

where

$$\bar{\boldsymbol{\varepsilon}}_- = \frac{1}{m_-} \int_{\Omega_-} \boldsymbol{\varepsilon} d\Omega, \quad \bar{\boldsymbol{\varepsilon}}_+ = \frac{1}{m_+} \int_{\Omega_+} \boldsymbol{\varepsilon} d\Omega.$$

Finally, we maximize $\varphi(\boldsymbol{\varepsilon}_0, \mathbf{t})$ and the right hand side of the inequality over $\mathbf{t}$. Then the inequality (57) becomes

$$w_0(\boldsymbol{\varepsilon}_0) \geq \mathcal{PW}.$$

Here,

$$\mathcal{PW} = \max_{t_i \in \Theta} \left(\min_{m_- \bar{\epsilon}_- + m_+ \bar{\epsilon}_+ = \epsilon_0} W^t(\bar{\epsilon}_-, \bar{\epsilon}_+) + \varphi(\mathbf{t}, \epsilon_0) \right) \quad (58)$$

and

$$W^t(\bar{\epsilon}_-, \bar{\epsilon}_+) = m_- w_-^t(\bar{\epsilon}_-) + m_+ w_+^t(\bar{\epsilon}_+),$$

the average strains $\bar{\epsilon}_\pm$ are defined by (20) and satisfy the restriction (21), and the set Θ of admissible translator parameters is determined in Subsection 4.3. The function $\mathcal{PW}$ is called the translation bound.

4.2. Translation-optimal strains in the phases

Here we find minimizing average strains $\bar{\epsilon}_\pm$. Optimal (maximizing) translator parameters are defined in Subsection 4.3. Since the function W^t is the convex function of strains $\bar{\epsilon}_\pm$, the minimization with respect to $\bar{\epsilon}_\pm$ is carried out by the direct differentiating W^t at fixed ϵ_0 . Taking into account (56), we obtain

$$\frac{\partial}{\partial \bar{\epsilon}_\pm} (W^t + \boldsymbol{\lambda} : (m_- \bar{\epsilon}_- + m_+ \bar{\epsilon}_+ - \epsilon_0)) = m_\pm (\mathbf{C}_\pm : (\bar{\epsilon}_\pm - \epsilon_\pm^p) - \mathbf{T} : \bar{\epsilon}_\pm + \boldsymbol{\lambda}) = 0$$

where $\boldsymbol{\lambda}$ is the second order tensor of Lagrange multipliers by the restriction (21). Minimizers $\bar{\epsilon}_-$ and $\bar{\epsilon}_+$ are to be found from the system of equations

$$\begin{cases} (\mathbf{C}_+ - \mathbf{T}) : \bar{\epsilon}_+ - \mathbf{C}_+ : \epsilon_+^p = (\mathbf{C}_- - \mathbf{T}) : \bar{\epsilon}_- - \mathbf{C}_- : \epsilon_-^p \\ m_- \bar{\epsilon}_- + m_+ \bar{\epsilon}_+ = \epsilon_0 \end{cases}$$

They are:

$$\begin{aligned} \bar{\epsilon}_- &= (m_- \mathbf{C}_+ + m_+ \mathbf{C}_- - \mathbf{T})^{-1} : ((\mathbf{C}_+ - \mathbf{T}) : \epsilon_0 - m_+ \llbracket \mathbf{C} : \epsilon^p \rrbracket), \\ \bar{\epsilon}_+ &= (m_- \mathbf{C}_+ + m_+ \mathbf{C}_- - \mathbf{T})^{-1} : ((\mathbf{C}_- - \mathbf{T}) : \epsilon_0 + m_- \llbracket \mathbf{C} : \epsilon^p \rrbracket), \end{aligned} \quad (59)$$

4.3. Domain of admissible translator parameters

The translation parameters vary in a set defined by several constraints, see [43, 15]: (i) by definition of the translator (53), the translator parameters are non-negative, and (ii) they are restricted by the requirement of convexity of w^t , that is by nonnegativity of the quadratic forms

$$\begin{aligned} \epsilon : (\mathbf{C}_\pm - \mathbf{T}) : \epsilon &= (\lambda_\pm + 2\mu_\pm)(\epsilon_{11}^2 + \epsilon_{22}^2 + \epsilon_{33}^2) + \\ &\quad 2(\lambda_\pm + t_3)\epsilon_{11}\epsilon_{22} + 2(\lambda_\pm + t_2)\epsilon_{11}\epsilon_{33} + 2(\lambda_\pm + t_1)\epsilon_{22}\epsilon_{33} + \\ &\quad 2(2\mu_\pm - t_3)\epsilon_{12}^2 + 2(2\mu_\pm - t_2)\epsilon_{13}^2 + 2(2\mu_\pm - t_1)\epsilon_{23}^2. \end{aligned} \quad (60)$$

The Hessian of (60) with respect of entries of ε is

$$H = 2 \begin{pmatrix} \lambda_{\pm} + 2\mu_{\pm} & \lambda_{\pm} + t_3 & \lambda_{\pm} + t_2 & 0 & 0 & 0 \\ \lambda_{\pm} + t_3 & \lambda_{\pm} + 2\mu_{\pm} & \lambda_{\pm} + t_1 & 0 & 0 & 0 \\ \lambda_{\pm} + t_2 & \lambda_{\pm} + t_1 & \lambda_{\pm} + 2\mu_{\pm} & 0 & 0 & 0 \\ 0 & 0 & 0 & 2(2\mu_{\pm} - t_3) & 0 & 0 \\ 0 & 0 & 0 & 0 & 2(2\mu_{\pm} - t_2) & 0 \\ 0 & 0 & 0 & 0 & 0 & 2(2\mu_{\pm} - t_1) \end{pmatrix} \quad (61)$$

It is non-negative-definite if

$$|t'_i| \leq 1, \quad i = 1, 2, 3 \quad (62)$$

$$2t'_1 t'_2 t'_3 - ((t'_1)^2 + (t'_2)^2 + (t'_3)^2) + 1 \geq 0, \quad (63)$$

where $t'_i = \frac{\lambda_{\pm} + t_i}{\lambda_{\pm} + 2\mu_{\pm}}$.

Inequality (63) shows that if one of the translator parameters t'_i equals unity then other two parameters must be equal to each other. Positivity of translator parameters together with equation (62) show that the admissible translator parameters are in the range

$$\Theta = \{t_i : t_i \in [0; 2\mu], \quad i = \overline{1, 3}, \quad \mu = \min\{\mu_-, \mu_+\}, \text{ and inequality (63) holds} \}.$$

Recall that we assumed $\mu_- < \mu_+$ in laminates construction, further we follow this assumption.

4.4. The optimal laminates and the choice of translator parameters

Now we have to find optimal translator parameters $t_1, t_2, t_3 \in \Theta$ to compute (58). We do not find translator parameters by straight maximization in (58). Instead, following approach suggested in [42, 43] and used in [1, 16], we assume that the lower bound is exact and attained by laminates which can be referred to as trial microstructures at this stage. We use compatibility conditions (23) and (24) and the properties of the strains ε_+ in optimal laminates to find translator parameters in various domains of strain space. The attainability of the lower bound with the use of optimal laminates is proved in the next subsection.

Depending on ε_0 , the translator parameters may lie inside the domain Θ or on various parts of its boundary. On one hand, the optimal translator parameters maximize the translated energy. On the other hand we expect that

the lower bound is attainable by one of the optimal laminated microstructure. Then, by the laminates analysis of Section 3, the translation-optimal average strain $\bar{\epsilon}_+$ in (59) is spherical or the difference of the translation-optimal average strains

$$\Delta\bar{\epsilon} = \bar{\epsilon}_+ - \bar{\epsilon}_- = (m_- \mathbf{C}_+ + m_+ \mathbf{C}_- - \mathbf{T})^{-1} : ((\mathbf{C}_- - \mathbf{C}_+) : \epsilon_0 + \llbracket \mathbf{C} : \epsilon^p \rrbracket) \quad (64)$$

satisfies compatibility conditions (23) or (24). Since the condition (24) corresponds to the second-rank laminates, an additional restriction on the translator parameters is that the tensor $\bar{\epsilon}_+$ is axisymmetric in this case. Different domains of external strains correspond to different optimal laminates and, thus, to different strains $\bar{\epsilon}_\pm$. This, in accordance with (59), gives different sets of the translator parameters.

The difference (64) can be rewritten in the form

$$\Delta\bar{\epsilon} = \bar{\epsilon}_+ - \bar{\epsilon}_- = -(m_- \mathbf{C}_+ + m_+ \mathbf{C}_- - \mathbf{T})^{-1} : \mathbf{q}_0, \quad (65)$$

where $\mathbf{q}_0 = \llbracket \mathbf{C} \rrbracket : \epsilon_0 - \llbracket \mathbf{C} : \epsilon^p \rrbracket = \llbracket \mathbf{C} \rrbracket : \mathbf{e}_0$. Then it is convenient to present the results through the eigenvalues q_i ($i = 1, 2, 3$) of $\mathbf{q}_0$ instead of ϵ_0 . We assume that tensors $\mathbf{t}$ and $\mathbf{q}_0$ have the same principal directions $\mathbf{e}_1$, $\mathbf{e}_2$ and $\mathbf{e}_3$. Then, by (59) and (65), the strain tensors $\bar{\epsilon}_\pm$ and the difference $\Delta\bar{\epsilon}$ have the same principal directions. This simplifies finding t_1 , t_2 , t_3 .

The calculation of the translator parameters leads to the following results. Let q_i be ordered such that $|q_3| \geq |q_1|, |q_2|$. Then all possible microstructures and corresponding translator parameters can be shown on the plane δ_1^q, δ_2^q , where $\delta_1^q = q_1/q_3$, $\delta_2^q = q_2/q_3$. Note that $|\delta_i^q| \leq 1$.

The top half $\delta_1^q \leq \delta_2^q$ of square $|\delta_i^q| \leq 1$ is divided into domains Ψ_i^q ($i = 1, 2, \dots, 7$), and each domain is characterized by some laminate microstructure

and by a set of values of the translator parameters:

$$\begin{aligned}
& t_1 = t_2 = t_3 = 2\mu_- & \text{if } \mathbf{q}_0 \in \Psi_1^q, \\
& t_1 = 2\mu_-, \quad t_2 = t_3 = \frac{2\delta_1^q(\mu_- + \bar{\mu}) + \bar{\lambda}(2\delta_1^q - \delta_2^q - 1)}{1 + \delta_2^q} & \text{if } \mathbf{q}_0 \in \Psi_2^q, \\
& t_1 = 2(\delta_2^q - 1)\bar{\lambda} + 2\delta_2^q\bar{\mu}, \quad t_2 = t_3 = (\delta_1^q - 1)\bar{\lambda} + 2\delta_1^q\bar{\mu} & \text{if } \mathbf{q}_0 \in \Psi_3^q, \\
& t_1 = 2\mu_-, \quad t_2 = t_3 = 0 & \text{if } \mathbf{q}_0 \in \Psi_4^q, \\
& t_1 = \frac{2\bar{\mu}(\bar{\lambda}(\delta_1^q - 2\delta_2^q + 1) - 2\delta_2^q\bar{\mu})}{\bar{\lambda}(1 - \delta_1^q) - 2\bar{\mu}}, \quad t_2 = t_3 = 0 & \text{if } \mathbf{q}_0 \in \Psi_5^q, \\
& t_1 = t_2 = 0, \quad t_3 = \frac{2\bar{\mu}(2\delta_2^q(\bar{\lambda} + \bar{\mu}) - \bar{\lambda}(1 + \delta_1^q))}{\bar{\lambda}(1 - \delta_1^q) + 2\bar{\mu}\delta_1^q} & \text{if } \mathbf{q}_0 \in \Psi_6^q, \\
& t_1 = t_2 = 0, \quad t_3 = 2\mu_- & \text{if } \mathbf{q}_0 \in \Psi_7^q,
\end{aligned} \tag{66}$$

where $\bar{\mu} = m_+\mu_- + m_-\mu_+$, $\bar{\lambda} = m_+\lambda_- + m_-\lambda_+$ and

