Universität Stuttgart
Mathematisches Institut A
Angewandte Analysis

1. Lehrstuhl
Pfaffenwaldring 57
D–70569 Stuttgart

http://www.mathematik.uni-stuttgart.de/mathA/lst1/

Estimates on the mixture function for multiphase problems in elasticity *

Alexander Mielke†

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1 Introduction

In the theory of shape memory alloys and other crystallographic problems it is the basic assumption, that each mesoscopic part of the crystal can choose to be in one of the n allowed phases. We distinguish these phases by their stored–energy densities

$$W(E, e_i) = \tfrac{1}{2}\langle\!\langle S_i[E-A_i], E-A_i\rangle\!\rangle + \alpha_i, \qquad i = 1, \ldots, n,$$

where $e_i \in \mathbb{R}^n$ is the ith unit vector and $E = \nabla_{\mathrm{sym}} u = \frac{1}{2}(\nabla u + \nabla u^T) \in \mathbb{R}^{d\times d}_{\mathrm{sym}}$ is the linearized strain tensor.

On a macroscopic level it is often desirable to describe the evolution of the phase portions $c \in P^n = \mathrm{conv}(P^n_{\mathrm{pure}})$ with $P^n_{\mathrm{pure}} = \{e_1, \ldots, e_n\}$ using a mixture theory, see [KMS99, KuM99, Lev98, MTL98, HaG99]. Here we do not consider the evolution problem of c for time-dependent processes, but only the mixture function $W(E, c)$ which is defined in (2.1). This function is derived mathematically solely from the functions $W(\cdot, e_i)$, $i = 1, \ldots, n$, without using any further physical modeling. Hence, $W(E, c)$ is given as the minimal energy in a representative volume element where the minimization is done over all possible mesoscopic arrangements of the phases with given volume fraction $c \in P^n$ and all mesoscopic deformations with macroscopic strain E, see [AvM89, SmW98].

If the elastic tensors are identical (i.e., $S_i = S$) the mixture function takes the form

$$W(E, c) = \sum_{i=1}^{n} c_i W(E, e_i) + w_{\mathrm{mix}}(c), \quad c = (c_1, \ldots, c_n)^T,$$

where $w_{\mathrm{mix}} : P^n \to (-\infty, 0]$ is convex and satisfies $w_{\mathrm{mix}}(e_i) = 0$. While $w_{\mathrm{mix}}(\theta e_i + (1-\theta)e_j)$ can be given explicitly for each $\theta \in [0, 1]$ and all $i \neq j$ (see [Koh91]), it is not known how to compute $w_{\mathrm{mix}}(c)$ in the general case. Here we provide upper and lower estimates for $w_{\mathrm{mix}}(c)$ in terms of the function $\psi : \mathbb{R}^n_* = \{\, \eta \in \mathbb{R}^n : \langle \eta, e_*\rangle = 0 \,\} \to \mathbb{R}$ given by

$$\psi(\eta) = \min\{\, \langle T^{-1}(\omega) S[A^\eta]\omega, S[A^\eta]\rangle : \omega \in \mathbb{S}^{d-1} \,\} \quad \text{with } A^\eta = \sum_{j=1}^{n} \eta_j A_j$$

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†Mathematisches Institut A, Universität Stuttgart, Germany

where $T(\omega)$ is the acoustic tensor. With $\mathbb{M}(c) = \mathrm{diag}(c) - c\otimes c$ and $m = (n^2-n)/2$ we obtain the lower bound

$$w^{\mathrm{low}}(c) = \min\{ \sum_{j=1}^{m} \psi(\eta^{(j)}) : \eta^{(j)} \in \mathbb{R}^n_*,\ \sum_{j=1}^{m} \eta^{(j)}\otimes\eta^{(j)} = \mathbb{M}(c) \}. \tag{1.1}$$

An upper bound is every function $w^{\mathrm{upp}} : P^n \to \mathbb{R}$ satisfying $w^{\mathrm{upp}}(e_i) \geq 0$ and

$$w^{\mathrm{upp}}(\theta c^{(1)} + (1-\theta)c^{(2)}) \geq \theta w^{\mathrm{upp}}(c^{(1)}) + (1-\theta)w^{\mathrm{upp}}(c^{(2)}) + \theta(1-\theta)\psi(c^{(1)}-c^{(2)}).$$

The theory uses $\mathbb{H}$–measures for minimizing sequences of optimal arrangements of the phase mixture. We follow the lines in [Koh91, SmW98]. The lower estimate is obtained by relaxing the set of $\mathbb{H}$–measures whereas the upper estimate relies on the mixing formula for laminated $\mathbb{H}$–measures.

In particular, we show that the function $w_{\mathrm{mix}} : P^n \to \mathbb{R}$ takes the form

$$w_{\mathrm{mix}}(c) = \langle\!\langle B, \mathbb{M}(c)\rangle\!\rangle \quad \text{with } B \in \mathbb{R}^{n\times n}_{\mathrm{sym}},$$

if the transformation strains satisfy $A_j = A_0 + a_j A$.

