Rank one plus a null-Lagrangian is an inherited property of two-dimensional compliance tensors under homogenization.

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Proc. Royal Soc. Edinburgh, Vol. 128A, pp. 283-299, 1998

Abstract

Assume that the local compliance tensor of an elastic composite in two space dimensions is equal to a rank-one tensor plus a null-Lagrangian (there is only one symmetric one in 2-D). The purpose of this paper is to prove that the effective compliance tensor has the same representation: rank-one plus the null-Lagrangian. This statement generalizes the well-known result of Hill [14, 15] that a composite of isotropic phases with a common shear modulus is necessarily elastically isotropic and shares the same shear modulus. It also generalizes the surprising discovery in [1] that under a certain condition on the pure crystal moduli the shear modulus of an isotropic polycrystal is uniquely determined. The present paper sheds light on this effect by placing it in a more general framework and using some elliptic PDE theory rather than the translation method. Our results allow us to calculate the polycrystalline G-closures of the special class of crystals under consideration. Our analysis is contrasted with a two dimensional model problem for shape-memory polycrystals. We show that the two problems can be thought of as "elastic percolation" problems, one elliptic, one hyperbolic.

1 Introduction

Consider an open domain $\Omega \subset \mathbb{R}^2$ occupied by an inhomogeneous periodic composite with the compliance tensor $S(x/\varepsilon)$ at every point $x \in \Omega$. When $\varepsilon \to 0$ the local compliance $S(x/\varepsilon)$ oscillates faster and faster, so that in the limit the whole set Ω will look like a *homogeneous* elastic material with the compliance S^*, called the effective compliance of the composite. To characterize S^* mathematically we need to introduce the following notation. Let Q be the unit area torus (i.e. a square with periodic boundary conditions). Let

$$\mathcal{J} = \{\sigma \in L^2(Q;\mathbb{R}^{2\text{x}2}) | \sigma^t = \sigma; \text{ and } \mathbf{div}\, \sigma = 0\} \tag{1.1}$$

be a divergence-free subspace of the space of square integrable functions on Q with values in the space of symmetric 2x2 matrices. Physically the subspace $\mathcal{J}$ represents the space of periodic stress fields in the absence of body forces. Let $\langle f \rangle$ denote the average value of an arbitrary function f over Q. Then for any 2x2 symmetric matrix σ^*

$$(S^*\sigma^*, \sigma^*) = \inf_{\substack{\sigma \in \mathcal{J} \\ \langle \sigma \rangle = \sigma^*}} \int_Q (S(x)\sigma(x), \sigma(x))dx. \tag{1.2}$$

Given $S(x)$ this variational formulation allows one to estimate the effective compliance S^*.

In practice one is interested in obtaining information about S^* given some information about the local compliance $S(x)$. The question we'll be concerned with is the *exact* results on S^* rather than some inequalities. One of the earliest examples of that type is the result of Hill [14, 15] (see also [10, 17]). It says that if you mix, possibly infinitely many, isotropic materials with the same shear moduli in prescribed proportion then the effective composite is isotropic and has uniquely determined bulk and shear moduli. In two dimensions this result follows from our analysis as a particular case. We discuss it in section 4.1.

A more recent example comes from a polycrystal problem discussed in [1]. If the pure crystal compliance S_0 is orthotropic and satisfies a certain relation, then the upper and lower shear modulus bounds pinch at a uniquely defined shear modulus.

If one wants to extend this particular result to a wider class of materials one would hope that there is an easier way than first finding the optimal shear modulus bounds and then studying when they pinch — the method employed in [1]. And indeed there is a simple and direct way to do so. The idea is to use again the translation method, that originated in the work of Lurie and Cherkaev [16] and Tartar [22], as was done in [1]. But this time the simplicity will rule over optimality. We are going to obtain a pair of very simple and *suboptimal* bounds on the effective shear modulus, that still pinch at all the right places. The condition on S_0 we arrive at is that S_0 equals to a null-Lagrangian Φ plus a rank-one tensor $s_0 \otimes s_0$. Incidentally, this is equivalent to S_0 being orthotropic and $\Delta = 0$, where Δ is given in [1, formula (3.7)]. This means that the polycrystalline G-closure of such a special orthotropic material contains only materials of the same type. In other words the set of these special materials is closed under homogenization. In fact in section 4.2 we calculate that G-closure exactly.

These results motivate our next generalization. Assume that

$$S(x) = \Phi + s(x) \otimes s(x), \tag{1.3}$$

where we place no restrictions on $s(x)$ except the boundedness and the positive definiteness of the compliance $S(x)$ (this necessitates the matrix $s(x)$ to be positive definite itself). Then we prove that

$$S^* = \Phi + s^* \otimes s^*, \tag{1.4}$$

where s^* is again a positive definite 2x2 matrix. We can state this result as $S^* - \Phi$ is rank-1 whenever $S(x) - \Phi$ is rank-1 (see Theorem 4). In section 4.3 we also prove a related result that if the local elasticity tensor $C(x)$ is rank-2 and for every x there is a positive definite matrix spanning the null-space of $C(x)$ then C^* is also rank-2 with a positive definite matrix spanning its null-space. For this result to hold it is not necessary that $C(x)$ be orthotropic.