$$\begin{aligned}
\Psi_1^q &= \left\{ \mathbf{q}_0 : \begin{aligned} &\delta_2^q \leq 2\delta_1^q \frac{\bar{\mu} + \mu_- + \bar{\lambda}}{2\mu_- + \bar{\lambda}} - 1, \delta_2^q \leq 1, \\ &\delta_1^q \leq 2\delta_2^q \frac{\bar{\mu} + \mu_- + \bar{\lambda}}{2\mu_- + \bar{\lambda}} - 1, \delta_1^q \leq 1 \end{aligned} \right\}, \\
\Psi_2^q &= \left\{ \mathbf{q}_0 : \begin{aligned} &\delta_2^q \geq 2\delta_1^q \frac{\bar{\mu} + \mu_- + \bar{\lambda}}{2\mu_- + \bar{\lambda}} - 1, \delta_2^q \geq \frac{\bar{\lambda} + 2\mu_-}{\bar{\lambda} + 2\bar{\mu}}, \\ &\delta_2^q \leq 1, \delta_2^q \leq 2\delta_1^q \frac{\bar{\mu} + \mu_- + \bar{\lambda}}{\bar{\lambda}} - 1 \end{aligned} \right\}, \\
\Psi_3^q &= \left\{ \mathbf{q}_0 : \delta_1^q \geq \frac{\bar{\lambda}}{\bar{\lambda} + 2\bar{\mu}}, \delta_2^q \geq \frac{\bar{\lambda}}{\bar{\lambda} + 2\bar{\mu}}, \delta_1^q \leq \frac{\bar{\lambda} + 2\mu_-}{\bar{\lambda} + 2\bar{\mu}}, \delta_2^q \leq \frac{\bar{\lambda} + 2\mu_-}{\bar{\lambda} + 2\bar{\mu}} \right\}, \\
\Psi_4^q &= \left\{ \mathbf{q}_0 : \begin{aligned} &\delta_2^q \leq 1, \delta_2^q \geq \frac{\bar{\lambda}(\bar{\mu} - \mu_-)\delta_1^q + \bar{\lambda}(\bar{\mu} + \mu_-) + 2\bar{\mu}\mu_-}{2\bar{\mu}(\bar{\lambda} + \bar{\mu})}, \\ &\delta_2^q \geq 2\delta_1^q \frac{\bar{\mu} + \mu_- + \bar{\lambda}}{\bar{\lambda}} - 1, \delta_1^q \geq -1 \end{aligned} \right\}, \\
\Psi_5^q &= \left\{ \mathbf{q}_0 : \begin{aligned} &\delta_2^q \leq \frac{\bar{\lambda}(\bar{\mu} - \mu_-)\delta_1^q + \bar{\lambda}(\bar{\mu} + \mu_-) + 2\bar{\mu}\mu_-}{2\bar{\mu}(\bar{\lambda} + \bar{\mu})}, \\ &\delta_2^q \geq \frac{\bar{\lambda}(\delta_1^q + 1)}{2(\bar{\lambda} + \bar{\mu})}, \delta_1^q \leq \frac{\bar{\lambda}}{\bar{\lambda} + 2\bar{\mu}}, \delta_1^q \geq -1 \end{aligned} \right\}, \\
\Psi_6^q &= \left\{ \mathbf{q}_0 : \begin{aligned} &\delta_2^q \leq \frac{\bar{\lambda}(\delta_1^q + 1)}{2(\bar{\lambda} + \bar{\mu})}, \delta_1^q \leq -1, \\ &\delta_2^q \geq \frac{\delta_1^q(\bar{\lambda}(\mu_- + \bar{\mu}) + 2\mu_- \bar{\mu}) + \bar{\lambda}(\bar{\mu} - \mu_-)}{2\bar{\mu}(\bar{\lambda} + \bar{\mu})} \end{aligned} \right\}, \\
\Psi_7^q &= \left\{ \mathbf{q}_0 : \begin{aligned} &\delta_2^q \geq \delta_1^q, \delta_1^q \geq -1, \\ &\delta_2^q \leq \frac{\delta_1^q(\bar{\lambda}(\mu_- + \bar{\mu}) + 2\mu_- \bar{\mu}) + \bar{\lambda}(\bar{\mu} - \mu_-)}{2\bar{\mu}(\bar{\lambda} + \bar{\mu})} \end{aligned} \right\}.
\end{aligned} \tag{67}$$

In the domain Ψ_1^q the tensor $\mathbf{q}_+$ is spherical and all eigenvalues of the strain difference tensor $\Delta\bar{\boldsymbol{\varepsilon}}$ have the same sign. The microstructure is the third-rank laminates.

In the domain Ψ_2^q the tensor $\mathbf{q}_+$ is axisymmetric, $\mathbf{q}_+ = q_k \mathbf{e}_1 \mathbf{e}_1 + q(\mathbf{E} - \mathbf{e}_1 \mathbf{e}_1)$, the differences of the eigenvalues of $\bar{\boldsymbol{\varepsilon}}_{\pm}$ are such that $\Delta\bar{\varepsilon}_1 = 0$ and $\Delta\bar{\varepsilon}_2 \Delta\bar{\varepsilon}_3 > 0$. The microstructure is the direct second-rank laminates.

In the domains Ψ_4^q and Ψ_7^q the strain tensor $\bar{\boldsymbol{\varepsilon}}_+$ is axisymmetric and the eigenvalues of the tensor $\Delta\bar{\boldsymbol{\varepsilon}}$ differ from zero and have different signs. Thus, a vector $\boldsymbol{\tau}$ exists such that $\Delta\bar{\boldsymbol{\varepsilon}} : \boldsymbol{\tau} \boldsymbol{\tau} = 0$. The microstructures are skew

Figure 3: Type of optimal microstructures, which energy attains the lower bound, in dependence on δ_1^q and δ_2^q

second-rank laminates. In the domain Ψ_4^q $\mathbf{q}_+ = q_k \mathbf{e}_1 \mathbf{e}_1 + q(\mathbf{E} - \mathbf{e}_1 \mathbf{e}_1)$, one of the normals lies in the plane passing through the eigenvectors $\mathbf{e}_1$ and $\mathbf{e}_2$ of $\boldsymbol{\varepsilon}_0$ and the other normal lies in the plane passing through the vectors $\mathbf{e}_1$ and $\mathbf{e}_3$. In the domain Ψ_7^q $\mathbf{q}_+ = q_k \mathbf{e}_3 \mathbf{e}_3 + q(\mathbf{E} - \mathbf{e}_3 \mathbf{e}_3)$, one normal lies in the plane passing through the vectors $\mathbf{e}_1$ and $\mathbf{e}_3$ and the other one lies in the plane passing through $\mathbf{e}_2$ and $\mathbf{e}_3$.

In the domain Ψ_3^q , tensor $\bar{\boldsymbol{\varepsilon}}_+$ has different eigenvalues and the eigenvalues of the tensor $\Delta \bar{\boldsymbol{\varepsilon}}$ are $\Delta \bar{\varepsilon}_1 = \Delta \bar{\varepsilon}_2 = 0$, $\Delta \bar{\varepsilon}_3 \neq 0$. The microstructure is a simple laminates with the normal $\mathbf{n} = \mathbf{e}_3$.

In the domains Ψ_5^q and Ψ_6^q the eigenvalues of the strain difference tensor are $\Delta \bar{\varepsilon}_2 = 0$ and $\Delta \bar{\varepsilon}_1 \Delta \bar{\varepsilon}_3 < 0$. The microstructures are simple laminates with the normals lying in the plane passing through $\mathbf{e}_1$ and $\mathbf{e}_3$.

The remaining cases are obtained by permutation of indices. The domains and microstructures are shown in Fig. 3.

4.5. The attainability of the lower bound

We prove that the lower bound

$$\mathcal{PW} = m_- w_-^t(\mathbf{t}, \bar{\boldsymbol{\varepsilon}}_-) + m_+ w_+^t(\mathbf{t}, \bar{\boldsymbol{\varepsilon}}_+) + \varphi(\mathbf{t}, \boldsymbol{\varepsilon}_0),$$

where $\mathbf{t}$ is determined by (66) in domains (67), can be attained by the optimal laminates, i.e. the equation (7)

$$\mathcal{PW} = \mathcal{J}_{wm} = \mathcal{LW}$$

holds if the strains averaged over the phases in the laminate equal to translation-optimal strains $\bar{\boldsymbol{\varepsilon}}_-$ and $\bar{\boldsymbol{\varepsilon}}_+$.

At first, we note that since the jumps of strains across the interfaces in optimal laminates are defined by the relationships like (33) or (36), and the translator parameters are defined in (66), then the equality holds

$$\int_{\Omega} \varphi(\mathbf{t}, \boldsymbol{\varepsilon}) d\Omega = \varphi(\mathbf{t}, \boldsymbol{\varepsilon}_0). \quad (68)$$

Secondly, from the transmitting formula (49) it follows that the local strains in the phase “—” on every sublevel are related with the strain $\bar{\boldsymbol{\varepsilon}}_-$ can be represented as

$$\boldsymbol{\varepsilon}_1^{(j)} = \bar{\boldsymbol{\varepsilon}}_- + \sum_{i=2}^n \alpha_i^{(j)} (\mathbf{K}_-(\mathbf{n}^{(i-1)}) - \mathbf{K}_-(\mathbf{n}^{(i)})) : \mathbf{q}_+,$$

where parameters $\alpha_i^{(j)}$ depend on the volume fractions of the sublayers on all levels (we do not need their explicit expressions).

In the domains $\Psi_1^q, \Psi_2^q, \Psi_4^q$ and Ψ_7^q where the second- and third-rank laminates are optimal, the translator is determined by tensors $\mathbf{t} = 2\mu_- \mathbf{E}$, $\mathbf{t} = (2\mu_- - t)\mathbf{e}_1 \mathbf{e}_1 + t\mathbf{E}$, $\mathbf{t} = 2\mu_- \mathbf{e}_1 \mathbf{e}_1$ and $\mathbf{t} = 2\mu_- \mathbf{e}_3 \mathbf{e}_3$, respectively. Therefore the Hessian (61) has zero eigenvalues in these domains, and

$$(\mathbf{C}_- - \mathbf{T}) : (\mathbf{K}_-(\mathbf{n}^{(i-1)}) - \mathbf{K}_-(\mathbf{n}^{(i)})) : \mathbf{q}_+ = 0. \quad (69)$$

in the case of optimal laminates. Then from (56) and (69) it follows that the difference $\boldsymbol{\varepsilon}_1^{(j)} - \bar{\boldsymbol{\varepsilon}}_-$ is such that

$$w_-^t(\mathbf{t}, \boldsymbol{\varepsilon}_1^{(j)}) = w_-^t(\mathbf{t}, \bar{\boldsymbol{\varepsilon}}_-) \quad (70)$$

where the fact is also used that the transformation strain is spherical.

Now, assuming that the average strains in the laminates are $\bar{\boldsymbol{\varepsilon}}_-$ and $\bar{\boldsymbol{\varepsilon}}_+$, we show that the energy of the optimal laminates

$$\mathcal{LW} = \sum_{i=1}^n \frac{m_1^{(i)}}{m_2^{(i)}} \prod_{j=i}^n m_2^{(j)} w_-^t(\boldsymbol{\varepsilon}_1^{(i)}) + m_+ w_+(\bar{\boldsymbol{\varepsilon}}_+) \quad (71)$$

equals to the lower bound.

We add and subtract $\varphi(\mathbf{t}, \boldsymbol{\varepsilon}_0)$ to the right-hand side of (71) and, using (68), bring $\mathcal{LW}$ to the form

$$\mathcal{LW} = \sum_{i=1}^n \frac{m_1^{(i)}}{m_2^{(i)}} \prod_{j=i}^n m_2^{(j)} w_-^t(\mathbf{t}, \boldsymbol{\varepsilon}_1^{(i)}) + m_+ w_+^t(\mathbf{t}, \bar{\boldsymbol{\varepsilon}}_+) + \varphi(\mathbf{t}, \boldsymbol{\varepsilon}_0).$$

Then we express the strains $\boldsymbol{\varepsilon}_1^{(i)}$ through the average $\bar{\boldsymbol{\varepsilon}}_-$ and, using the relationship (70) and the equality $m_- = \sum_{i=1}^n \frac{m_1^{(i)}}{m_2^{(i)}} \prod_{j=i}^n m_2^{(j)}$, obtain

$$\mathcal{LW} = m_- w_-^t(\mathbf{t}, \bar{\boldsymbol{\varepsilon}}_-) + m_+ w_+^t(\mathbf{t}, \bar{\boldsymbol{\varepsilon}}_+) + \varphi(\mathbf{t}, \boldsymbol{\varepsilon}_0),$$

which is equal to $\mathcal{PW}$.