2 Definition of the mixture function

We have given the n stored–energy densities $W(F, e_j)$, $j = 1, \ldots, n$, which are assumed to be quasiconvex. The **mixture function** for given volume fraction $c \in P$ is defined via

$$\begin{aligned} W(F,c) = \inf\Big\{ \textstyle\int_{Q^d} W(F+\nabla\varphi(y), \chi(y))\,\mathrm{d}y : \varphi \in W^{1,p}_{\mathrm{per}}(Q^d),& \\ \chi(y) \in P^n_{\mathrm{pure}}, \textstyle\int_{Q^d} \chi(y)\,\mathrm{d}y = c \Big\},& \end{aligned} \tag{2.1}$$

where $Q^d = (0,1)^d \subset \mathbb{R}^d$. It can be shown (cf. [Mie00]) that for each $c \in P^n$ the function $F \mapsto W(F,c)$ is quasiconvex and for each F the function $c \mapsto W(F,c)$ is convex.

Here we are interested in the special case of linearized elasticity where additionally each phase has the same elastic tensor S:

$$W(F, e_j) = \tfrac{1}{2}\langle\!\langle S[E-A_j], E-A_j\rangle\!\rangle + \alpha_j. \tag{2.2}$$

Here $E = \frac{1}{2}(F+F^T) - I$ is the linearized strain, A_j is the transformation strain, and α_j is the height of the well (which usually depends on the temperature T assumed to be constant here).

Proposition 2.1 *If all $W(F, e_j)$, $j = 1, \ldots, n$, have the form (2.2) then the mixture function takes the form $W(F,c) = \sum_{j=1}^n c_j W(F, e_j) + w_{\mathrm{mix}}(c)$, where the mixture term $w_{\mathrm{mix}} : P^n \to \mathbb{R}$ is convex and given by*

$$\begin{aligned} w_{\mathrm{mix}}(c) = \inf\Big\{ \textstyle\int_{Q^d} \langle\!\langle S[\nabla_{\mathrm{sym}}\varphi], \tfrac{1}{2}\nabla_{\mathrm{sym}}\varphi - \sum_{j=1}^n \chi_j(y)A_j\rangle\!\rangle\,\mathrm{d}y :& \\ \textstyle\int_{Q^d} \chi(y)\,\mathrm{d}y = c, \chi(y) \in P^n_{\mathrm{pure}}, \varphi \in W^{1,2}_{\mathrm{per}}(Q^d) \Big\}.& \end{aligned} \tag{2.3}$$

This form follows immediately using the quadratic structure of $W(F,e_j)$, $\int \nabla_{\rm sym}\varphi\,{\rm d}y = 0$, $\int \chi(y)\,{\rm d}y = c$ and $\sum \chi_j(y) \equiv 1$.

Since φ appears quadratically in $w_{\rm min}(c)$ we may eliminate it by first minimizing with respect to φ and keeping χ fixed. This is done most easily using Fourier series

$$\varphi(y) = \sum_{\xi\in\Gamma_*} \varphi_\xi {\rm e}^{{\rm i}\langle\xi,y\rangle}, \quad \chi(y) = \sum_{\xi\in\Gamma} \chi_\xi {\rm e}^{{\rm i}\langle\xi,y\rangle}, \quad \chi_0 = c,$$

where $\Gamma = (2\pi\mathbb{Z})^d$ and $\Gamma_* = \Gamma\setminus\{0\}$. Inserting this form into $w_{\rm mix}(c)$ we find a decoupling between different ξ's and thus $\varphi_\xi = \overline{\varphi}_{-\xi} \in \mathbb{C}^d$ can be found by minimizing

$$\tfrac12 \langle\!\langle S[{\rm i}\xi\otimes_{\rm sym}\varphi_\xi], {\rm i}\xi\otimes_{\rm sym}\varphi_\xi\rangle\!\rangle - {\rm Re}\langle\!\langle S[{\rm i}\xi\otimes_{\rm sym}\phi_\xi], \sum_j (\chi_\xi)_j A_j\rangle\!\rangle. \tag{2.4}$$

After some elementary calculations we arrive at

$$w_{\rm min}(c) = \inf\{\, I(\chi) : \int_{Q^d} \chi(y)\,{\rm d}y = c, \chi(y) \in P^n_{\rm pure}\}$$

with $I(\chi) = -\frac12 \sum_{\xi\in\Gamma_*} \langle T(\xi)^{-1} S[\sum_{j=1}^n (\chi_\xi)_j A_j]\xi, S[\sum_{j=1}^n (\chi_\xi)_j A_j]\xi\rangle$. Here the acoustic tensor $T(\xi)$ is defined via $\langle T(\xi)u,u\rangle = \langle\!\langle S[\xi\otimes_{\rm sym}u], \xi\otimes_{\rm sym}u\rangle\!\rangle$ and thus is homogeneous of degree 2 in $\xi\in\mathbb{R}^d$. Introducing $\widehat{G}, G(\xi) \in \mathbb{R}^{n\times n}_{\rm sym}$ via

$$G(\xi)_{jk} = \tfrac12 \langle T(\xi)^{-1} S[A_j]\xi, S[A_k]\xi\rangle, \quad \widehat{G}_{jk} = \tfrac12 \langle\!\langle S[A_j], A_k\rangle\!\rangle$$

we obtain the final formula

$$I(\chi) = -\sum_{\xi\in\Gamma_*} \langle\!\langle G(\xi), \overline{\chi}_\xi\otimes\chi_\xi\rangle\!\rangle \text{ where } \chi(y) = \sum_{\xi\in\Gamma} \chi_\xi {\rm e}^{{\rm i}\langle\xi,y\rangle}.$$