It is curious that the orthotropic materials of the type (1.4) have also appeared as a distinguished class of materials in the problem of energy minimizing microstructures for composites made of two anisotropic phases [11]. Generically, the optimal microstructures may not have smooth curved interfaces. However, if the compliance tensor of the matrix phase is given by (1.4), then we get a large variety of interesting optimal microstructures. The Vigdergauz construction [13, 23, 24] and the confocal ellipse construction [5, 12, 19, 20, 21, 22, 25] are among them.

There is another microstructure-independent relation uncovered in [1]. Unfortunately it lies outside of the scope of this paper. Yet, an attentive reader would appreciate the parallel. If the original crystal has square symmetry and the polycrystal is isotropic then its bulk and shear moduli are given explicitly as a function of bulk and two shear moduli of the original crystal. It turns out [18] that *any* polycrystal made with a square crystal has to possess square symmetry and that the two effective shear moduli lie on the hyperbola in the (μ_1^*, μ_2^*) plane [17, 18]:

$$\mu_1^0 \mu_2^0 (\mu_1^* + k)(\mu_2^* + k) = \mu_1^* \mu_2^* (\mu_1^0 + k)(\mu_2^0 + k),$$

where k is the bulk and μ_1^0, μ_2^0 are shear moduli of the original crystal. The effective bulk modulus of such a polycrystal is equal to k. See [17, 18] for the detailed account of these results.

Now we would like to point out to the connection of our work with the recent results on shape-memory polycrystals in [6]. Both works can be viewed as results on an elastic percolation problem. In both works a single crystal is assumed to have some "easy" (stress-free) eigenstrains. If a given strain does not produce stresses in the polycrystal then each individual grain must undergo one of the "easy" strains. Then we say that the given strain "percolates".

The distinction between our results and those in [6] is that we are dealing with "elliptic percolation" (elliptic PDEs, positive definite matrices), and the dimensionality of the set of "percolating strains" is microstructure-independent. At the same time Bhattacharya and Kohn are dealing in [6] with "hyperbolic percolation" (hyperbolic PDEs, indefinite matrices), and the dimensionality of the set of "percolating strains" is microstructure-dependent.

We must note that "hyperbolicity" in [6] is not accidental. It appears naturally from the kinematic compatibility between austenite and martensite variants in a pure shape memory crystal. Therefore, our setting can not arise in the framework of [6]. See section 4.3 for a rigorous discussion on these issues.

2 The translation bounds

2.1 Preliminaries

We begin by representing our fourth order tensors as matrices of self-adjoint operators on the space of symmetric 2x2 matrices. We choose the basis of the underlying linear space to be the same as in [1] and [17, 18]:

$$\mathbf{a_1} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \mathbf{a_2} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \mathbf{a_3} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{2.1}$$

The translation tensors Φ are all those constant symmetric fourth order tensors that for all $\sigma \in \mathcal{J}$ satisfy

$$\langle(\Phi\sigma, \sigma)\rangle = (\Phi\langle\sigma\rangle, \langle\sigma\rangle), \tag{2.2}$$

where $\mathcal{J}$ is given by (1.1). In the above basis all such tensors have a representation [1, 2, 7, 17, 18] $\Phi = tT$, where t is an arbitrary scalar and

$$T = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{2.3}$$

The tensor T has several useful properties besides (2.2).

1. T is rotation invariant:
$$\mathcal{R}^t T \mathcal{R} = T, \tag{2.4}$$
where $\mathcal{R}$ is defined by its action on an arbitrary symmetric 2x2 matrix ξ by
$$\mathcal{R}\xi = R\xi R^t \tag{2.5}$$
and R is a rotation ($R \in SO(2)$).

2. $T^{-1} = T$;

3. $T\xi = -R_\perp \xi R_\perp^t$, where
$$R_\perp = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{2.6}$$

4. The identity $(T\xi, \xi) = -2\det\xi$ holds for any symmetric 2x2 matrix ξ ;

5. $T\xi = -\xi^{-1}\det\xi$ for all invertible symmetric matrices ξ.

6. Let $e(v) = \frac{1}{2}(\nabla v + (\nabla v)^t)$ be the linear strain then

$$\langle (Te(v), e(v))\rangle \quad \geq \quad (T\langle e(v)\rangle, \langle e(v)\rangle). \tag{2.7}$$

The last property will be used in the lower bound derived using the standard variational principle:

$$(C^*e^*, e^*) = \inf_{\substack{e\in\mathcal{E}\\ \langle e\rangle = e^*}} \int_Q (C(x)e(x), e(x))dx. \tag{2.8}$$

Here $C^* = (S^*)^{-1}$, $C(x) = (S(x))^{-1}$ and

$$\mathcal{E} = \{e \in L^2(Q; \mathbb{R}^{2\text{x}2}) | \exists v \in H^1(Q; \mathbb{R}^2) : e(x) = \frac{1}{2}(\nabla v + (\nabla v)^t)\} \tag{2.9}$$

is the subspace of elastic linear strains in L^2.