4.6. Optimal energy

The common values of the upper $\mathcal{LW}(m_+, \boldsymbol{\varepsilon}_0)$ and lower $\mathcal{PW}(m_+, \boldsymbol{\varepsilon}_0)$ bounds of the energy define the optimal energy $\mathcal{J}_{wm}(m_+, \boldsymbol{\varepsilon}_0)$ as it is noted in (7). The formulas for the optimal energy $\mathcal{J}_{wm}(m_+, \boldsymbol{\varepsilon}_0)$ are obtained by substitution of optimal t_i into expression for $\mathcal{PW}$. The resulting formulas, however, are bulky and not instructive. We show them here but for a special but representative case of zero eigenstrain $\boldsymbol{\varepsilon}_\pm^p = 0$ and zero Poisson's ratio:

$$\begin{aligned}
\mathcal{J}_{wm} &= \frac{\mu_-(\mu_+ + 2\mu_-)}{\bar{\mu} + 2\mu_-}(\varepsilon_1 + \varepsilon_2 + \varepsilon_3)^2 - 2\mu_-(\varepsilon_1\varepsilon_2 + \varepsilon_2\varepsilon_3 + \varepsilon_1\varepsilon_3) & \text{if } \mathbf{q}_0 \in \Psi_1^q \\
\mathcal{J}_{wm} &= (\mu_+ + \mu_- - \bar{\mu})\varepsilon_1^2 + \frac{\mu_-(\mu_+ + \mu_-)}{\bar{\mu} + \mu_-}(\varepsilon_2 + \varepsilon_3)^2 - 2\mu_-\varepsilon_2\varepsilon_3 & \text{if } \mathbf{q}_0 \in \Psi_2^q \\
\mathcal{J}_{wm} &= (\mu_+ + \mu_- - \bar{\mu})(\varepsilon_1^2 + \varepsilon_2^2) + \frac{\mu_-\mu_+}{\bar{\mu}}\varepsilon_3^2 & \text{if } \mathbf{q}_0 \in \Psi_3^q \\
\mathcal{J}_{wm} &= \frac{\mu_-\mu_+}{\bar{\mu}}\varepsilon_1^2 + \frac{\mu_-(\mu_+ + \mu_-)}{\bar{\mu} + \mu_-}(\varepsilon_2 + \varepsilon_3)^2 - 2\mu_-\varepsilon_2\varepsilon_3 & \text{if } \mathbf{q}_0 \in \Psi_4^q \\
\mathcal{J}_{wm} &= \frac{\mu_-\mu_+}{\bar{\mu}}(\varepsilon_1^2 + \varepsilon_3^2) + (\mu_+ + \mu_- - \bar{\mu})\varepsilon_2^2 & \text{if } \mathbf{q}_0 \in \Psi_5^q \cup \Psi_6^q \\
\mathcal{J}_{wm} &= \frac{\mu_-(\mu_+ + \mu_-)}{\bar{\mu} + \mu_-}(\varepsilon_1 + \varepsilon_2)^2 + \frac{\mu_-\mu_+}{\bar{\mu}}\varepsilon_3^2 - 2\mu_-\varepsilon_1\varepsilon_2 & \text{if } \mathbf{q}_0 \in \Psi_7^q
\end{aligned}$$

where the domains Ψ_i^q are derived easily from (67) (see also [5, 6]).

4.7. Comments on optimal regimes

1. The boundaries of the domains Ψ_i^q , derived from the optimality of the translated energy, coincide with the lines of change of the type of optimal microstructures. Namely, at the boundary CD the structure parameter β_1 in third-rank laminates tends to zero and the third-rank laminates degenerate into second-rank laminates. At the boundaries AF , AD and EH one of the structure parameters of the second rank laminates tends to zero and the second-rank laminates degenerate into simple laminates. At the boundaries AB and AE , when moving from Ψ_1^q to Ψ_6^q or from Ψ_2^q to Ψ_4^q , the condition (31) holds and correspondingly, direct laminates are turned into skew laminates.

2. In the degenerative case $m_+ = 0$ the arrangement of the domains Ψ_i^q does not change in general, but in the opposite case $m_- = 0$ the boundaries AF and AD move to the boundary $\delta_2^q = 1$ and the point D tends to the corner point $\delta_1^q = \delta_2^q = 1$. This implies that only simple laminates are optimal when the concentration of the softer phase m_- tends to zero.

3. We have shown that minimal energy at any external strain corresponds to an optimal laminate structure. The minimal energy of the optimal microstructures forms a multi-faced surface that is explicitly described by simple analytic formulas. Thus, we obtained a parametric representation for the quasiconvex envelope of two-well Lagrangian for elastic energy in 3D and have described the minimizing sequences (fields in optimal laminates) for this problem.

5. Phase transformations limit surfaces

The phase transformations limit surfaces are formed by the strains at which phase transformation can occur at first time on a given strain path. This means that the microstructure with an infinitesimal volume fraction of one of the phases has a minimal energy in comparison with other microstructures.

Recall that the energy of an elastic body undergoing phase transformations is determined by (6) as

$$\mathcal{J}_f(\boldsymbol{\varepsilon}_0) = \inf_{0 \leq m_+ \leq 1} \mathcal{F}_m$$

where the minimum of the free energy at given external strains and volume fractions of the phases is

$$\mathcal{F}_m = f_-^0 + m_+ \gamma + \mathcal{J}_{wm}(m_+, \boldsymbol{\varepsilon}_0). \quad (72)$$

and $\mathcal{J}_{wm}(m_+, \boldsymbol{\varepsilon}_0)$ is the optimal strain energy that is exact lower bound of the strain energy at given m_+ and $\boldsymbol{\varepsilon}_0$.

Considering phase transformation requires an additional minimization of (72) with respect to the volume fraction m_+ . Since the optimal strain energy coincides with the energy of one of the optimal laminates, it is convenient to minimize the energy using the lamination formulae. As a result the dependencies $m_+(\boldsymbol{\varepsilon}_0)$ and stress-strain diagrams can be constructed on the path of the phase transformation at $0 \leq m_+ \leq 1$ (see, e.g., example of such a strategy for the case of simple laminates in [38]).

Further we focus on the transformation limit surfaces construction for the direct and reverse phase transformations. After taking the interaction energy

$$E = m_+(\gamma_* + \frac{1}{2} \mathbf{e}_0 : \mathbf{M}_-^{(n)} : \mathbf{e}_0), \quad n = 1, 2, 3$$

of the optimal laminates (i.e. of the optimal rank n and normals) instead of $\mathcal{F}_m$, we obtain that the limit surfaces are formed by all strains $\boldsymbol{\varepsilon}_0$ at which one of the minimizing volume fractions tends to zero,

$$\left. \frac{\partial E(\boldsymbol{\varepsilon}_0, m_+)}{\partial m_+} \right|_{m_+=0} = 0, \quad (73)$$

or to unit,

$$\left. \frac{\partial E(\boldsymbol{\varepsilon}_0, m_+)}{\partial m_+} \right|_{m_+=1} = 0. \quad (74)$$

The initial undeformed state corresponds to the phase with a lower chemical energy f^0 . We will refer to this phase as to the parent phase. Note also that we accept that $\mu_- < \mu_+$. Therefore, if the shear module of the parent phase is greater than the shear module of a new phase, then parent and new phases are the phases “+” and “−”, respectively; $\gamma = f_+^0 - f_-^0 < 0$. The equation (74) determines the direct transformation limit surface (from “+” to “−”), and the equation (73) determines the reverse transformation limit surface (from “−” to “+”).

If the shear module of the parent phase is less than the shear module of a new phase, then parent and new phases are the phases “−” and “+”, respectively; $\gamma = f_+^0 - f_-^0 > 0$. The direct transformation surface for the transformation from “−” to “+” is determined by the equation (73), and the equation (74) determines the reverse transformation limit surface for the transformation from “+” to “−”.

It can be derived (see Appendix E) that for all optimal laminates

$$\frac{\partial E}{\partial m_+} = \gamma_* + \frac{1}{2}(\mathbf{q}_+ : \llbracket \mathbf{C} \rrbracket^{-1} : \mathbf{q}_+ + \mathcal{K}_{max}(\mathbf{q}_+)) = 0 \quad (75)$$

where the dependence of $\mathcal{K}_{max}$ on eigenvalues of $\mathbf{q}_+$ is given by one of the formulae (34), (37), (41), (45) or (47), depending on eigenvalues of $\mathbf{q}_+$.

The equation (75) is a restriction on $\mathbf{q}_+$ at all equilibrium volume fractions m_+ . This is the Maxwell relation for the equilibrium interface expressed in terms of strains on one side of the interface [52] that additionally corresponds to the external PTZ boundary, i.e. with the strain $\boldsymbol{\varepsilon}_+$ belonging to the PTZ boundary (see, e.g., [62, 40, 34] or [36] and references therein).

The substitution of $\mathbf{q}_+ = \mathbf{M}^{(n)} : \llbracket \mathbf{C} \rrbracket^{-1} : \mathbf{q}_0$ with the optimal rank, normals and $m_+ = 0$ or $m_+ = 1$ into (75) results in the equation of the limit surfaces in the space of eigenvalues q_{0i} of the tensor $\mathbf{q}_0 = \sum_{i=1}^3 q_{0i} \mathbf{e}_i \mathbf{e}_i$.

The choice of the rank and the normals depends on the external strains. The space of eigenvalues of the tensor $\mathbf{q}_0 = \sum_{i=1}^3 q_{0i} \mathbf{e}_i \mathbf{e}_i$ is divided into domains which correspond to domains Ψ_i^q ($i = 1, 2, \dots, 7$). Different optimal laminates and different relationships between the tensor $\mathbf{q}_+$ and external strains

ε_0 (different tensors $\mathbf{M}_-^{(n)}$) correspond to different domains Ψ_i^q . Thus, the transformation surfaces are combinations of parts which correspond to the nucleation of different optimal laminates.

If $m_+ \rightarrow 1$ then $m_- \rightarrow 0$ and, by (12) and (13), $\mathbf{q}_+ = \mathbf{q}_0$. The equation (75) becomes the equation of the limit surface of the nucleation of a phase “−”, the phase with the less shear module. The space is divided into domains corresponding Ψ_3^q , Ψ_5^q and Ψ_6^q since only first-rank laminates are optimal, $\mathcal{K}_{max}$ is determined by (33) or (37) (see also comment 2 in Subsection 4.7). The limit surface is formed by ellipsoids in strain space. Note that the limit surface in this case coincides with the external PTZ boundary.

Other optimal laminates may correspond to the nucleation of the phase “+” ($m_+ \rightarrow 0$), the phase with a greater shear module. For example, in the case of the optimal skew second-rank laminates $\mathbf{q}_+ = (q_k - q)\mathbf{k}\mathbf{k} + q\mathbf{E}$. The equation (75) takes the form

$$2\gamma_* + \frac{(q_k + 2q)^2}{9\llbracket k \rrbracket} + \frac{(q_k - q)^2}{3\llbracket \mu \rrbracket} + \mathcal{K}_{max} = 0 \quad (76)$$

where $\mathcal{K}_{max}$ is given by (41).

By (12), the relation between $\mathbf{q}_0$ and $\mathbf{q}_+$ is

$$\mathbf{q}_0 = \{\mathbf{I} + m_- \llbracket \mathbf{C} \rrbracket : (\beta \mathbf{K}_-(\mathbf{n}^{(1)}) + (1 - \beta) \mathbf{K}_-(\mathbf{n}^{(2)}))\} : \mathbf{q}_+$$

where $\beta = m_1^{(1)}/m_-$. For the optimal skew second-rank laminates $\mathbf{k}$ is one of the eigenvectors of $\mathbf{q}_0$. Let $\mathbf{k} = \mathbf{e}_1$. Then from (39) and (40) it follows at $m_+ = 0$ ($m_- = 1$) that

$$q_{01} = q_k + \frac{1}{2\mu_-} (\llbracket \lambda \rrbracket (q_k - q) + 2\llbracket \mu \rrbracket ((1 - \nu_-)q_k - \nu_- q)) \quad (77)$$

$$q_{02} = q + \frac{1}{2\mu_-} (\llbracket \lambda \rrbracket (q_k - q) + 2\beta \llbracket \mu \rrbracket ((1 - \nu_-)q - \nu_- q_k)) \quad (78)$$

$$q_{03} = q + \frac{1}{2\mu_-} (\llbracket \lambda \rrbracket (q_k - q) + 2(1 - \beta) \llbracket \mu \rrbracket ((1 - \nu_-)q - \nu_- q_k)). \quad (79)$$

From (78) and (79) it follows that

$$q_{02} + q_{03} = 2q + \frac{1}{2\mu_-} (2\llbracket \lambda \rrbracket (q_k - q) + 2\llbracket \mu \rrbracket ((1 - \nu_-)q - \nu_- q_k)). \quad (80)$$

Given q_{01} , q_{02} and q_{03} , equations (77) and (80) determine q and q_k in dependence on q_{01} and $q_{02} + q_{03}$. After substitution of these dependencies

into (76) we obtain the equation of a cylindrical surface in space of q_{01} , q_{02} and q_{03} . Thus, the skew second-rank laminate nucleation surface is a part of the cylindrical surface restricted by the domain Ψ_4^q . Boundaries of Ψ_4^q correspond to $\beta = 0$ and 1 and to the strains when $q_k = 0$.