The term in (2.4) is bounded from below by $-\frac12 \langle\!\langle S[\sum_{j=1}^n (\chi_\xi)_j A_j], \sum_{k=1}^n (\overline{\chi}_\xi)_k A_k\rangle\!\rangle$ (minimize over $E = \overline{E}^T \in \mathbb{C}^{d\times d}$ instead of ${\rm i}\xi\otimes_{\rm sym}\varphi_\xi$). Adding up these terms we arrive at the lower estimate $I(\chi) \geq -\langle\!\langle \widehat{G}, \sum_{\xi\in\Gamma_*} \chi_\xi\otimes\overline{\chi}_\xi\rangle\!\rangle = -\langle\!\langle \widehat{G}, \mathbb{M}(c)\rangle\!\rangle$, (use that $\chi(y)\in P^n_{\rm pure}$ gives $\int_{Q^d} \chi(y)\otimes\chi(y)\,{\rm d}y = \sum_{\xi\in\Gamma} \chi_\xi\otimes\chi_{-\xi} = {\rm diag}(c)$). Thus, we found the rather simple bounds

$$0 \geq w_{\rm mix}(c) \geq -\langle\!\langle \widehat{G}, \mathbb{M}(c)\rangle\!\rangle. \tag{2.5}$$

Another form of the mixture function is sometimes used in engineering [KMS99, KuM99, Lev98], which uses the averaged transformation strain $A^c = \sum_{j=1}^n c_j A_j$:

$$W(E,c) = \tfrac12 \langle\!\langle S[E-A^c], E-A^c\rangle\!\rangle + \sum_{j=1}^n c_j\alpha_j + \widehat{w}_{\rm mix}(c).$$

A simple calculation shows that $\widehat{w}_{\rm mix}$ is related to $w_{\rm mix}$ by $w_{\rm mix}(c) = \widehat{w}_{\rm mix}(c) - \langle\!\langle \widehat{G}, \mathbb{M}(c)\rangle\!\rangle$ and satisfies the simple bounds $0 \leq \widehat{w}_{\rm mix}(c) \leq \langle\!\langle \widehat{G}, \mathbb{M}(c)\rangle\!\rangle$.

3 The $\mathbb{H}$–measure associated with χ

The function $\chi : Q^d \to P^n_{\rm pure}$ defines a microstructure of pure phases having the volume average $c = \int_{Q^d} \chi(y)\,{\rm d}y$. We associate to each function χ a matrix–valued measure $\mu = \widetilde{\mu}(\chi)$ on the unit sphere $\mathbb{S}^{d-1}$. The values of μ will lie in the set $\mathbb{H}^n_{\geq 0}$ of positive semidefinite Hermitian matrices. For any Borel measurable $\Sigma \subset \mathbb{S}^{d-1}$ we let $\mu(\Sigma) =$

$\sum_{\xi\in\Gamma_*,\xi/|\xi|\in\Sigma}\chi_\xi\otimes\overline{\chi}_\xi \in \mathbb{H}^n_{\geq 0}$. Thus, μ measures the correlation between the oscillations in direction $\omega\in\mathbb{S}^{d-1}$ of the different components. The measure is a homogeneous $\mathbb{H}$–measure in the sense of [Tar90], when the generating sequence $u^{(n)}(x)=\chi(nx)-c$ is considered.

Introducing the linear functional

$$J:\mathrm{meas}(\mathbb{S}^{d-1},\mathbb{H}^n_{\geq 0})\to\mathbb{R};\ \mu\mapsto J(\mu)=-\int_{\omega\in\mathbb{S}^{d-1}}\langle\!\langle G(\omega),\mu(\mathrm{d}\omega)\rangle\!\rangle \tag{3.1}$$

we obtain the relation $I(\chi)=J(\widehat{\mu}(\chi))$. Moreover, the symmetry $G(-\omega)=G(\omega)$ tells us that J depends only on the real part of μ. We consider the map

$$\widehat{\mu}:\mathrm{L}^\infty(Q^d,P^n_{\mathrm{pure}})\to\mathrm{meas}(\mathbb{S}^{d-1},\mathbb{P}^n);\ \chi\mapsto\widehat{\mu}(\chi)=\mathrm{Re}\widetilde{\mu}(\chi),$$

where $\mathbb{P}^n=\{\,B\in\mathbb{R}^{n\times n}:B=B^T,\ B \text{ positive semidefinite}\,\}$. Then each $\mu=\widehat{\mu}(\chi)$ satisfies (with $e_*=(1,\dots,1)^T$)

$$\begin{array}{ll}\text{(i)} & \mu(\Sigma)e_*=0 \text{ for all } \Sigma\subset\mathbb{S}^{d-1}\\ \text{(ii)} & \mu(\mathbb{S}^{d-1})=\mathbb{M}(c) \text{ where } c=\int\chi(y)\,\mathrm{d}y\\ \text{(iii)} & \mu(-\Sigma)=\mu(\Sigma)\in\mathbb{P}^n \text{ for all } \Sigma\subset\mathbb{S}^{d-1}.\end{array} \tag{3.2}$$