2.2 Bounds

Now we are ready to prove some *suboptimal* bounds on the effective tensors of polycrystals. These simple bounds will still allow us to recover a result in [1] about the uniqueness of a shear modulus of an isotropic polycrystal made with a special orthotropic pure crystal. We present this new argument to motivate our generalization developed in the next section. Let us assume that

$$S(x) = \mathcal{R}(x)S_0\mathcal{R}^t(x), \tag{2.10}$$

where S_0 is the single crystal compliance and $\mathcal{R}(x)$ is given by (2.5) for every $x \in Q$.

The upper bound on C^* is obtained from (1.2) and (2.2):

$$(S^*\sigma^*, \sigma^*) = \inf_{\substack{\sigma\in\mathcal{J}\\ \langle\sigma\rangle = \sigma^*}} \int_Q ((S(x) - tT)\sigma(x), \sigma(x))dx + t(T\sigma^*, \sigma^*). \tag{2.11}$$

If we now choose the scalar t such that $S(x) - tT$ is positive semidefinite, then we get our upper bound:

$$(S^*\sigma^*, \sigma^*) \geq t(T\sigma^*, \sigma^*). \tag{2.12}$$

Since we will be interested in the shear modulus bounds we assume that $\det\sigma^* < 0$. Then, to get the best upper bound we must choose t as large as possible. Since T is rotation invariant then $S(x) - tT$ is positive semidefinite if and only if $S_0 - tT$ is positive semidefinite. In other words $1/t$ is the largest eigenvalue of TS_0^{-1}.

The lower bound is obtained from (2.8) and (2.7):

$$(C^*e^*, e^*) \geq \inf_{\substack{e\in\mathcal{E}\\ \langle e\rangle = e^*}} \int_Q ((C(x) - qT)e(x), e(x))dx + q(Te^*, e^*) \geq q(Te^*, e^*). \tag{2.13}$$

The last inequality holds if $C(x) - qT$ is positive semidefinite. Again we are only interested in the "shear" fields e^*, namely those for which $\det e^* < 0$. Then the obtained lower bound is best when q is as large as possible, which is equivalent to $1/q$ being the largest eigenvalue of S_0T.

Finally,we need to relate t and q in order to study when the two bounds "pinch", i.e. when the set of tensors satisfying the bounds has empty interior in the space of all fourth order tensors with Hooke's law symmetries. This is done by the following simple lemma:

Lemma 1 *The operator S_0T has exactly two positive eigenvalues and one negative. Call them $\lambda_1^+ \geq \lambda_2^+ > 0 > \lambda^-$. Then*

$$q = 1/\lambda_1^+, \tag{2.14}$$

$$t = \lambda_2^+. \tag{2.15}$$

Proof. Since T has one negative and two positive eigenvalues then so does $(S_0)^{1/2}T(S_0)^{1/2}$ by the law of inertia. But this matrix has the same eigenvalues as $(S_0)^{1/2}[(S_0)^{1/2}T(S_0)^{1/2}](S_0)^{-1/2}$, which is just S_0T. Another observation is that $(S_0T)^{-1} = TS_0^{-1}$ and therefore the operator TS_0^{-1} has eigenvalues $1/\lambda_2^+ \geq 1/\lambda_1^+ > 0 > 1/\lambda^-$. Now the lemma follows from our definitions of $1/q$ and $1/t$ as largest eigenvalues of S_0T and TS_0^{-1} respectively.□

Corollary 1 *The inequality $tq \leq 1$ holds (since $\lambda_1^+ \geq \lambda_2^+$). It becomes equality if and only if S_0T has a double eigenvalue.*

The proof is obvious.

Finally, if we assume that S^* is isotropic then our bounds say:

$$\frac{1}{2\mu^*} \geq t, \tag{2.16}$$

$$2\mu^* \geq q. \tag{2.17}$$

Thus, the upper bound is equal to the lower bound whenever $tq = 1$. So we have just proved a theorem:

Theorem 1 *An isotropic polycrystal made out of a pure crystal with compliance S_0 has a uniquely determined shear modulus if S_0T has a double eigenvalue.*

Remark 1 *The converse of the statement is not true. In fact, for a pure crystal with square symmetry the isotropic polycrystal's shear (and bulk) modulus is uniquely determined [1], yet S_0T does not have a double eigenvalue (unless S_0 is isotropic). This is not surprising since we didn't use optimal bounds for Theorem 1. For the insight and generalization of that other phenomenon from [1] we refer the reader to [17, 18].*

Remark 2 *Notice that if S_0T has a double eigenvalue, say $\lambda_1^+ = \lambda_2^+ = t$, then $S_0T - tI$ is rank-1. Multiplying on the right by T, we see that $S_0 - tT$ is rank-1. In order to check if a given tensor S_0 has that property one needs to compute the adjoint of $S_0 - tT$, set it equal to zero and eliminate t. Then one finds that S_0 must be orthotropic and $\Delta = 0$, where Δ is given in [1, formula (3.7)].*

Now we are ready to formulate an intermediate generalization of our result.