Other optimal laminates can be considered analogously. The parts of the limit surface that correspond to the first rank laminates are parts of the ellipsoid

$$\gamma_* + \frac{1}{2}(\mathbf{q}_0 : \llbracket \mathbf{C} \rrbracket^{-1} : \mathbf{q}_0 - \mathcal{K}_{max}^+(\mathbf{q}_0)) = 0$$

where $\mathcal{K}_{max}^+(\mathbf{q}_0)$ is the maximum of $\mathbf{q}_0 : \mathbf{K}_+(\mathbf{n}) : \mathbf{q}_0$, where $\mathbf{K}_+$ is defined by the elasticity tensor $\mathbf{C}_+$ [34]. The limit surfaces for the direct second-rank laminates are cylinders. The limit surfaces for the third-rank laminates are the triangles, as for the ellipsoidal nuclei [52, 36, 39] (see Appendix E for details).

6. Results and discussion

Transformation surfaces are formed by second order surfaces (cylindrical and ellipsoids or hyperboloid, depending on the sign-definiteness of the jump $\llbracket \mathbf{C} \rrbracket$) and planes (for the third-rank laminates). Examples of the cross-sections of the direct and reverse transformation limit surfaces by the plane $\varepsilon_1 = \varepsilon_2$ are shown in the Figures 4–7. The cross-sections correspond to axisymmetric external strains. The material parameters are indicated in the captions. The curves “1” are the direct transformation surfaces, the curves “2” are the reverse transformation surfaces.

Also, envelope of the nucleation surfaces for equilibrium nuclei of different geometries (planar layers, elliptical cylinders, ellipsoids) with interfaces which satisfy the local thermodynamic equilibrium condition (the Maxwell relation) obtained earlier [52, 40, 38, 39, 7, 8] are shown.

Given transformation strain and the “temperature” γ , the position of the transformation surfaces with respect to the origin of coordinates (zero external strain) and the shape of the limit surfaces (closed or unclosed) depend on the relation between elastic moduli of the phases. This in turn affects the type of the microstructure that appear on the path of direct and reverse transformations.

The surfaces are closed if the jump of the elasticity tensor is sign-definite (Fig. 4, 5) and unclosed if the jump is not a sign-definite tensor (Fig. 6, 7).

Figure 4: Cross section of phase transition surfaces by surface $\varepsilon_1 = \varepsilon_2$. Material parameters are $f_0^- - f_0^+ = 0.5$, $k_+ = 39$, $k_- = 78$, $\mu_+ = 15$, $\mu_- = 30$, $\varepsilon_+^p = 0$, $\varepsilon_-^p = 0.1$

If the shear module of the parent phase is greater than the shear module of a new phase then the limit surfaces surround the coordinate origin (Fig. 4). The transformation takes place at both stretching and compression. When the direct transformation surface (curve “1” in Fig. 4) is reached on the straining path from the unstrained state, the layers of a new phase “-” nucleate inside the parent phase “+”. The orientation of the layer depends on the strain state, according to formulae (31)–(43). It may be a “direct” laminate with layers oriented perpendicular to the direction of maximal stretch like a normal crack, or inclined laminate like shear bands, and the angle depends on the strains.

The reverse transformation “-” $\rightarrow$ “+” occurs during unloading. The reverse transformation limit surface (the curve 2) corresponds to third-rank laminates equivalent to the ellipsoidal nuclei, simple direct laminates, direct second-rank laminates equivalent to cylinder nuclei and skew second-rank laminates. The skew second-rank laminates replace direct second-rank laminates (points E and E') or simple laminates (points B and B'). This means

Figure 5: Cross section of phase transition surfaces by surface $\varepsilon_1 = \varepsilon_2$. Material parameters are $f_0^+ - f_0^- = 0.5$, $k_+ = 78$, $k_- = 39$, $\mu_+ = 30$, $\mu_- = 15$, $\varepsilon_+^p = 0.1$, $\varepsilon_-^p = 0$

that the equilibrium cylinders or layers do not provide the minimum of energy in this part of strain space, even if they satisfy thermodynamic equilibrium conditions and their local instability was not found. We emphasize that that skew second-rank laminates make the transformation surface convex.

If the shear module of the parent phase is less then the shear module of a new phase then the limit surfaces are shifted with respect to the coordinates origin (Fig. 5). As opposite to the previous case, there are linear straining paths which start from the origin and do not cross the direct transformation limit surface; no direct phase transformation in such cases whatever the values of strains are. The free energy of one-phase state is always less than the energy of two-phase state at these paths. Third-rank laminates (equivalent to the ellipsoids), direct (equivalent to cylinders) and skew second-rank laminates and simple laminates (simple layers) correspond to the direct transformation limit surface in this case. Direct and inclined simple laminates correspond to the reverse transformation limit surface.

Note that strains inside the phase “+” are spherical in the third-rank

Figure 6: Cross section of phase transition surfaces by surface $\varepsilon_1 = \varepsilon_2$. Material parameters are $f_0^- - f_0^+ = 0.5$, $k_+ = 39$, $k_- = 78$, $\mu_+ = 30$, $\mu_- = 15$, $\varepsilon_+^p = 0$, $\varepsilon_-^p = 0.1$

laminates as well as inside equilibrium ellipsoid. Therefore the energy is not affected by increasing the shear module in the case of ellipsoids nucleation. This explains different geometry of microstructures on the paths of direct and reverse transformations at different relations of the shear moduli.

If the jump of the elasticity tensor is not sign-definite then the transformation surface are unclosed, opposite to the case of the sign-definite jump of the elasticity tensor (Fig. 6, 7). As it is in the case of the sign-definite jump of the elasticity tensor, one of the limit surfaces corresponds to simple laminates, another one to the laminates of the first, second and third ranks, and one can see that the skew second-rank laminates affect the transformation limit surfaces.

Figure 7: Cross section of phase transition surfaces by surface $\varepsilon_1 = \varepsilon_2$. Material parameters are $f_0^+ - f_0^- = 0.5$, $k_+ = 39$, $k_- = 78$, $\mu_+ = 30$, $\mu_- = 15$, $\varepsilon_+^p = 0.1$, $\varepsilon_-^p = 0$

7. Conclusions

In the present paper we constructed phase transformation limit surfaces in strain space basing on exact energy lower bounds for elastic two-phase composites and demonstrated that the optimal laminates construction may be an effective tool for transformation surfaces construction. These surfaces define external strains at which a two-phase microstructure minimizes the free energy at an infinitesimal volume fraction of one of the phases. The case of isotropic phases was considered. To construct the limit surfaces we solved two problems. At first, the sequential laminates with minimal energy were studied in detail. Then the lower bound was constructed basing on translation method. The coincidence of the energy of optimal laminates and the lower bound was demonstrated. We also noted that the minimizing strains in one of the phases must belong to the external PTZ-boundary that is in agreement with earlier observations [41, 37, 26, 46, 47].

The solution showed that there are new regimes of optimality of microstructures in comparison with the asymptotic cases considered in other papers, namely, so-called skew laminates are the minimizers in some part of strain space. The case of optimal skew laminates also complements more general solution for anisotropic materials considered in [15].

It was also shown that the transformation limit surfaces only partly coincide with the envelope of the nucleation surfaces constructed earlier by the semi-inverse method for planar, cylindrical and ellipsoidal nuclei. It was noted that such an envelope may be nonconvex and namely skew second-rank laminates, which do not correspond to any of above-mentioned nuclei, make the transformation surface convex in such a case.

We showed that the limit surfaces can be closed or unclosed, depending on the jump of the sign-definiteness of elasticity tensor. We also demonstrated that microstructures of various types correspond to the direct and reverse transformations, and the type of the microstructure depends on the relation between shear moduli of the phases.

Appendix A. Transmitting tensor $\mathbf{M}_-^{(n)}$

Below we derive the expression (13) for the transmitting tensor $\mathbf{M}^{(n)}$ and prove the Proposition 1 about its sign-definiteness.

A1. Derivation of the transmitting tensor $\mathbf{M}_-^{(n)}$

We start with considering *rank-1 laminates* which consist of simple layers 1 and 2. Let $m_1^{(1)} = m_-$ and $m_2^{(1)} = m_+$ are the volume fractions of the layers occupied by the materials “−” and “+”, $\mathbf{n}^{(1)}$ is the normal to the layers, $\boldsymbol{\varepsilon}_1^{(1)}$, $\boldsymbol{\varepsilon}_2^{(1)}$ and $\boldsymbol{\sigma}_1^{(1)}$, $\boldsymbol{\sigma}_2^{(1)}$ are the strains and stresses inside the layers 1 and 2. The following relationships are satisfied:

$$m_1^{(1)}\boldsymbol{\varepsilon}_1^{(1)} + m_2^{(1)}\boldsymbol{\varepsilon}_2^{(1)} = \boldsymbol{\varepsilon}_2^{(2)}, \quad m_1^{(1)}\boldsymbol{\sigma}_1^{(1)} + m_2^{(1)}\boldsymbol{\sigma}_2^{(1)} = \boldsymbol{\sigma}_2^{(2)}, \quad (\text{A.1})$$

$$\boldsymbol{\sigma}_1^{(1)} = \mathbf{C}_- : (\boldsymbol{\varepsilon}_1^{(1)} - \boldsymbol{\varepsilon}_-^p), \quad \boldsymbol{\sigma}_2^{(1)} = \mathbf{C}_2^{(1)} : (\boldsymbol{\varepsilon}_2^{(1)} - \boldsymbol{\varepsilon}_2^{p(1)}), \quad (\text{A.2})$$

$$\mathbf{C}_2^{(1)} = \mathbf{C}_+, \quad \boldsymbol{\varepsilon}_2^{p(1)} = \boldsymbol{\varepsilon}_+^p. \quad (\text{A.3})$$

Average strain $\boldsymbol{\varepsilon}_0 = \boldsymbol{\varepsilon}_2^{(2)}$ and stresses, $\boldsymbol{\sigma}_0 = \boldsymbol{\sigma}_2^{(2)}$ are related as

$$\boldsymbol{\sigma}_0 = \mathbf{C}_0 : (\boldsymbol{\varepsilon}_0 - \boldsymbol{\varepsilon}_0^p) \quad (\text{A.4})$$

where effective elasticity tensor $\mathbf{C}_0 = \mathbf{C}_2^{(2)}$ and effective transformation strain $\boldsymbol{\varepsilon}_0^p = \boldsymbol{\varepsilon}_2^{p(2)}$ are to be found. Note that in the case of higher rank laminates

$\boldsymbol{\varepsilon}_2^{(2)}$ and $\boldsymbol{\sigma}_2^{(2)}$ are unknown strains and stresses averaged within the rank-1 sublayer. That is why we keep super- and subscripts denoting the rank and number of a layer even in the case of the rank-1 laminate.