For each $c\in P^n$ we define the subsets of matrix–valued measures

$$\mathcal{H}(c)=\mathrm{closure}\{\,\widehat{\mu}(\chi):\int_{Q^d}\chi(y)\,\mathrm{d}y=c\,\},$$
$$\widehat{\mathcal{H}}(c)=\{\,\mu\in\mathrm{meas}(\mathbb{S}^{d-1},\mathbb{P}^n):(3.2)\text{ holds}\,\}.$$

Clearly, $\mathcal{H}(c)\subset\widehat{\mathcal{H}}(c)$ and $\widehat{\mathcal{H}}(c)$ is convex. The function w_{mix} can now be expressed as

$$w_{\mathrm{mix}}(c)=\inf\{\,J(\mu):\mu\in\mathcal{H}(c)\,\}. \tag{3.3}$$

Constructing $\mathcal{H}^{\mathrm{inn}}(c)$ and $\mathcal{H}^{\mathrm{out}}$ with $\mathcal{H}^{\mathrm{inn}}(c)\subset\mathcal{H}(c)\subset\mathcal{H}^{\mathrm{out}}(c)$ we obtain upper and lower bounds for w_{mix} if $\mathcal{H}(c)$ in the infimum is replaced by $\mathcal{H}^{\mathrm{inn}}(c)$ and $\mathcal{H}^{\mathrm{out}}$, respectively.

The difficulty in calculating $w_{\mathrm{mix}}(c)$ is reminiscent to calculating $\mathcal{H}(c)$. Until now there are only very few methods to generate suitably large subclasses of $\mathcal{H}(c)$. In section 4 we will use $\mathcal{H}^{\mathrm{out}}=\widehat{\mathcal{H}}(c)$ to obtain a lower bound. In section 5 the lamination mixture formula for $\mathbb{H}$–measures (see theorem 5.1) is employed to find upper bounds.

4 A lower estimate

To improve the trivial lower bound in (2.5) we let

$$w^{\mathrm{low}}(c)=\inf\{\,\int_{\mathbb{S}^{d-1}}\langle\!\langle G(w),\mu(\mathrm{d}w)\rangle\!\rangle:\mu\in\widehat{\mathcal{H}}(c)\,\}$$

which provides a lower bound for $w_{\mathrm{mix}}(c)$. Since $\widehat{H}(c)$ is characterized solely by algebraic conditions it is easier to calculate $w^{\mathrm{low}}(c)$ than $w_{\mathrm{mix}}(c)$. In particular, following [SmW98] we will show that the calculation of $w^{\mathrm{low}}(c)$ can be reduced to a finite dimensional minimization problem. (It is an open problem to find more algebraic restriction on $\mu\in\mathcal{H}(c)$ in order to make $\widehat{\mathcal{H}}(c)$ smaller and to increase $w^{\mathrm{low}}(c)$.)

Since the mapping $J : \mathrm{meas}(\mathbb{S}^{d-1}, \mathbb{H}^n_{\geq 0}) \to \mathbb{R}$ given in (3.1) is linear and since $\widehat{\mathcal{H}}(c)$ is convex, closed and bounded, we can apply the Krein–Milman theorem which states that J attains its minimum on the extremal points of $\widehat{\mathcal{H}}(c)$:

$$\mathrm{ex}(\widehat{\mathcal{H}}(c)) = \{\, \mu \in \widehat{\mathcal{H}}(c) : \widehat{\mathcal{H}} \setminus \{\mu\} \text{ is convex} \,\}.$$

Recalling $m = (n^2-n)/2$ and using the Dirac measure $\delta_\omega \in \mathrm{meas}(\mathbb{S}^{d-1}, \mathbb{R})$ this set can be characterized as follows.