Theorem 2 *Let $S(x)$ be smooth (C^3 is enough) and uniformly positive definite tensor field on Q. If for some $t \in \mathbb{R}$ the translated local compliance $S(x) - tT$ is rank-1 and S^* is the corresponding effective compliance tensor, then $S^* - tT$ is also rank-1.*

Notice that we have already proved this theorem for the case when $S(x)$ is an isotropic polycrystal. The complete proof follows in the next section. The Theorem 4 in section 3.3 gets rid of the smoothness assumptions, and Theorem 5 describes all possible effective tensors S^* of a polycrystal.

3 Generalizations.

3.1 PDE background.

Before we begin, we would like to recall one theorem from the theory of elliptic PDEs. Let $A(x) \in C^3(Q)$ be symmetric positive definite nxn matrix valued function. And let $(A(x)\xi, \xi) \geq \alpha|\xi|^2$ for some $\alpha > 0$ and all $\xi \in \mathbb{R}^n$. Consider a scalar second order elliptic differential operator L acting on the Sobolev space $H^2(Q)$: For any $u \in H^2(Q)$ let

$$Lu = A_{ij}(x)\frac{\partial^2 u}{\partial x_i \partial x_j} \tag{3.1}$$

define the action of L, where we use the summation over repeated indices convention. Then

$$L^* v = \mathbf{div\ div}\ (A(x)v) = \frac{\partial^2}{\partial x_i \partial x_j}(A_{ij}(x)v) \tag{3.2}$$

is its formal adjoint.

We remark that all elements of the function spaces above are functions on the torus Q and therefore periodic by definition of the function spaces themselves. The following theorem provides the solvability condition for the equation $Lu = f$.

THEOREM **3**

1. *The equation $L^* m = 0$, $m \in H^2(Q)$, $\langle m \rangle = 1$ has a unique solution $m(x)$.*
2. *There exists a constant $\overline{m} > 0$ and a constant $M > 0$ such that the inequality $\overline{m} \le m(x) \le M$ holds for all $x \in Q$.*
3. *If $f \in L^2(Q)$ then the equation $Lu = f$, $u \in H^2(Q)$, $\langle u \rangle = 0$ has a unique solution if and only if*

$$\langle mf \rangle = \int_Q m(x) f(x) dx = 0. \tag{3.3}$$

Parts 1 and 3 of the theorem were proved in [4], while part 2 was proved in [3, Proposition 3.1].

3.2 The proof of Theorem 2.

Now let us start again from the beginning. Let us assume first that the field $S(x)$ is of class C^3 and that $S(x) = s(x) \otimes s(x) + tT$. We also require that $S(x)$ be strictly positive definite. One can show that the conditions $0 < t < -(Ts(x), s(x))$ are necessary and sufficient for $S(x)$ to be strictly positive definite. In the above we regarded S and T as operators on the three dimensional space of 2x2 symmetric matrices, while s was considered a vector in that space. On the other hand, if we view $s(x)$ as a 2x2 matrix then the condition $(Ts(x), s(x)) < 0$ becomes $\det s(x) > 0$. Thus, without loss of generality we can regard $s(x)$ as strictly positive definite 2x2 matrix field of class C^3.

In order to prove Theorem 2 we start with the variational principle (1.2):

$$(S^*\sigma^*, \sigma^*) = \inf_{\substack{\sigma \in \mathcal{J} \\ \langle \sigma \rangle = \sigma^*}} \int_Q (s(x), \sigma(x))^2 dx + t(T\sigma^*, \sigma^*). \tag{3.4}$$

At this point we'll make an essential use of the two-dimensionality. We represent the symmetric divergence-free field σ by the Airy stress potential ϕ: $\sigma = R_\perp \nabla\nabla\phi R_\perp^t$, where $R_\perp$ is given by (2.6). Then our variational principle (3.4) becomes:

$$((S^* - tT)\sigma^*, \sigma^*) = \inf_{\phi_0 \in H^2(Q)} \int_Q (\hat{s}(x), \nabla\nabla\phi)^2 dx \tag{3.5}$$

where

$$\phi_0(x) = \phi(x) - \frac{1}{2}(R_\perp^t \sigma^* R_\perp x, x) \tag{3.6}$$

and

$$\hat{s}(x) = R_\perp^t s(x) R_\perp. \tag{3.7}$$

If we now write down the Euler-Lagrange equation for the variational problem (3.5) we obtain the following PDE:

$$\mathbf{div}\,\mathbf{div}\,(\hat{s}(x)(\hat{s}(x),\nabla\nabla\phi)) = 0. \tag{3.8}$$