Following relationships for the rank-1 laminate were presented in [38]. We repeat the derivations to have the notation consistent with further considerations of higher ranks laminates. From (A.1) and (10) it follows that

$$\boldsymbol{\varepsilon}_2^{(2)} = \boldsymbol{\varepsilon}_2^{(1)} - m_1^{(1)}(\boldsymbol{\varepsilon}_2^{(1)} - \boldsymbol{\varepsilon}_1^{(1)}) = \boldsymbol{\varepsilon}_2^{(1)} + m_1^{(1)}\mathbf{K}_-(\mathbf{n}^{(1)}) : \mathbf{q}_2^{(1)} \quad (\text{A.5})$$

where

$$\mathbf{q}_2^{(1)} = \left(\mathbf{C}_2^{(1)} - \mathbf{C}_1^{(1)} \right) : \boldsymbol{\varepsilon}_2^{(1)} - \left(\mathbf{C}_2^{(1)} : \boldsymbol{\varepsilon}_2^{p(1)} - \mathbf{C}_1^{(1)} : \boldsymbol{\varepsilon}_1^{p(1)} \right)$$

Equation (A.5) can be rewritten as

$$\left(\left(\mathbf{C}_2^{(1)} - \mathbf{C}_1^{(1)} \right)^{-1} + m_1^{(1)}\mathbf{K}_-(\mathbf{n}^{(1)}) \right) : \mathbf{q}_2^{(1)} = \mathbf{e}_2^{(2)}$$

where

$$\mathbf{e}_2^{(2)} = \boldsymbol{\varepsilon}_2^{(2)} - \left(\mathbf{C}_2^{(1)} - \mathbf{C}_1^{(1)} \right)^{-1} : \left(\mathbf{C}_2^{(1)} : \boldsymbol{\varepsilon}_2^{p(1)} - \mathbf{C}_1^{(1)} : \boldsymbol{\varepsilon}_1^{p(1)} \right)$$

Then

$$\mathbf{q}_2^{(1)} = \mathbf{L}_-^{(1)}(\mathbf{n}^{(1)}, m_1^{(1)}) : \mathbf{e}_2^{(2)} \quad (\text{A.6})$$

where

$$\mathbf{L}_-^{(1)}(\mathbf{n}^{(1)}, m_1^{(1)}) = \left(\left(\mathbf{C}_2^{(1)} - \mathbf{C}_1^{(1)} \right)^{-1} + m_1^{(1)}\mathbf{K}_-(\mathbf{n}^{(1)}) \right)^{-1}.$$

By (A.3),

$$\begin{aligned} \mathbf{q}_2^{(1)} &= \llbracket \mathbf{C} \rrbracket : \boldsymbol{\varepsilon}_2^{(1)} - \llbracket \mathbf{C} : \boldsymbol{\varepsilon}^p \rrbracket = \mathbf{q}_+ \\ \mathbf{e}_2^{(2)} &= \boldsymbol{\varepsilon}_2^{(2)} - \llbracket \mathbf{C} \rrbracket^{-1} : \llbracket \mathbf{C} : \boldsymbol{\varepsilon}^p \rrbracket \\ \mathbf{L}_-^{(1)}(\mathbf{n}^{(1)}, m_1^{(1)}) &= \left(\llbracket \mathbf{C} \rrbracket^{-1} + m_1^{(1)}\mathbf{K}_-(\mathbf{n}^{(1)}) \right)^{-1}. \end{aligned} \quad (\text{A.7})$$

Since $\boldsymbol{\varepsilon}_2^{(2)} = \boldsymbol{\varepsilon}_0$, from (A.7) it follows that

$$\mathbf{e}_2^{(2)} = \boldsymbol{\varepsilon}_0 - \llbracket \mathbf{C} \rrbracket^{-1} : \llbracket \mathbf{C} : \boldsymbol{\varepsilon}^p \rrbracket \equiv \mathbf{e}_0$$

Finally (A.6) takes the form of the dependence of $\mathbf{q}_+$ on external strain and microstructure parameters $m_1^{(1)}$, $\mathbf{n}^{(1)}$:

$$\mathbf{q}_+ = \mathbf{L}_-^{(1)}(\mathbf{n}^{(1)}, m_1^{(1)}) : \mathbf{e}_0 \quad (\text{A.8})$$

To relate $\boldsymbol{\sigma}_2^{(2)}$ and $\boldsymbol{\varepsilon}_2^{(2)}$, we note that from (A.1) and (A.2) it follows that

$$\boldsymbol{\sigma}_2^{(2)} = \mathbf{C}_- : (\boldsymbol{\varepsilon}_2^{(2)} - \boldsymbol{\varepsilon}_-^p) + m_2^{(1)} \mathbf{q}_2^{(1)} \quad (\text{A.9})$$

After substituting (A.8) into (A.9) we derive that

$$\boldsymbol{\sigma}_2^{(2)} = \mathbf{C}_2^{(2)} : (\boldsymbol{\varepsilon}_2^{(2)} - \boldsymbol{\varepsilon}_2^{p(2)})$$

where the effective elasticity tensor and effective transformation strain of the rank-1 laminate

$$\mathbf{C}_2^{(2)} = \mathbf{C}_- + m_2^{(1)} \mathbf{L}_-^{(1)} \quad (\text{A.10})$$

$$(\boldsymbol{\varepsilon}_2^p)^{(2)} = \boldsymbol{\varepsilon}_-^p + m_2^{(1)} \left(\mathbf{C}_2^{(2)} \right)^{-1} : \mathbf{L}_-^{(1)} : [\mathbf{C}]^{-1} : \mathbf{C}_+ : [\boldsymbol{\varepsilon}^p] \quad (\text{A.11})$$

Further we will use the tensors (A.10) and (A.11) as the elasticity tensor and transformation tensor of a homogenized rank-1 sublayer of higher rank laminates.

Rank-2 laminates are characterized by the volume fraction $m_1^{(2)}$ of the simple layers of the phase “−” and the volume fraction $m_2^{(2)}$ of the mixed layers which themselves are rank-1 laminates characterized by the volume fractions $m_1^{(1)}$ and $m_2^{(1)}$ of the sublayers “−” and “+”; $\mathbf{n}^{(2)}$ and $\mathbf{n}^{(1)}$ are the normals to the macrolayers and to sublayers inside rank-1 layers, respectively.

The volume fractions satisfy the relationships:

$$m_1^{(2)} + m_2^{(2)} = 1, \quad m_1^{(1)} + m_2^{(1)} = 1, \quad m_2^{(1)} m_2^{(2)} = m_+.$$

Then

$$m_1^{(2)} + m_1^{(1)} m_2^{(2)} = m_1^{(1)} + m_1^{(2)} m_2^{(1)} = m_-.$$

Strains $\boldsymbol{\varepsilon}_1^{(2)}$, $\boldsymbol{\varepsilon}_1^{(1)}$, $\boldsymbol{\varepsilon}_2^{(2)}$, $\boldsymbol{\varepsilon}_2^{(1)}$ and stresses $\boldsymbol{\sigma}_1^{(2)}$, $\boldsymbol{\sigma}_1^{(1)}$, $\boldsymbol{\sigma}_2^{(2)}$, $\boldsymbol{\sigma}_2^{(1)}$ satisfy the relationships

$$\begin{aligned} m_1^{(1)} \boldsymbol{\varepsilon}_1^{(1)} + m_2^{(1)} \boldsymbol{\varepsilon}_2^{(1)} &= \boldsymbol{\varepsilon}_2^{(2)}, & m_1^{(2)} \boldsymbol{\varepsilon}_1^{(2)} + m_2^{(2)} \boldsymbol{\varepsilon}_2^{(2)} &= \boldsymbol{\varepsilon}_2^{(3)} = \boldsymbol{\varepsilon}_0, \\ m_1^{(1)} \boldsymbol{\sigma}_1^{(1)} + m_2^{(1)} \boldsymbol{\sigma}_2^{(1)} &= \boldsymbol{\sigma}_2^{(2)}, & m_1^{(2)} \boldsymbol{\sigma}_1^{(2)} + m_2^{(2)} \boldsymbol{\sigma}_2^{(2)} &= \boldsymbol{\sigma}_2^{(3)} = \boldsymbol{\sigma}_0, \\ \boldsymbol{\sigma}_1^{(1)} &= \mathbf{C}_- : (\boldsymbol{\varepsilon}_1^{(1)} - \boldsymbol{\varepsilon}_-^p), & \boldsymbol{\sigma}_2^{(1)} &= \mathbf{C}_2^{(1)} : (\boldsymbol{\varepsilon}_2^{(1)} - \boldsymbol{\varepsilon}_2^{p(1)}), \\ \boldsymbol{\sigma}_1^{(2)} &= \mathbf{C}_- : (\boldsymbol{\varepsilon}_1^{(2)} - \boldsymbol{\varepsilon}_-^p), & \boldsymbol{\sigma}_2^{(2)} &= \mathbf{C}_2^{(2)} : (\boldsymbol{\varepsilon}_2^{(2)} - \boldsymbol{\varepsilon}_2^{p(2)}), \end{aligned}$$

where $\mathbf{C}_2^{(1)} = \mathbf{C}_+$, $\boldsymbol{\varepsilon}_2^{p(1)} = \boldsymbol{\varepsilon}_+^p$, $\mathbf{C}_2^{(2)}$ and $\boldsymbol{\varepsilon}_2^{p(2)}$ are defined by (A.10) and (A.11).

The equation (A.6) expresses $\mathbf{q}_2^{(1)} = \mathbf{q}_+$ through $\mathbf{e}_2^{(2)}$ defined by (A.7). Now we have to express $\mathbf{e}_2^{(2)}$ through $\boldsymbol{\varepsilon}_0$. Considering rank-1 sublayer as a homogenized layer with the effective elasticity tensor $\mathbf{C}_2^{(2)}$ and effective transformation strain $\boldsymbol{\varepsilon}_2^{p(2)}$ defined by (A.10) and (A.11) we derive similar to (A.6) that

$$\mathbf{q}_2^{(2)} = \mathbf{L}_-^{(2)} \left(\mathbf{n}^{(2)}, m_1^{(2)} \right) : \mathbf{e}_2^{(3)}, \quad (\text{A.12})$$

where by the definition

$$\mathbf{q}_2^{(2)} = \left(\mathbf{C}_2^{(2)} - \mathbf{C}_- \right) : \boldsymbol{\varepsilon}_2^{(2)} - \left(\mathbf{C}_2^{(2)} : \boldsymbol{\varepsilon}_2^{p(2)} - \mathbf{C}_- : \boldsymbol{\varepsilon}_-^p \right), \quad (\text{A.13})$$

$$\mathbf{e}_2^{(3)} = \boldsymbol{\varepsilon}_0 - \left(\mathbf{C}_2^{(2)} - \mathbf{C}_- \right)^{-1} : \left(\mathbf{C}_2^{(2)} : \boldsymbol{\varepsilon}_2^{p(2)} - \mathbf{C}_- : \boldsymbol{\varepsilon}_-^p \right), \quad (\text{A.14})$$

$$\mathbf{L}_-^{(2)} = \left(\left(\mathbf{C}_2^{(2)} - \mathbf{C}_- \right)^{-1} + m_1^{(2)} \mathbf{K}_- (\mathbf{n}^{(2)}) \right)^{-1}. \quad (\text{A.15})$$

From (A.10) and (A.11) it follows that

$$\begin{aligned} \mathbf{C}_2^{(2)} - \mathbf{C}_- &= m_2^{(1)} \mathbf{L}_-^{(1)}, \\ \mathbf{C}_2^{(2)} : \boldsymbol{\varepsilon}_2^{p(2)} - \mathbf{C}_- : \boldsymbol{\varepsilon}_-^p &= \left(\mathbf{C}_2^{(2)} - \mathbf{C}_- \right) : \boldsymbol{\varepsilon}_-^p + \mathbf{C}_2^{(2)} : \left(\boldsymbol{\varepsilon}_2^{p(2)} - \boldsymbol{\varepsilon}_-^p \right) \\ &= m_2^{(1)} \mathbf{L}_-^{(1)} : \left(\boldsymbol{\varepsilon}_-^p + \llbracket \mathbf{C} \rrbracket^{-1} : \mathbf{C}_+ : \llbracket \boldsymbol{\varepsilon}^p \rrbracket \right) = m_2^{(1)} \mathbf{L}_-^{(1)} : \llbracket \mathbf{C} \rrbracket^{-1} : \llbracket \mathbf{C} : \boldsymbol{\varepsilon}^p \rrbracket, \\ \left(\mathbf{C}_2^{(2)} - \mathbf{C}_- \right)^{-1} : \left(\mathbf{C}_2^{(2)} : \boldsymbol{\varepsilon}_2^{p(2)} - \mathbf{C}_- : \boldsymbol{\varepsilon}_-^p \right) &= \llbracket \mathbf{C} \rrbracket^{-1} : \llbracket \mathbf{C} : \boldsymbol{\varepsilon}^p \rrbracket \end{aligned}$$

Then, by (A.13)–(A.15), with $\mathbf{e}_2^{(2)}$ defined by (A.7) and with the use of (A.6),

$$\begin{aligned} \mathbf{q}_2^{(2)} &= m_2^{(1)} \mathbf{L}_-^{(1)} : \mathbf{e}_2^{(2)} = m_2^{(1)} \mathbf{q}_2^{(1)} = m_2^{(1)} \mathbf{q}_+, \quad (\text{A.16}) \\ \mathbf{e}_2^{(3)} &= \boldsymbol{\varepsilon}_0 - \llbracket \mathbf{C} \rrbracket^{-1} : \llbracket \mathbf{C} : \boldsymbol{\varepsilon}^p \rrbracket = \mathbf{e}_0, \\ \mathbf{L}_-^{(2)} &= m_2^{(1)} \left(\llbracket \mathbf{C} \rrbracket^{-1} + m_1^{(1)} \mathbf{K}_- (\mathbf{n}^{(1)}) + m_1^{(2)} m_2^{(1)} \mathbf{K}_- (\mathbf{n}^{(2)}) \right)^{-1}. \end{aligned}$$