Proposition 4.1 *We have $\mu \in \mathrm{ex}(\widehat{\mathcal{H}}(c))$ if and only if there exist $\omega_1, \ldots, \omega_m \in \mathbb{S}^{d-1}$ and $\eta_1, \ldots, \eta_m \in \mathbb{R}^n_*$ such that $\mu = \sum_{j=1}^m \widehat{\delta}_{\xi_j} \eta_j \otimes \eta_j$, where $\widehat{\delta}_\xi = \frac{1}{2}(\delta_\xi + \delta_{-\xi})$.*

Proof. Assume that $\mathbb{S}^{d-1}$ contains $m+1$ pairwise disjoint symmetric Σ_j (i.e. $\Sigma_j = -\Sigma_j$), such that $\mu(\Sigma_j) \neq 0$. Since all $\mu(\Sigma_j)$ lie in the m–dimensional linear space $\{M \in \mathbb{R}^{n\times n}_{\mathrm{sym}} : Me_* = 0\}$ the equation $\sum_{j=1}^{m+1} \alpha_j \mu(\Sigma_j) = 0$ has a nontrivial solution $(\alpha_1, \ldots, \alpha_{m+1}) \in \mathbb{R}^{m+1} \setminus \{0\}$. We may assume $|\alpha_j| \leq 1$ and define the two measures $\mu^\pm \in \widehat{\mathcal{H}}(c)$ via $\mu^\pm(\Sigma) = (1 \pm \alpha_j)\mu(\Sigma)$ if $\Sigma \subset \Sigma_j$ and $\mu^\pm(\Sigma) = \mu(\Sigma)$ if $\Sigma \cap \bigcup_{j=1}^m \Sigma_j = \emptyset$. Clearly, $\mu^+ \neq \mu^-$ and $\mu = \frac{1}{2}(\mu^+ + \mu^-)$. Thus, μ cannot be extremal. We conclude that extremal measures take the form $\mu = \sum_{j=1}^m \widehat{\delta}_{\omega_j} M_j$ with $M_j \in \mathbb{P}^n_* = \{M \in \mathbb{P}^n : Me_* = 0\,\}$.

Now assume $\sum_{j=1}^m \mathrm{rank}\, M_j > m$, then as above $\sum_{j=1}^m \alpha_j M_j = 0$ has a nontrivial solution with $|\alpha_j| \leq 1$. The measures $\mu^\pm = \sum_{j=1}^m (1+\alpha_j)\widehat{\delta}_{\xi_j} M_j$ are different, lie in $\widehat{\mathcal{H}}(c)$ and satisfy $\mu = \frac{1}{2}(\mu^+ + \mu^-)$. Thus, μ was no extremal measure. We conclude $\sum_{j=1}^m \mathrm{rank}\, M_j \leq m$ and together with $M_j = \sum_{i=1}^{m_j} a_{j,i} \otimes a_{j,i}$ where $m_j = \mathrm{rank}\, M_j$ the result follows. ∎

To formulate the main result of this section we define $\psi : \mathbb{R}^n \to \mathbb{R}$ via

$$\psi(\eta) = \inf\{\, -\langle\!\langle G(\omega), \eta \otimes \eta \rangle\!\rangle : \omega \in \mathbb{S}^{d-1} \,\}.$$

Moreover, let $\mathbb{E}^n_* = \{\eta \otimes \eta \in \mathbb{P}^n_* : \eta \in \mathbb{S}^{n-1}, \langle \eta, e_* \rangle = 0\}$ and $\mathbb{K}^n_* = \{M \in \mathbb{P}^n_* : \mathrm{tr}\, M = 1\}$. Then $\mathbb{K}^n_* = \mathrm{conv}(\mathbb{E}^n_*)$ and $\mathbb{E}^n_* = \mathrm{ex}(\mathbb{K}^n_*)$. The set $\mathbb{E}^n_*$ is a smooth manifold of dimension $(n-2)$. The set $\mathbb{K}^n_*$ lies in an affine subspace of $\mathbb{R}^{n\times n}$ of dimension $(n^2-n)/2 - 1$ and has nonempty interior with respect to this subspace.

Finally we define $\Psi : \mathbb{K}^n_* \to \mathbb{R}$ to be the largest convex function which satisfies $\Psi(\eta \otimes \eta) = \psi(\eta)$ for $\eta \otimes \eta \in \mathbb{E}^n_*$, namely

$$\Psi(M) = \min\Big\{ \sum_{j=1}^m \alpha_j \psi(\eta_j) : \alpha_j \geq 0, \sum_{j=1}^m \alpha_j = 1, \eta_j \otimes \eta_j \in \mathbb{E}^n_*, \sum_{j=1}^m \alpha_j \eta_j \otimes \eta_j = M \Big\}. \tag{4.1}$$

Here again $m = (n^2-n)/2$ by the standard theory of finite–dimensional convexity and the fact that $\mathbb{K}^n_*$ lies in a $(m-1)$–dimensional affine subspace of $\mathbb{R}^{n\times n}$.

In fact, we may extend ψ to $\psi : \mathbb{R}^n_* \to \mathbb{R}$ naturally such that $\psi(\alpha\eta) = \alpha^2 \psi(\eta)$, and similarly we may extend Ψ into $\Psi : \mathbb{P}^n_* \to \mathbb{R}$ such that $\Psi(\alpha M) = \alpha \Psi(M)$ for $\alpha \geq 0$.

Theorem 4.2 *We have the formula $w^{\mathrm{low}}(c) = \Psi(\mathbb{M}(c))$.*

The proof follows by combining the Krein–Milman theorem and the definition of Ψ.