According to Theorem 3 part 1 (with $A(x) = \hat{s}(x)$) there is a constant $c \in \mathbb{R}$ such that

$$(\hat{s}(x),\nabla\nabla\phi) = cm(x), \tag{3.9}$$

where $m(x)$ is the unique positive solution of the homogeneous equation

$$\mathbf{div}\,\mathbf{div}\,(\hat{s}(x)m) = 0, \quad m \in L^2(Q), \quad \|m\| = 1, \tag{3.10}$$

and $\|m\|$ is the $L^2(Q)$ norm of m. The equation (3.9) can also be written as

$$(\hat{s}(x),\nabla\nabla\phi_0) = cm(x) - (s(x),\sigma^*). \tag{3.11}$$

Then part 3 of the Theorem 3 says that it has a solution if and only if the right hand side is orthogonal to $m(x)$ in $L^2(Q)$:

$$\int_Q cm^2(x) - (s(x),\sigma^*)m(x)dx = 0. \tag{3.12}$$

Since $\|m\| = 1$ it follows that

$$c = (s^*,\sigma^*), \tag{3.13}$$

where

$$s^* = \int_Q s(x)m(x)dx. \tag{3.14}$$

Substituting this value of c into (3.9) and recalling the variational principle (3.5) we finally obtain

$$(S^*\sigma^*,\sigma^*) = (s^*,\sigma^*)^2 + t(T\sigma^*,\sigma^*). \tag{3.15}$$

Thus we have proved Theorem 2. In fact, we have obtained a representation for S^* according to (3.15). Now we are ready to get rid of the superfluous smoothness assumption that we needed in order to use Theorem 3.

3.3 Smoothness in Theorem 2 is redundant.

THEOREM 4 *Let $S(x) = s(x)\otimes s(x)+tT$ be a measurable, bounded, positive definite local compliance tensor in two space dimensions. (The positive definiteness is equivalent to $0 < t < 2\det s(x)$ for almost all $x \in Q$.) Let S^* denote the corresponding effective compliance. Then*

$$S^* = s^*\otimes s^* + tT, \tag{3.16}$$

where s^* is given by (3.14) and $m(x)$ is the unique positive solution of (3.10). Moreover s^* is necessarily positive definite with $\det s^* > \frac{1}{2}t > 0$ (otherwise S^* would not be positive definite).

We have already proved the theorem under some smoothness assumptions. To get rid of them we use a type of density argument. Consider a sequence $s_\varepsilon \in C^3$ such that it stays uniformly bounded and converges almost everywhere to $s \in L^\infty$. Then the two variational principles (1.2) and (2.8) give the estimates:

$$(S^*_\varepsilon\sigma^*,\sigma^*) \le \int_Q (S_\varepsilon(x)\sigma(x),\sigma(x))dx, \quad \sigma \in \mathcal{J}, \quad \langle\sigma\rangle = \sigma^*, \tag{3.17}$$

$$((S_\varepsilon^*)^{-1}e^*, e^*) \le \int_Q ((S_\varepsilon(x))^{-1}e(x), e(x))dx, \quad e \in \mathcal{E}, \quad \langle e\rangle = e^*, \tag{3.18}$$

where $S_\varepsilon = s_\varepsilon \otimes s_\varepsilon + tT$.

Our conditions guarantee that S_ε^* stays strictly and uniformly positive definite and bounded. Therefore we may select a subsequence, again denoted by S_ε^*, that converges to a limit S_0^*. Also, both $S_\varepsilon(x)$ and $(S_\varepsilon(x))^{-1}$ converge to their respective limits $S(x)$ and $(S(x))^{-1}$. Passing to the limit in the above inequalities and taking infima again we obtain

$$(S_0^*\sigma^*, \sigma^*) \le (S^*\sigma^*, \sigma^*) \tag{3.19}$$

and

$$((S_0^*)^{-1}e^*, e^*) \le ((S^*)^{-1}e^*, e^*), \tag{3.20}$$

where S^* is the effective compliance corresponding to the local nonsmooth compliance $S(x)$. From the last two inequalities which hold for all choices of e^* and σ^*, we obtain that

$$S_0^* = S^*. \tag{3.21}$$

Thus the whole sequence S_ε^* converges to S^* even without taking a subsequence.