From (A.16) and (A.12) it follows that

$$\mathbf{q}_+ = \frac{1}{m_2^{(1)}} \mathbf{q}_2^{(2)} = \mathbf{M}_-^{(2)} : \mathbf{e}_0$$

where

$$\mathbf{M}_-^{(2)} = \frac{1}{m_2^{(1)}} \mathbf{L}_-^{(2)} = \left(\llbracket \mathbf{C} \rrbracket^{-1} + m_1^{(1)} \mathbf{K}_- (\mathbf{n}^{(1)}) + m_1^{(2)} m_2^{(1)} \mathbf{K}_- (\mathbf{n}^{(2)}) \right)^{-1}.$$

Average stress $\boldsymbol{\sigma}_0 = \boldsymbol{\sigma}_2^{(3)}$ and strain $\boldsymbol{\varepsilon}_0 = \boldsymbol{\varepsilon}_2^{(3)}$ are related by (A.4) with the effective elasticity tensor and effective transformation strain

$$\begin{aligned}\mathbf{C}_0 &= \mathbf{C}_2^{(3)} = \mathbf{C}_- + m_2^{(2)} \mathbf{L}_-^{(2)} = \mathbf{C}_- + m_+ \mathbf{M}_-^{(2)} \\ \boldsymbol{\varepsilon}_2^{p(3)} &= \boldsymbol{\varepsilon}_-^p + m_+ \left(\mathbf{C}_2^{(3)} \right)^{-1} : \mathbf{M}_-^{(2)} : \llbracket \mathbf{C} \rrbracket^{-1} : \mathbf{C}_+ : \llbracket \boldsymbol{\varepsilon}^p \rrbracket\end{aligned}$$

Considering rank-3 laminates, we derive that $\mathbf{q}_2^{(3)} = m_2^{(2)} \mathbf{q}_2^{(2)} = m_2^{(2)} m_2^{(1)} \mathbf{q}_+$ and finally, for rank-n laminates, come to the formula (16) and then to the formulae (12)–(15) and (18). Note that $\mathbf{M}_-^{(1)} = \mathbf{L}_-^{(1)}$ and (12) reduces to (A.8) at $n = 1$.

A2. The proof of the Proposition 1 (the sign of $\mathbf{M}^{(n)}$)

Obviously, if $\llbracket \mathbf{C} \rrbracket > 0$ then $\mathbf{M}^{(n)} > 0$. Let $\llbracket \mathbf{C} \rrbracket < 0$. From the identities [53]

$$\mathbf{K}_+ : \llbracket \mathbf{C} \rrbracket : \mathbf{K}_- = \mathbf{K}_- : \llbracket \mathbf{C} \rrbracket : \mathbf{K}_+ = -\llbracket \mathbf{K} \rrbracket$$

it follows that [64]

$$(\mathbf{I} + \mathbf{K}_- : \llbracket \mathbf{C} \rrbracket) : (\mathbf{I} - \mathbf{K}_+ : \llbracket \mathbf{C} \rrbracket) = \mathbf{I}.$$

This provides the existence of the inverse tensors $(\llbracket \mathbf{C} \rrbracket^{-1} + \mathbf{K}_-)^{-1}$ and $(\llbracket \mathbf{C} \rrbracket^{-1} - \mathbf{K}_+)^{-1}$. Particularly,

$$(\llbracket \mathbf{C} \rrbracket^{-1} + \mathbf{K}_-)^{-1} = \llbracket \mathbf{C} \rrbracket - \llbracket \mathbf{C} \rrbracket : \mathbf{K}_+ : \llbracket \mathbf{C} \rrbracket \leq \llbracket \mathbf{C} \rrbracket < 0$$

and, thus,

$$\llbracket \mathbf{C} \rrbracket^{-1} + \mathbf{K}_- < 0. \quad (\text{A.17})$$

Since $\beta^i < 1$ and $m_- < 1$, from (A.17) it follows that

$$\beta^i \llbracket \mathbf{C} \rrbracket^{-1} + m_- \beta^i \mathbf{K}_- (\mathbf{n}^{(i)}) < 0. \quad (\text{A.18})$$

Summation of the inequalities (A.18) from $i = 1$ till $i = n$ with taking into account (15) gives

$$\llbracket \mathbf{C} \rrbracket^{-1} + m_- \sum_{i=1}^n \beta^{(i)} \mathbf{K}_- (\mathbf{n}^{(i)}) < 0$$

where from it follows that $\mathbf{M}_-^{(n)}$ exists and $\mathbf{M}_-^{(n)} < 0$.

Appendix B. Energy equivalence of laminates with permuted normals. Rank reduction

B1. Derivation of the transmitting formula (49)

The difference $\boldsymbol{\varepsilon}_1^{(i)} - \boldsymbol{\varepsilon}_1^{(i-1)}$ can be written down as

$$\boldsymbol{\varepsilon}_1^{(i)} - \boldsymbol{\varepsilon}_1^{(i-1)} = (\boldsymbol{\varepsilon}_1^{(i)} - \boldsymbol{\varepsilon}_2^{(i)}) - (\boldsymbol{\varepsilon}_1^{(i-1)} - \boldsymbol{\varepsilon}_2^{(i-1)}) + (\boldsymbol{\varepsilon}_2^{(i)} - \boldsymbol{\varepsilon}_2^{(i-1)}) \quad (\text{B.1})$$

Since $\boldsymbol{\varepsilon}_2^{(i)} = m_1^{(i-1)}\boldsymbol{\varepsilon}_1^{(i-1)} + m_2^{(i-1)}\boldsymbol{\varepsilon}_2^{(i-1)}$ and $1 - m_2^{(i-1)} = m_1^{(i-1)}$, the last summand transforms to

$$\boldsymbol{\varepsilon}_2^{(i)} - \boldsymbol{\varepsilon}_2^{(i-1)} = m_1^{(i-1)}(\boldsymbol{\varepsilon}_1^{(i-1)} - \boldsymbol{\varepsilon}_2^{(i-1)})$$

and the representation (B.1) takes the form

$$\boldsymbol{\varepsilon}_1^{(i)} - \boldsymbol{\varepsilon}_1^{(i-1)} = (\boldsymbol{\varepsilon}_1^{(i)} - \boldsymbol{\varepsilon}_2^{(i)}) - m_2^{(i-1)}(\boldsymbol{\varepsilon}_1^{(i-1)} - \boldsymbol{\varepsilon}_2^{(i-1)}) \quad (\text{B.2})$$

Then the transmitting formula (49) follows from (B.2) if it is taken into account that

$$\begin{aligned} \boldsymbol{\varepsilon}_1^{(i)} - \boldsymbol{\varepsilon}_2^{(i)} &= \mathbf{K}_-(\mathbf{n}^{(i)}) : \mathbf{q}_2^{(i)}, \quad \boldsymbol{\varepsilon}_1^{(i-1)} - \boldsymbol{\varepsilon}_2^{(i-1)} = \mathbf{K}_-(\mathbf{n}^{(i-1)}) : \mathbf{q}_2^{(i-1)}, \\ \mathbf{q}_2^{(i)} &= \mathbf{q}_+ \prod_{j=1}^{i-1} m_2^{(j)}, \quad \mathbf{q}_2^{(i-1)} = \mathbf{q}_+ \prod_{j=1}^{i-2} m_2^{(j)} \end{aligned}$$

B2. The proof of the Proposition 2

Let $\mathbf{q}_+^A$ and $\mathbf{q}_+^B$ are the tensors $\mathbf{q}_+$ in the laminate A and B with permuted normals $\mathbf{n}^{(k)}$ and $\mathbf{n}^{(k+1)}$, respectively. Then, by (12) and (13),

$$\begin{aligned} &\left([\mathbf{C}]^{-1} + m_- \sum_{i=1, i \neq k, k+1}^n \beta^{(i)} \mathbf{K}_-(\mathbf{n}^{(i)}) \right. \\ &\quad \left. + m_- \left(\beta_A^{(k)} \mathbf{K}_-(\mathbf{n}_A^{(k)}) + \beta_A^{(k+1)} \mathbf{K}_-(\mathbf{n}_A^{(k+1)}) \right) \right) : \mathbf{q}_+^A = \mathbf{e}_0 \quad (\text{B.3}) \end{aligned}$$

$$\begin{aligned} &\left([\mathbf{C}]^{-1} + m_- \sum_{i=1, i \neq k, k+1}^n \beta^{(i)} \mathbf{K}_-(\mathbf{n}^{(i)}) \right. \\ &\quad \left. + m_- \left(\beta_B^{(k)} \mathbf{K}_-(\mathbf{n}_B^{(k)}) + \beta_B^{(k+1)} \mathbf{K}_-(\mathbf{n}_B^{(k+1)}) \right) \right) : \mathbf{q}_+^B = \mathbf{e}_0 \quad (\text{B.4}) \end{aligned}$$

If $k \geq 2$ then, by (14),

$$\beta_{A,B}^{(k)} = \frac{m_{1A,B}^{(k)}}{m_-} \prod_{j=1}^{j=k-1} m_2^{(j)}, \quad \beta_{A,B}^{(k+1)} = \frac{m_{1A,B}^{(k+1)} m_{2A,B}^{(k)}}{m_-} \prod_{j=1}^{j=k-1} m_2^{(j)}.$$

Then due to (50)

$$\beta_B^{(k)} = \beta_A^{(k+1)} \quad \text{and} \quad \beta_B^{(k+1)} = \beta_A^{(k)}.$$

and, thus,

$$\beta_A^{(k)} \mathbf{K}_-(\mathbf{n}_A^{(k)}) + \beta_A^{(k+1)} \mathbf{K}_-(\mathbf{n}_A^{(k+1)}) = \beta_B^{(k)} \mathbf{K}_-(\mathbf{n}_B^{(k)}) + \beta_A^{(k+1)} \mathbf{K}_-(\mathbf{n}_A^{(k+1)})$$

If $i < k$ then the coefficients $\beta^{(i)}$ do not depend on the volume fractions on the k -th and $k+1$ -th levels. If $i > k+1$ then the coefficients $\beta_{A,B}^{(i)}$ depend on the volume fractions on the k -th and $k+1$ -th levels through the products $m_{2A,B}^{(k)} m_{2A,B}^{(k+1)}$. From (50) it follows that

$$m_{2B}^{(k)} m_{2B}^{(k+1)} = m_{2B}^{(k)} (1 - m_{1B}^{(k+1)}) = m_{2B}^{(k)} - m_{1A}^{(k)} = 1 - m_{1A}^{(k+1)} m_{2A}^{(k)} - m_{1A}^{(k)} = m_{2A}^{(k)} m_{2A}^{(k+1)}. \quad (\text{B.5})$$

Thus, the product $m_2^{(k)} m_2^{(k+1)}$ does not change and

$$\beta_B^{(i)} = \beta_A^{(i)}, \quad i \neq k, k+1$$

From (B.5) it also follows that relationships (50) do not contradict the restriction $\prod_{i=1}^n m_{2B}^{(i)} = m_+$.

If $k = 1$ then $\beta_{A,B}^{(1)} = \frac{m_{1A,B}^{(1)}}{m_-}$ and $\beta_{A,B}^{(2)} = \frac{m_1^{(2)} m_{2A,B}^{(1)}}{m_-}$. By (50), $\beta_B^{(1)} = \beta_A^{(2)}$ and $\beta_B^{(2)} = \beta_A^{(1)}$. By (B.5), the product $m_2^{(1)} m_2^{(2)}$ does not change after the permutation of the normals. Thus, $\beta_B^{(i)} = \beta_A^{(i)}$, $i > 2$.

Finally from (B.3), (B.4) follows that $\mathbf{M}_{B-}^{(n)} = \mathbf{M}_{A-}^{(n)}$, $\mathbf{q}_+^B = \mathbf{q}_+^A \equiv \mathbf{q}_+$, and, by (19), $W_B^{(n)} = W_A^{(n)}$.