It should be noted that we do not need the function Ψ on the whole set $\mathbb{K}^n_*$. Since

$$\mathbb{M}(c) = \mathrm{diag}(c) - c \otimes c = \tfrac{1}{2} \textstyle\sum_{i,j=1}^n c_i c_j (e_i - e_j) \otimes (e_i - e_j), \tag{4.2}$$

we have $[\,\mathrm{tr}\, \mathbb{M}(c)]^{-1} \mathbb{M}(c) \in \mathrm{conv}\{\, \frac{1}{2}(e_i - e_j) \otimes (e_i - e_j) \in \mathbb{E}^n_* : i \neq j \,\} \subset \mathbb{K}^n_*$.

In the case $n = 3$ the dimension $m-1$ equals 2 and $\mathbb{K}^n_*$ can be identified with a circle, see [SmW98]. Formula (1.1) is obtained by extending (4.1) homogeneously.

5 Upper Bounds

To improve the trivial upper bound $w_{\rm mix}(c) \leq 0$ we need to find a suitable inner approximation of $\mathcal{H}(c)$. In fact, in light of the Krein–Milman theorem it would be sufficient to characterize (or approximate) its extremal points.

Their is no general theory to describe $\mathcal{H}(c)$ suitably, however the **lamination mixture formula**, which is due to [AvM89, Tar90, Koh91], allows us to construct new $\mathbb{H}$–measures as mixture of two given ones.

Theorem 5.1 *Assume $\mu^{(1)} \in \mathcal{H}(c^{(1)}), \mu^{(2)} \in \mathcal{H}(c^{(2)}), \theta \in (0,1)$ and $\omega \in \mathbb{S}^{d-1}$, then*

$$\mu = \theta\mu^{(1)} + (1-\theta)\mu^{(2)} + \theta(1-\theta)(c^{(2)}-c^{(1)})\otimes(c^{(2)}-c^{(1)})\widehat{\delta}_\omega \in \mathcal{H}(\theta c^{(1)} + (1-\theta)c^{(2)}).$$

This formula implies convexity of $\mathcal{H}(c)$, since mixing with $c^{(1)} = c^{(2)} = c$ does not generate an additional quadratic term. Another immediate consequence is the estimate

$$w_{\rm mix}(\theta c^{(1)}+(1-\theta)c^{(2)}) \leq \theta w_{\rm mix}(c^{(1)}) + (1-\theta)w_{\rm mix}(c^{(2)}) + \theta(1-\theta)\psi(c^{(1)}-c^{(2)}). \tag{5.1}$$

Because of $\psi(\eta) \leq 0$ this implies better bounds than simple convexity. Starting with $0 \in \mathcal{H}(e_j)$ we may inductively apply this formula to obtain nontrivial bounds.

It was first observed by R.V. Kohn [Koh91] that this approach gives $w_{\rm mix}$ exactly in the case of two phases only, namely

$$w_{\rm mix}(\theta e_j + (1-\theta)e_k) = \theta(1-\theta)\psi(e_j-e_k). \tag{5.2}$$

This result follows immediately since the lower and upper bounds for $w_{\rm mix}(c)$ coincide. Our theorem 6.2 generalizes this fact to the case of n phases, if all transformation strains lie on one straight line.

By applying (5.1) with $c^{(1)} = \theta e_j + (1-\theta)e_k$ and $c^{(2)} = e_l$ we obtain a bound for all points in $\mathrm{conv}\{e_j, e_k, e_l\}$. Proceeding like this we obtain a first upper bound.

Proposition 5.2 *For $c \in P^n$ define $c^{(k)} = (c_1+\ldots+c_k)^{-1}(c_1e_1+\ldots+c_ke_k)$, then*

$$w_{\rm mix}(c) \leq \sum_{j=2}^{n} \tfrac{(c_1+\ldots+c_{j-1})c_j}{c_1+\ldots+c_j}\,\psi(c^{(j-1)}-c^{(j)}). \tag{5.3}$$

By permutation of the points $e_1, \ldots, e_n$ we can generate other upper bounds.

Of course, the upper bound in the right–hand side of (5.3) may be further reduced by applying (5.1) again. In fact, in typical cases it needs infinitely many applications of the lamination formula to reach the lowest level. This corresponds to infinite sequential lamination, see [SmW98].

In principle, the definition $w^{\rm upp}(c) = \max\{\, \widetilde{w}(c) : \widetilde{w} \text{ satisfies } (5.1), \widetilde{w}(e_j) \leq 0,\ j = 1, \ldots, n\,\}$ defines the best upper bound for $w(c)$ which can be obtained from lamination. For practical purposes it is better to write $w^{\rm upp}$ as a minimum, since then each candidate $\overline{w}$ provides a true upper bound

$$w^{\rm upp}(c) = \min\{\, \overline{w}(c) : \overline{w} \text{ satisfies (5.4)},\ \overline{w}(e_j) \geq 0 \text{ for } j = 1, \ldots, n\,\},$$

where now the condition reads

$$\overline{w}(\theta c^{(1)}+(1-\theta)c^{(2)}) \geq \theta\overline{w}(c^{(1)}) + (1-\theta)\overline{w}(c^{(2)}) + \theta(1-\theta)\psi(c^{(1)}-c^{(2)}). \tag{5.4}$$