Now we are going to obtain a representation for S^* using the fact that it is a limit of $S_\varepsilon^* = s_\varepsilon^* \otimes s_\varepsilon^* + tT$. The matrix s_ε^* is given via m_ε by (3.14) and (3.10), with $s(x)$ replaced by $s_\varepsilon(x)$. Since $\|m_\varepsilon\| = 1$, we may extract a subsequence (denoted by m_ε again) that converges weakly in $L^2(Q)$ to $m_0(x)$. Since s_ε converges strongly, we have

$$s_\varepsilon^* \to \int_Q s(x)m_0(x)dx = s^* \tag{3.22}$$

We observe that $s^* \ne 0$, otherwise S^* would be equal to tT, which is not positive semidefinite and contradicts (3.21). The same weak-strong argument shows that $m_0(x)$ is a weak solution of

$$\mathbf{div}\,\mathbf{div}\ (\hat{s}(x)m_0(x)) = 0. \tag{3.23}$$

Now we are going to prove that m_ε converges strongly to m_0. The following argument will also be used to show uniqueness in (3.10). From the limit equation (3.23) it follows that $e(x) = s(x)m_0(x)$ satisfies the two-dimensional strain compatibility condition:

$$\frac{\partial^2 e_{11}}{\partial x_2^2} + \frac{\partial^2 e_{22}}{\partial x_1^2} = 2\frac{\partial^2 e_{12}}{\partial x_1 \partial x_2}. \tag{3.24}$$

Thus, $e(x) = e(u)$ for some function u. We are going to use $e(u)$ as a test field in the variational principle (2.8). We have

$$S^* = s^* \otimes s^* + tT. \tag{3.25}$$

Therefore, using properties 2,4 and 5 of T and inverting (3.25),

$$C^* = \frac{1}{t}\Big(\frac{(\det s^*)^2}{2\det s^* - t}(s^*)^{-1} \otimes (s^*)^{-1} + T\Big). \tag{3.26}$$

Similarly, since

$$S(x) = s(x) \otimes s(x) + tT, \tag{3.27}$$

we have

$$C(x) = \frac{1}{t}\Big(\frac{(\det s(x))^2}{2\det s(x) - t}(s(x))^{-1} \otimes (s(x))^{-1} + T\Big). \tag{3.28}$$

Substituting the test field $e(u)$ together with the above formulas into the variational principle (2.8) and using (3.22), we obtain after a simple calculation:

$$\frac{2\det s^*}{2\det s^* - t} \le \int_Q \frac{2m_0^2(x)\det s(x)}{2\det s(x) - t}dx. \tag{3.29}$$

Observe, that m_0 does not depend on t and that t is an arbitrary number from the interval

$$t \in (0, 2\inf_{x\in Q} \det s(x)). \tag{3.30}$$

Therefore, the inequality will remain valid if we pass to the limit as $t \to 0^+$. We obtain $\|m_0\| \ge 1$. But m_0 was the weak limit of m_ε with $\|m_\varepsilon\| = 1$. Thus $\|m_0\| \le 1$. Combining the inequalities, we get that $\|m_0\| = 1$. Therefore the subsequence m_ε converges to m_0 strongly in $L^2(Q)$.

Now we need to establish the uniqueness of m_0 — a solution of (3.10). Suppose we have two linearly independent solutions m_1 and m_2 of (3.10) both giving rise to the same s^* (we have already showed that s^* is uniquely defined by the limiting process). Now, consider $m(x) = \alpha_1 m_1 + \alpha_2 m_2$. Due to the linearity of (3.10), any linear combination of m_1 and m_2 will be a solution as well. Then repeat the previous calculation with the test field $e = m(x)s(x)$ with the average value $e^* = (\alpha_1 + \alpha_2)s^*$:

$$(\alpha_1 + \alpha_2)^2 \le \|\alpha_1 m_1 + \alpha_2 m_2\|^2 = \alpha_1^2 + \alpha_2^2 + 2(m_1, m_2)\alpha_1\alpha_2, \tag{3.31}$$

where we used the fact that $\|m_1\| = \|m_2\| = 1$ in the last equality. Equivalently, choosing α_1 and α_2 positive, we obtain

$$(m_1, m_2) \ge 1. \tag{3.32}$$

This is possible if and only if m_1 and m_2 are linearly dependent. The Theorem 4 is proved. In particular, it says that the periodic problem (3.10) has a unique weak solution m_0 even in the case of merely measurable coefficients. Our result also shows that the whole sequence m_ε converges L^2-strong to m_0.

4 Applications.

4.1 The result of Hill.

One application is a generalization of Hill's results [14, 15] (see also [10, 17]) that a composite made of isotropic components having the same shear modulus μ is necessarily isotropic with the bulk modulus being uniquely determined by the volume factions of components and their elastic properties. Such a composite has a compliance given by

$$S(x) = (\frac{1}{4k(x)} + \frac{1}{4\mu})I \otimes I + \frac{1}{2\mu}T, \tag{4.1}$$

where $k(x)$ is a local bulk modulus. Generalizing Hill's result we assume that

$$S(x) = \alpha(x)A \otimes A + \beta T, \tag{4.2}$$

where A is a constant symmetric positive definite 2x2 matrix, α is a positive and bounded scalar function and β is a positive number. In this case our "cell problem" (3.10) has a simple solution

$$m(x) = m_0\Big(\alpha(x)\Big)^{-1/2}, \tag{4.3}$$

where m_0 is a constant. Substituting it into (3.14) and (3.15) we obtain

$$S^* = H(\alpha(x))A \otimes A + \beta T, \tag{4.4}$$

where $H(f(x)) = \langle f^{-1}(x)\rangle^{-1}$ is the harmonic mean of $f(x)$. If we set $A = I$ and substitute $\alpha = (4k(x))^{-1} + (4\mu)^{-1}$ and $\beta = 1/(2\mu)$, then we see that any such composite must be isotropic and we recover Hill's result.