B3. The proof of the Proposition 3 (rank reduction)

At first we consider the case

$$\mathbf{K}_-(\mathbf{n}^{(1)}) : \mathbf{q}_+ = \mathbf{K}_-(\mathbf{n}^{(2)}) : \mathbf{q}_+ \quad (\text{B.6})$$

By the transmitting formula (49)

$$\boldsymbol{\varepsilon}_1^{(2)} - \boldsymbol{\varepsilon}_1^{(1)} = m_2^{(1)} (\mathbf{K}_-(\mathbf{n}^{(2)}) - \mathbf{K}_-(\mathbf{n}^{(1)})) : \mathbf{q}_+ = 0.$$

Then $\boldsymbol{\varepsilon}_1^{(1)} = \boldsymbol{\varepsilon}_1^{(2)} \equiv \boldsymbol{\varepsilon}_{1*}^{(1)}$. Therefore the strain energy will not change if one replace rank-2 sub-level of the rank- n laminate by the rank-1 laminate with the strains $\boldsymbol{\varepsilon}_{1*}^{(1)}$ and $\boldsymbol{\varepsilon}_{2*}^{(1)} = \boldsymbol{\varepsilon}_+$ and the volume fractions $m_{1*}^{(1)} = m_1^{(2)} + m_1^{(1)} m_2^{(2)}$ and $m_{2*}^{(1)} = m_2^{(1)} m_2^{(2)}$. This in turn means that the rank- n laminate can be replaced by the rank- $(n-1)$ laminate without changing the energy.

If $\mathbf{K}_-(\mathbf{n}^{(i)}) : \mathbf{q}_+ = \mathbf{K}_-(\mathbf{n}^{(j)}) : \mathbf{q}_+$ then permutating sequentially the normal $\mathbf{n}^{(i)}$ with the normals $\mathbf{n}^{(i-1)}$, $\mathbf{n}^{(i-2)}$, etc. and permutating the normal $\mathbf{n}^{(j)}$ with the normals $\mathbf{n}^{(j-1)}$, $\mathbf{n}^{(j-2)}$, etc. until the normals $\mathbf{n}^{(i)}$, $\mathbf{n}^{(j)}$ will appear at the first two levels, and changing the volume fractions by the rule (50) we will finally reduce (51) to the case (B.6).

B4. Optimal laminates of ranks higher than 3

We show that the optimal laminates with the rank higher than three are energy equivalent to the optimal laminates with the rank not more than 3. This means that in 3D-case maximum required rank is 3.

Indeed, even if $n = 3$, then only one case remains to be unreduced to lower rank laminates, namely the case 3(b) with spherical $\mathbf{q}_+$ in Appendix C. So, only spherical tensors may be considered as trial $\mathbf{q}_+$ if $n > 3$, and the condition $\mathbf{q}_+ : \mathbf{K}_-(\mathbf{n}_i); \mathbf{q}_+ = \text{const } i = 1, 2 \dots n$ is fulfilled in this case for any set of normals. But the energy of the laminate does not depend on the rank if the tensor $\mathbf{q}_+$ is spherical. Indeed, if $\mathbf{q}_+ = q\mathbf{E}$ then, by (12), (46) and (15)

$$\begin{aligned} \mathbf{e}_0 &= \left([\mathbf{C}]^{-1} : \mathbf{E} + m_- cq \sum_{i=1}^n \beta^{(i)} \mathbf{n}^{(i)} \otimes \mathbf{n}^{(i)} \right), \\ \text{tr } \mathbf{e}_0 &= \mathbf{E} : [\mathbf{C}]^{-1} : \mathbf{E} + m_- cq. \end{aligned}$$

Thus, if at given $\boldsymbol{\varepsilon}_0$ the tensor $\mathbf{q}_+$ is spherical then q does not depend on the rank. Then, by (11), the energy

$$E_q = \frac{1}{2} m_+ q \text{tr } \mathbf{e}_0$$

also does not depend on the rank.

Appendix C. The choice of laminates

If we restrict the consideration by the laminates of the first, second and third rank than the following cases can be considered depending on the relations between the eigenvalues of the tensor $\mathbf{q}_+$.

1. *Rank-1 laminates.* This case is denoted as the case *I* in Section 3. The normal is uniquely determined by the eigenvalues of $\mathbf{q}$ at all $\mathbf{q}_+$ from the condition of the maximum of the quadratic form $\mathcal{K}_-(\mathbf{n}, \mathbf{q}_+)$.

2. *Rank-2 laminates.* The conditions (27) and (28) are to be satisfied at two normals $\mathbf{n}^{(1)}$ and $\mathbf{n}^{(2)}$. From (34), (41), (43) and (47) one can see that the equality

$$\mathcal{K}_-(\mathbf{n}^{(1)}, \mathbf{q}_+) = \mathcal{K}_-(\mathbf{n}^{(2)}, \mathbf{q}_+) = \max_{\mathbf{n}: |\mathbf{n}|=1} \mathcal{K}_-(\mathbf{n} | \mathbf{q}_+), \quad \mathbf{n}^{(2)} \nparallel \mathbf{n}^{(1)}$$

is possible in four cases:

- (a) The eigenvalues of $\mathbf{q}_+$ are different, one of the inequalities (31) holds and both normals are determined by the equation (32), but differ by the sign of one of the component:

$$n_{max}^{(2)} = -n_{max}^{(1)}, \quad n_{min}^{(2)} = n_{min}^{(1)}, \quad n_{mid}^{(1,2)} = 0$$

or

$$n_{max}^{(2)} = n_{max}^{(1)}, \quad n_{min}^{(2)} = -n_{min}^{(1)}, \quad n_{mid}^{(1,2)} = 0$$

By (33), in both cases not only

$$\mathbf{q}_+ : \mathbf{K}_-(\mathbf{n}^{(1)}) : \mathbf{q}_+ = \mathbf{q}_+ : \mathbf{K}_-(\mathbf{n}^{(2)}) : \mathbf{q}_+ \quad (\text{C.1})$$

but also

$$\mathbf{K}_-(\mathbf{n}^{(1)}) : \mathbf{q}_+ = \mathbf{K}_-(\mathbf{n}^{(2)}) : \mathbf{q}_+$$

Thus, by the Proposition 3, the rank can be lowered without changing the strain energy, and the case 2(a) can be reduced to the the rank-1 laminate.

- (b) The tensor $\mathbf{q}_+$ is axisymmetric, $\mathbf{q}_+ = q(\mathbf{E} - \mathbf{k} \otimes \mathbf{k}) + q_k \mathbf{k} \otimes \mathbf{k}$, and the eigenvalues q and q_k satisfy (38). Two unit unequal normals have to satisfy the equality (C.1). Then any two different normals with equal projections onto the axe $\mathbf{k}$ determined by (39) can be taken as $\mathbf{n}^{(1)}$ and $\mathbf{n}^{(2)}$. One can take the normals such that the vectors $\mathbf{k}$, $\mathbf{n}^{(1)}$ and

$\mathbf{n}^{(2)}$ will be noncoplanar. Then the vectors $\mathbf{e}^{(1)} = \mathbf{k} \times \frac{\mathbf{k} \times \mathbf{n}^{(1)}}{|\mathbf{k} \times \mathbf{n}^{(1)}|}$ and $\mathbf{e}^{(2)} = \mathbf{k} \times \frac{\mathbf{k} \times \mathbf{n}^{(2)}}{|\mathbf{k} \times \mathbf{n}^{(2)}|}$ in formula (40) for $\mathbf{K}_-(\mathbf{n}^{(1),(2)}) : \mathbf{q}_+$ are different, and $\mathbf{K}_-(\mathbf{n}^{(1)}) : \mathbf{q}_+ \neq \mathbf{K}_-(\mathbf{n}^{(2)}) : \mathbf{q}_+$. The rank reduction condition (B.6) is not fulfilled.

- (c) The tensor $\mathbf{q}_+$ is axisymmetric, and the eigenvalues q and q_k do not satisfy (38). By (42), (43), only the case

$$|q_k| < |q|$$

allows two different normals $\mathbf{n}^{(1)}$ and $\mathbf{n}^{(2)}$, and both normals are perpendicular to the axe $\mathbf{k}$.

- (d) The tensor $\mathbf{q}_+$ is spherical, $\mathbf{q}_+ = q\mathbf{E}$. In the case of the rank-2 laminate this is just a particular case of the case 2(c) with $q_k = q$.

3. Rank-3 laminates

Three noncoplanar vectors of normals have to satisfy the equalities

$$\mathbf{q}_+ : \mathbf{K}_-(\mathbf{n}^{(1)}) : \mathbf{q}_+ = \mathbf{q}_+ : \mathbf{K}_-(\mathbf{n}^{(2)}) : \mathbf{q}_+ = \mathbf{q}_+ : \mathbf{K}_-(\mathbf{n}^{(3)}) : \mathbf{q}_+. \quad (\text{C.2})$$

and provide the maximum of the quadratic form $\mathbf{q}_+ : \mathbf{K}_-(\mathbf{n}) : \mathbf{q}_+$. This cannot be the case if the eigenvalues of $\mathbf{q}_+$ are different or if the tensor $\mathbf{q}_+$ is axisymmetric and eigenvalues q and q_k do not satisfy (38) (by (42) and (43) only one normal $\mathbf{n} = \mathbf{k}$ or three coplanar normals lying in the plane perpendicular to the axe of $\mathbf{q}_+$ are possible).

Two cases remain:

- (a) The tensor $\mathbf{q}_+$ is axisymmetric, the eigenvalues q and q_k satisfy (38). To satisfy the first equality in (C.2) we choose the normals $\mathbf{n}^{(1)}$ and $\mathbf{n}^{(2)}$ such that

$$\mathbf{n}^{(1)} = n_k^{(1)}\mathbf{k} + n_1^{(1)}\mathbf{e}_1, \quad \mathbf{n}^{(2)} = n_k^{(2)}\mathbf{k} + n_2^{(2)}\mathbf{e}_2, \quad (\text{C.3})$$

where $(n_k^{(1)})^2 = (n_k^{(2)})^2$ and $(n_1^{(1)})^2 = (n_2^{(2)})^2$ are determined by (39), and $\mathbf{e}_1, \mathbf{e}_2, \mathbf{k}$ is an arbitrary orthonormal basis related with the axe $\mathbf{k}$. (To avoid misunderstanding note that subscripts 1, 2 (and k) denote

here the component of a vector, not a number of a layer.) Then the second equality in (C.2) is fulfilled if

$$\mathbf{n}^{(3)} = n_k^{(3)} \mathbf{k} + n_1^{(3)} \mathbf{e}_1, \quad (\text{C.4})$$

where

$$n_k^{(3)} = n_k^{(1)}, \quad n_1^{(3)} = -n_1^{(1)} \quad \text{or} \quad n_k^{(3)} = -n_k^{(1)}, \quad n_1^{(3)} = n_1^{(1)},$$

or

$$\mathbf{n}^{(3)} = n_k^{(3)} \mathbf{k} + n_2^{(3)} \mathbf{e}_2, \quad (\text{C.5})$$

where

$$n_k^{(3)} = n_k^{(1)}, \quad n_2^{(3)} = -n_2^{(2)} \quad \text{or} \quad n_k^{(3)} = -n_k^{(1)}, \quad n_2^{(3)} = -n_2^{(2)}.$$

By (40),

$$\begin{aligned} \mathbf{K}_-(\mathbf{n}^{(1)}) : \mathbf{q}_+ &= \frac{q_k - q}{2\mu_-} (n_k^2 \mathbf{k} \otimes \mathbf{k} - (1 - n_k^2) \mathbf{e}_1 \otimes \mathbf{e}_1), \\ \mathbf{K}_-(\mathbf{n}^{(2)}) : \mathbf{q}_+ &= \frac{q_k - q}{2\mu_-} (n_k^2 \mathbf{k} \otimes \mathbf{k} - (1 - n_k^2) \mathbf{e}_2 \otimes \mathbf{e}_2) \end{aligned}$$

and

$$\mathbf{K}_-(\mathbf{n}^{(1)}) : \mathbf{q}_+ = \mathbf{K}_-(\mathbf{n}^{(3)}) : \mathbf{q}_+ \quad \text{or} \quad \mathbf{K}_-(\mathbf{n}^{(2)}) : \mathbf{q}_+ = \mathbf{K}_-(\mathbf{n}^{(3)}) : \mathbf{q}_+ \quad (\text{C.6})$$

in the cases (C.4) or (C.5), respectively. If to change $\mathbf{n}^{(1)}$ or $\mathbf{n}^{(2)}$ by $\mathbf{n}^{(3)}$ in relationships (C.3)–(C.6) then the equality

$$\mathbf{K}_-(\mathbf{n}^{(1)}) : \mathbf{q}_+ = \mathbf{K}_-(\mathbf{n}^{(2)}) : \mathbf{q}_+ \quad (\text{C.7})$$

also becomes possible. Due to the equalities (C.6), (C.7), the rank can be lowered, the rank-3 laminate becomes equivalent to the rank-2 laminate if the tensor $\mathbf{q}_+$ is axisymmetric. Thus, the case 3(a) is energy equivalent to the case 2(b).