6 Examples

Proposition 6.1 *If $\psi(\eta) = \langle\!\langle B, \eta\otimes\eta \rangle\!\rangle$ for all $\eta \in \mathbb{R}^n_*$, then, $w_{\rm mix}(c) = \langle\!\langle B, \mathbb{M}(c) \rangle\!\rangle$.*

To proof this we first note that $w^{\rm low}(c) = \langle\!\langle B, \mathbb{M}(c)\rangle\!\rangle$ since in (1.1) every linear combination gives the same result by linearity. Similarly the upper bound (5.3) gives the same result. In fact, the assumption can be weakened severely by assuming $\psi(\eta) \geq \langle\!\langle B, \eta\otimes\eta\rangle\!\rangle$ with equality for those η which are needed in (5.3).

The n–well problem can be solved explicitly, when all transformation strains lie on one straight line in $\mathbb{R}^{n\times n}_{\rm sym}$, i.e., $A_j = A_0 + a_j A$ with $a_j \in \mathbb{R}$. The case $A_1{=}-A_3$ and $A_2{=}0$ is considered in [PAM98]. For $A^\eta = \sum_j \eta_j A_j$ with $\eta \in \mathbb{E}^n_*$ we find $A^\eta = \langle \eta, a\rangle A$ and

$$\psi(\eta) = -\gamma\langle a, \eta\rangle^2 = -\gamma\langle\!\langle a\otimes a, \eta\otimes\eta\rangle\!\rangle, \quad \gamma = \max\{\, \langle T(\omega)^{-1}S[A]\omega, S[A]\omega\rangle : \omega \in \mathbb{S}^{d-1}\,\}.$$

With proposition 6.1 we conclude the following exact formula.

Theorem 6.2 *If all $W(E, e_j)$ have the form (2.2) with $A_j{=}A_0 + a_jA$, then*

$$w_{\rm mix}(c) = -\gamma\langle\!\langle a\otimes a, \mathbb{M}(c)\rangle\!\rangle = -\gamma\Big[\textstyle\sum_{j=1}^n a_j^2 c_j - \langle a, c\rangle^2\Big].$$

The second example concerns the case of three wells but now $d = 2$ and

$$A_1 = \begin{pmatrix} a_{11} & 0 \\ 0 & a_{12} \end{pmatrix}, \quad A_2 = 0, \quad A_3 = \begin{pmatrix} a_{31} & 0 \\ 0 & a_{32} \end{pmatrix}.$$

The elasticity tensor is assumed to be isotropic, $S[E] = \lambda\,{\rm tr}\,(E)\mathbb{I} + 2\mu E$. We find

$$\langle\!\langle G(\omega), \eta\otimes\eta\rangle\!\rangle = \tfrac{1}{2}\Big[\tfrac{1}{\lambda+2\mu}(\lambda\,{\rm tr}\,A^\eta{+}2\mu\langle\omega, A^\eta\omega\rangle)^2 + 4\mu\big(|A^\eta\omega|^2{-}\langle\omega, A^\eta\omega\rangle^2\big)\Big].$$

Define $\rho, \kappa \in \mathbb{R}$ via $A^\eta = {\rm diag}((\rho{+}\kappa)/2, (\rho{-}\kappa)/2)$, then minimization over $\omega \in \mathbb{S}^1$ gives

$$\psi(\eta) = -\tfrac{1}{2}(\mu\kappa^2 + (\lambda{+}\mu)\rho^2) + \tfrac{\mu(\lambda+\mu)}{2(\lambda+2\mu)}(\max\{0, |\kappa|{-}|\rho|\})^2. \tag{6.1}$$

With $M = \eta\otimes\eta$ we find that $\Psi|_{\mathbb{E}^3_*}$ is the restriction of a piecewise linear function in (M_{11}, M_{13}, M_{33}). (These three variable uniquely determine $M \in \mathbb{P}^3_*$.)

We do not study the general situation but restrict to a typical case: $A_1 = \begin{pmatrix} 1 & 0 \\ 0 & 0\end{pmatrix}$ and $A_3 = \begin{pmatrix} 0 & 0 \\ 0 & a \end{pmatrix}$ with $a \neq 0$. Then, $\rho = \eta_1{+}a\eta_3$, $\kappa = \eta_1{-}a\eta_3$ and, for $M \in \mathbb{E}^3_*$, we have

$$\Psi(M) = \Psi^{\rm lin}(M) + 2\tfrac{\mu(\lambda+\mu)}{\lambda+2\mu}\begin{cases} \min\{M_{11}, a^2M_{33}\} & \text{for} \quad aM_{13} \geq 0, \\ 0 & \text{for} \quad aM_{13} \leq 0, \end{cases}$$

where $\Psi^{\rm lin}(M) = -\frac{1}{2}(\lambda{+}2\mu)(M_{11}{+}a^2M_{33}) - \lambda a M_{13}$.