4.2 The G-closure for the polycrystal is computed.

Now we return to our source of inspiration, the polycrystal. Assume that $S(x) = s(x) \otimes s(x) + tT$, with $s(x) = R(x)s_0R^t(x)$, where $R(x)$ is a rotation field and s_0 is fixed symmetric, positive definite 2x2 matrix. Then Theorem 4 tells us that S^* has the form (3.16). The polycrystal G-closure problem consists in identifying all possible values of s^* in (3.16) corresponding to some rotation field $R(x)$. The pure crystal moduli, characterized by s_0 are assumed fixed. See [17, 18] for another G-closure result for 2-D elastic polycrystals in the setting described in the introduction.

Our first observation comes from the linearity of the formula (3.14) and the equation (3.10). If a particular s^* belongs to the G-closure, then so do all of its rotations. Thus the G-closure is characterized by the eigenvalues of s^*. This allows us to represent the G-closure graphically as a subset of a two-dimensional (s_1^*, s_2^*)-plane of eigenvalues of s^*. Similarly, without loss of generality we may assume that s_0 is a diagonal matrix

$$s_0 = \begin{pmatrix} s_1 & 0 \\ 0 & s_2 \end{pmatrix}. \tag{4.5}$$

We are going to prove that s^* lies in the set bounded by two curves: the upper and the lower bounds. To get the upper bound we take a trace of the formula (3.14):

$$\mathbf{Tr} s^* = \int_Q (\mathbf{Tr} s_0) m(x) dx \leq \mathbf{Tr} s_0, \tag{4.6}$$

since $\|m\| = 1$.

To get the lower bound we use the fact that $e(x) = s(x)m(x)$ is a strain (see (3.24)), and properties 4 and 6 (see (2.7)) of the tensor T.

$$\langle (Ts(x)m(x), s(x)m(x)) \rangle \quad \geq \quad (Ts^*, s^*). \tag{4.7}$$

Equivalently,

$$\det s_0 \leq \det s^*, \tag{4.8}$$

since $\|m\| = 1$.

Geometrically, the set of eigenvalues of s^* satisfying the upper and the lower bounds (4.6) and (4.8) is shown in figure 1. To prove that this set is indeed a G-closure, we need to produce specific rotation fields $R(x)$ attaining the points on the boundary of our set. This is enough to show the attainability of every point of the set including its interior (see for example [9]).

To attain a straight line joining the points A and B in figure 1, we observe that the equality is attained in (4.6) if and only if $m(x) = 1$ identically on Q. It means, by (3.10) that $s(x)$ itself should be a strain. Next we observe that the matrices

$$e_1 = \begin{pmatrix} s_1 & 0 \\ 0 & s_2 \end{pmatrix} \tag{4.9}$$

and

$$e_2 = \begin{pmatrix} s_2 & 0 \\ 0 & s_1 \end{pmatrix} \tag{4.10}$$

are compatible as strains ($\det(e_1 - e_2) < 0$). It means that there are vectors $\mathbf{a}$ and $\mathbf{n}$ with $|\mathbf{n}| = 1$ such that

$$e_1 - e_2 = \frac{1}{2}(\mathbf{a} \otimes \mathbf{n} + \mathbf{n} \otimes \mathbf{a}). \tag{4.11}$$

Specifically,

$$\mathbf{n} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \quad \mathbf{a} = \sqrt{2}(s_1 - s_2) \begin{pmatrix} 1 \\ 1 \end{pmatrix}. \tag{4.12}$$