- (b) The tensor $\mathbf{q}_+$ is spherical. Then any three noncoplanar unit vectors can be the normals.

Therefore, there are four cases 1, 2(b), 2(c), 3(b) which represent all energy nonequivalent options to satisfy the conditions (26) and (25) by the choice of the rank and directions of normals in dependence of the eigenvalues of the tensor $\mathbf{q}_+$. In Section 3 this cases are I=1, II(a)=2(b), II(b)=2(c), and III=3(b).

Appendix D. Representation of the translator in a form of the quadratic form (54)

We note that the translator (53) can be written in the form of the convolution

$$\varphi(\mathbf{t}, \boldsymbol{\varepsilon}) = -\mathbf{t} : \text{Cof } \boldsymbol{\varepsilon} \quad (\text{D.1})$$

where the cofactor of the strain tensor is defined as

$$\text{Cof } \boldsymbol{\varepsilon} = \begin{cases} (\det \boldsymbol{\varepsilon}) \boldsymbol{\varepsilon}^{-T}, & \text{if } \det \boldsymbol{\varepsilon} \neq 0; \\ \varepsilon_i \varepsilon_j \mathbf{e}_k \otimes \mathbf{e}_k \text{ (no sum)}, & \text{if } \varepsilon_k = 0, \varepsilon_i, \varepsilon_j \neq 0 \text{ (} i \neq j \neq k \text{)}; \\ 0, & \text{otherwise.} \end{cases}$$

where ε_i and $\mathbf{e}_i$ are eigenvalues and corresponding eigenvectors of $\boldsymbol{\varepsilon}$.

The convolution (D.1), in turn, can be presented as a quadratic form [6]

$$\mathbf{t} : \text{Cof } \boldsymbol{\varepsilon} = -\frac{1}{2} \boldsymbol{\varepsilon} : \mathbf{T} : \boldsymbol{\varepsilon} \quad (\text{D.2})$$

where the fourth-rank translator tensor $\mathbf{T}$ depends on $\mathbf{t}$ as

$$\mathbf{T} = (\mathbf{t} \otimes \mathbf{E} + \mathbf{E} \otimes \mathbf{t}) + (\text{tr } \mathbf{t})(\mathbf{I} - \mathbf{E} \otimes \mathbf{E}) - (\mathbf{I} \cdot \mathbf{t} + \mathbf{t} \cdot \mathbf{I}). \quad (\text{D.3})$$

The formulae (D.2), (D.3) can be easily derived if to take into account that if the inverse $\boldsymbol{\varepsilon}^{-1}$ exists then by the Cayley – Hamilton theorem

$$\text{Cof } \boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^2 - I_1(\boldsymbol{\varepsilon}) \boldsymbol{\varepsilon} + I_2(\boldsymbol{\varepsilon}) \mathbf{E},$$

where the strain invariants $I_1(\boldsymbol{\varepsilon}) = \text{tr } \boldsymbol{\varepsilon}$ and $I_2(\boldsymbol{\varepsilon}) = \frac{1}{2}(I_1^2(\boldsymbol{\varepsilon}) - I_1(\boldsymbol{\varepsilon}^2))$ can be written as

$$I_1(\boldsymbol{\varepsilon}) = \mathbf{E} : \boldsymbol{\varepsilon}, \quad I_2(\boldsymbol{\varepsilon}) = \frac{1}{2}(\boldsymbol{\varepsilon} : \mathbf{E} \otimes \mathbf{E} : \boldsymbol{\varepsilon} - \boldsymbol{\varepsilon} : \mathbf{I} : \boldsymbol{\varepsilon}).$$

and if to use the identities

$$\begin{aligned} \mathbf{t} : \boldsymbol{\varepsilon}^2 &\equiv \frac{1}{2} \boldsymbol{\varepsilon} : (\mathbf{I} \cdot \mathbf{t} + \mathbf{t} \cdot \mathbf{I}) : \boldsymbol{\varepsilon}, \\ (\text{tr } \boldsymbol{\varepsilon}) \boldsymbol{\varepsilon} : \mathbf{t} &= \boldsymbol{\varepsilon} : \mathbf{E} \otimes \mathbf{t} : \boldsymbol{\varepsilon} = \frac{1}{2} \boldsymbol{\varepsilon} : (\mathbf{E} \otimes \mathbf{t} + \mathbf{t} \otimes \mathbf{E}) : \boldsymbol{\varepsilon} \end{aligned}$$

(cf. also with [15])

Appendix E. Derivation for the phase transformation surfaces construction

E1. Derivation of the equation (75)

Since

$$E = m_+(\gamma_* + \frac{1}{2}\mathbf{e}_0 : \mathbf{M}_-^{(n)} : \mathbf{e}_0),$$

the derivative

$$\frac{\partial E}{\partial m_+} = \gamma_* + \frac{1}{2}\mathbf{e}_0 : \mathbf{M}_-^{(n)} : \mathbf{e}_0 + \frac{1}{2}m_+\mathbf{e}_0 : \frac{\partial \mathbf{M}_-^{(n)}}{\partial m_+} : \mathbf{e}_0$$

By (13),

$$\begin{aligned} \frac{\partial \mathbf{M}_-^{(n)}}{\partial m_+} &= -\mathbf{M}_-^{(n)} : \frac{\partial}{\partial m_+} \left(\llbracket \mathbf{C} \rrbracket^{-1} + (1 - m_+) \sum_{i=1}^n \beta^{(i)} \mathbf{K}_-(\mathbf{n}^{(i)}) \right) : \mathbf{M}_-^{(n)} \\ &= \mathbf{M}_-^{(n)} : \left(\sum_{i=1}^n \beta^{(i)} \mathbf{K}_-(\mathbf{n}^{(i)}) \right) : \mathbf{M}_-^{(n)} \end{aligned}$$

Then, taking into account the equality $\mathbf{M}_-^{(n)} : \mathbf{e}_0 = \mathbf{q}_+$ we get

$$\begin{aligned} \frac{\partial E}{\partial m_+} &= \gamma_* + \frac{1}{2}\mathbf{q}_+ : \left(\llbracket \mathbf{C} \rrbracket^{-1} + (1 - m_+) \sum_{i=1}^n \beta^{(i)} \mathbf{K}_-(\mathbf{n}^{(i)}) + m_+ \sum_{i=1}^n \beta^{(i)} \mathbf{K}_-(\mathbf{n}^{(i)}) \right) : \mathbf{q}_+ \\ &= \gamma_* + \frac{1}{2}\mathbf{q}_+ : \left(\llbracket \mathbf{C} \rrbracket^{-1} + \sum_{i=1}^n \beta^{(i)} \mathbf{K}_-(\mathbf{n}^{(i)}) \right) : \mathbf{q}_+. \end{aligned} \tag{E.1}$$

By the optimality condition with respect to the parameters $\beta^{(i)}$ and the normals $\mathbf{n}^{(i)}$, $\mathbf{q}_+ : \mathbf{K}_-(\mathbf{n}^{(i)}) : \mathbf{q}_+ = \mathcal{K}_{max}(\mathbf{q}_+)$ at all normals $\mathbf{n}^{(i)}$. Then (E.1) takes the form (75):

$$\frac{\partial E}{\partial m_+} = \gamma_* + \frac{1}{2}(\mathbf{q}_+ : \llbracket \mathbf{C} \rrbracket^{-1} : \mathbf{q}_+ + \mathcal{K}_{max}(\mathbf{q}_+)).$$

E2. Nucleation of the third-rank laminate

In the case of the third-rank laminates $\mathbf{q}_+ = q\mathbf{E}$. The equation (75) takes form

$$2\gamma_* + q^2 \left(\frac{1}{\llbracket k \rrbracket} + c \right) = 0,$$

where $c = 3/(3k_- + 4\mu_-)$.

Thus, the field in the phase “+” in third-rank laminates is a constant, defined by material parameters, and it is

$$q = \pm \sqrt{-2\gamma_* \frac{\llbracket k \rrbracket}{1 + c\llbracket k \rrbracket}} \quad (\text{E.2})$$

By (12), the relation between $\mathbf{q}_+$ and $\mathbf{q}_0$ is

$$\mathbf{q}_0 = q(\mathbf{E} + c\llbracket \mathbf{C} \rrbracket : \sum_{i=1}^3 \beta^{(i)} \mathbf{n}^{(i)} \mathbf{n}^{(i)}) = q((1 + c\llbracket \lambda \rrbracket)\mathbf{E} + 2c\llbracket \mu \rrbracket \sum_{i=1}^3 \beta^{(i)} \mathbf{n}^{(i)} \mathbf{n}^{(i)}).$$

at $m_- = 1$.

The normals of the optimal third-rank laminate are directed along the principal directions of $\mathbf{q}_0$. Thus,

$$\begin{aligned} q_{01} &= q(1 + c(\llbracket \lambda \rrbracket + 2\beta^{(1)}\llbracket \mu \rrbracket)), \\ q_{02} &= q(1 + c(\llbracket \lambda \rrbracket + 2\beta^{(2)}\llbracket \mu \rrbracket)), \\ q_{03} &= q(1 + c(\llbracket \lambda \rrbracket + 2\beta^{(3)}\llbracket \mu \rrbracket)). \end{aligned} \quad (\text{E.3})$$

Summing these equations and using $\beta^{(1)} + \beta^{(2)} + \beta^{(3)} = 1$ we get

$$\text{tr} \mathbf{q}_0 = 3q(1 + c\llbracket k \rrbracket).$$

and after substitution of (E.2) it becomes

$$\text{tr} \mathbf{q}_0 = \pm 3\sqrt{-2\gamma_* \llbracket k \rrbracket (1 + \llbracket k \rrbracket c)} \quad (\text{E.4})$$

The equation (E.4) describes a plane in the space of the eigenvalues of external strains. The transformation surface lays on the plane and it is restricted by the requirement $\beta^{(i)} \geq 0$. From (E.3) the structural parameters are

$$\beta^{(i)} = \frac{1}{2\llbracket \mu \rrbracket} \left(\frac{1}{c} \left(\frac{q_{0i}}{q} - 1 \right) - \llbracket \lambda \rrbracket \right).$$

With taking into account $\llbracket \mu \rrbracket > 0$ and $c > 0$ the restriction becomes

$$\frac{q_{0i}}{q} \geq 1 + c\llbracket \lambda \rrbracket.$$

E3. Nucleation of direct second-rank laminates

By (12), the relation between $\mathbf{q}_0$ and $\mathbf{q}_+$ is

$$\mathbf{q}_0 = \{\mathbf{I} + m_- \llbracket \mathbf{C} \rrbracket : (\beta \mathbf{K}_-(\mathbf{n}^{(1)}) + (1 - \beta) \mathbf{K}_-(\mathbf{n}^{(2)}))\} : \mathbf{q}_+$$

where $\beta = m_1^{(1)}/m_-$. For the optimal laminates $\mathbf{k}$ is one of the eigenvectors of $\mathbf{q}_0$. Let $\mathbf{k} = \mathbf{e}_1$. Then from (43) and (44) it follows at $m_- = 1$ that

$$q_{01} = q_k + c \llbracket \lambda \rrbracket q \quad (\text{E.5})$$

$$q_{02} = q + c(\llbracket \lambda \rrbracket q + 2\beta \llbracket \mu \rrbracket \beta q) \quad (\text{E.6})$$

$$q_{03} = q + c(\llbracket \lambda \rrbracket q + 2(1 - \beta) \llbracket \mu \rrbracket q) \quad (\text{E.7})$$

From (E.6) (E.7) it follows that

$$q_{02} + q_{03} = 2q(1 + c \llbracket \lambda + \mu \rrbracket) \quad (\text{E.8})$$

Given q_{01} , q_{02} and q_{03} , equations (E.5) and (E.8) determine q and q_k in dependence on q_{01} and $q_{02} + q_{03}$. After substitution of these dependencies into (76) we obtain the equation of a cylindrical surface in space q_{01} , q_{02} , q_{03} . The nucleation surface is a part of the cylindrical surface restricted by the boundaries of Ψ_2^q which correspond to $\beta = 0$ and 1 and $q_k = 0$ and q .

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Figure 1_0930

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