If $a > 0$ we use the fact that the matrices M in $\mathbb{K}^3_*$ with $M_{13} \leq 0$ form a convex set which contains all $\mathbb{M}(c)$. Using (4.2) we obtain $w^{\rm low}_{a>0}(c) = \Psi^{\rm lin}(\mathbb{M}(c))$ for $a > 0$. By inspection of the arguments in proposition 6.1 we find that they also apply here and conclude, for $a > 0$,

$$w_{\mathrm{mix}}(c) = -\tfrac{\lambda+2\mu}{2}(c_1 - c_1^2 + a^2(c_3 - c_3^2)) + \lambda a c_1 c_3.$$

The case $a < 0$ is more interesting. To calculate $\Psi : \mathbb{K}^3_* \to \mathbb{R}$ we let $\Psi = \Psi^{\mathrm{lin}} + \frac{\mu(\lambda+\mu)}{\lambda+2\mu}\Psi^*$ with $\Psi^*(M) = 2\min\{M_{11}, a^2 M_{33}\}$ for $M \in \mathbb{E}^3_*$ and $M_{13} \le 0$. Since Ψ^* depends only on M_{11}, M_{13} and M_{33} we introduce coordinates in $\mathbb{K}^3_*$ as follows:

$$\begin{pmatrix} M_{11} \\ M_{13} \\ M_{33} \end{pmatrix} = \tfrac{1}{6}\begin{pmatrix} 2 \\ -1 \\ 2 \end{pmatrix} + \tfrac{\alpha}{6}\begin{pmatrix} 1 \\ 1 \\ -2 \end{pmatrix} + \tfrac{\beta}{2\sqrt{3}}\begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}, \quad \alpha^2 + \beta^2 \le 1.$$

Moreover, $(\alpha, \beta) = (\cos\phi, \sin\phi)$, $\phi \in [0, 2\pi)$, defines coordinates in $\mathbb{E}^3_*$. We have $M_{13}(\phi) \le 0$ and $\Psi^*(\phi) = \frac{2}{3}\min\{1 + \cos(\phi - \frac{\pi}{3}), a^2(1 - \cos\phi)\}$ for $\phi \in [0, 4\pi/3]$. A geometric consideration as in [SmW98] shows that, for $\alpha - \beta\sqrt{3} \le 1$ ($M_{13} \le 0$), $\Psi^*(\alpha, \beta)$ is obtained by interpolating between two points on $\mathbb{E}^3_*$:

$$\begin{gathered} \Psi^*(\alpha, \beta) = \theta\Psi^*(\phi_1) + (1-\theta)\Psi^*(\phi_2), \quad 0 \le \phi_1 \le \phi_2 \le 4\pi/3; \\ \alpha = \theta\cos\phi_1 + (1-\theta)\cos\phi_2, \quad \beta = \theta\sin\phi_1 + (1-\theta)\sin\phi_2; \\ (1-a^2)\sin(\phi_1 - \phi_2) + (a^2 - \tfrac{1}{2})(\sin\phi_1 - \sin\phi_2) - \tfrac{\sqrt{3}}{2}(\cos\phi_1 - \cos\phi_2) = 0. \end{gathered}$$

The last condition is the optimality condition. In the case $a = -1$ we find $\phi_2 = 4\pi/3 - \phi_1$ and $\Psi^*(M) = M_{11} + M_{33} - \sqrt{(M_{11}+M_{33})^2 - 4M_{13}^2}$. This leads to the lower bound

$$w^{\mathrm{low}}_{a=-1}(c) = \Psi^{\mathrm{lin}}(\mathbb{M}(c)) + \tfrac{\mu(\lambda+\mu)}{\lambda+2\mu}\Psi^*(\mathbb{M}(c)).$$

An upper estimate for the case $a = -1$ is obtained via the mixing formulae

$$\begin{aligned} w^{\mathrm{upp}}(\theta e_1 + (1-\theta)e_2) &= w^{\mathrm{upp}}(\theta e_3 + (1-\theta)e_2) = -\theta(1-\theta)\tfrac{1}{2}(\lambda+2\mu) \\ w^{\mathrm{upp}}(c) &= w^{\mathrm{upp}}\Big(\tfrac{c_1}{1-c_2}\begin{pmatrix} 1-c_2 \\ c_2 \\ 0 \end{pmatrix} + \tfrac{c_3}{1-c_2}\begin{pmatrix} 0 \\ c_2 \\ 1-c_2 \end{pmatrix}\Big) \\ &\le -\tfrac{\lambda+2\mu}{2}(c_1c_2 + c_2c_3) + c_1c_3\psi\Big(\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}\Big) \\ &= -\tfrac{\lambda+2\mu}{2}(c_1 - c_1^2 + c_3 - c_3^2) - \lambda c_1c_3 + 2\tfrac{\mu(\lambda+\mu)}{\lambda+2\mu}c_1c_3. \end{aligned}$$

It is not clear whether this upper bound can be improved using the mixing formula again. However, the theory in [SmW98] indicates, that it is very unlikely to decrease $w^{\mathrm{upp}}(c)$ such that $w^{\mathrm{upp}}(c) = w^{\mathrm{low}}(c)$.

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