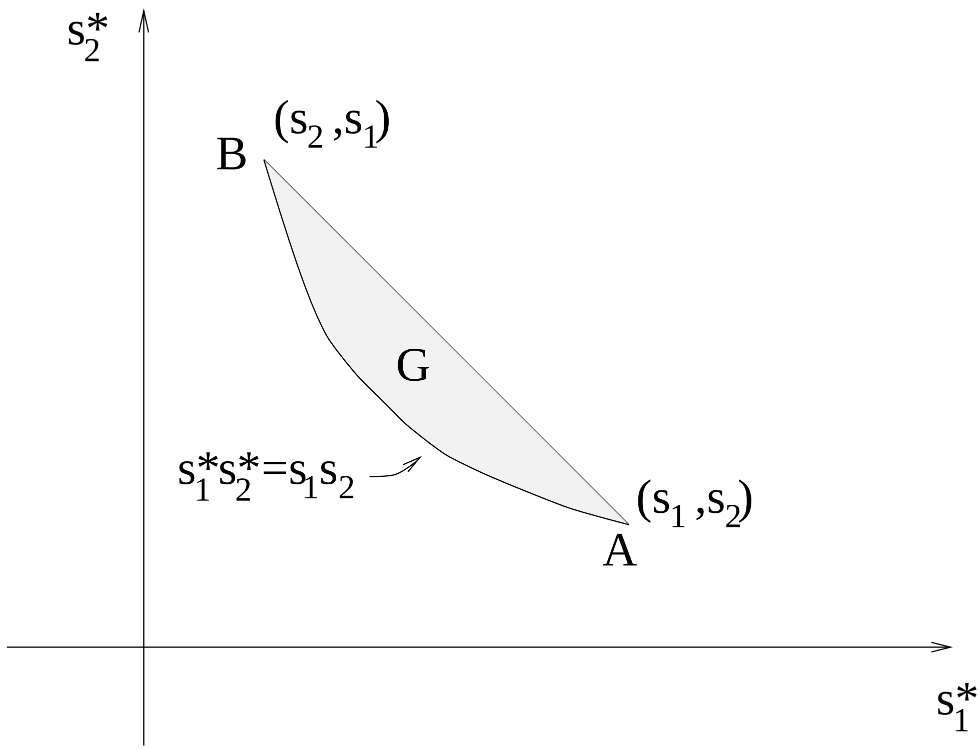

Figure 1: The G-closure.

Then, in order to achieve a point

$$s^* = \theta e_1 + (1-\theta)e_2, \quad \theta \in [0,1] \tag{4.13}$$

we are considering a rotation field taking values R_1 and R_2 as shown in figure 2. The arrows indicate the eigen-directions corresponding to the eigenvalue s_1. The rotations R_1 and R_2 are such that

$$R_1\mathbf{n} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad R_2 = R_1 R_\perp. \tag{4.14}$$

Equivalently R_1 and R_2 can be given explicitly

$$R_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}, \quad R_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}. \tag{4.15}$$

In order to attain a hyperbola joining the points A and B in figure 1, we observe that the equality is attained in (4.8) if and only if

$$\mathbf{curl}\,(s(x)m(x)) = 0, \tag{4.16}$$

(see e.g. [11, formula (3.5)]). To satisfy this condition we propose the rotation field $R(x)$ taking again two values I (the identity matrix) and $R_\perp$, while this time $m(x)$ will not be a constant but will also take two values denoted m_1 and m_2 as shown in figure 3. The arrows in the figure have the same meaning as in figure 2. Then the compatibility condition (4.16) will be satisfied if, for example

$$e_1 m_1 - e_2 m_2 = \begin{pmatrix} \alpha & 0 \\ 0 & 0 \end{pmatrix} \tag{4.17}$$

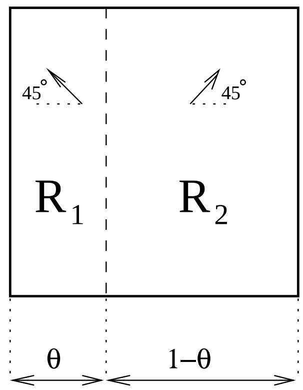

Figure 2: Microstructure attaining the upper bound. The arrows in the figure denote crystal orientation.

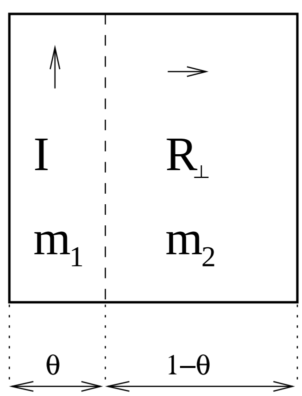

Figure 3: Microstructure attaining the lower bound. Again the arrows denote crystal orientation.

with m_1 and m_2 satisfying the additional constraint $\|m\| = 1$, or

$$\theta m_1^2 + (1-\theta)m_2^2 = 1 \tag{4.18}$$

and α being an arbitrary constant. Solving (4.17) and (4.18) for m_1 and m_2, we obtain

$$m_1 = \frac{s_1}{\sqrt{\theta s_1^2 + (1-\theta)s_2^2}}, \quad m_2 = \frac{s_2}{\sqrt{\theta s_1^2 + (1-\theta)s_2^2}} \tag{4.19}$$

and

$$s^* = \theta e_1 m_1 + (1-\theta) e_2 m_2 = \begin{pmatrix} \sqrt{\theta s_1^2 + (1-\theta)s_2^2} & 0 \\ 0 & \dfrac{s_1 s_2}{\sqrt{\theta s_1^2 + (1-\theta)s_2^2}} \end{pmatrix}. \tag{4.20}$$

As θ increases from 0 to 1, the s^* moves from the point B to point A along the hyperbola in figure 1.

Thus, we have proved the following G-closure theorem

THEOREM **5** *Let the pure crystal compliance S_0 have the form*

$$S_0 = s_0 \otimes s_0 + tT. \tag{4.21}$$

Then the polycrystalline G-closure of this crystal is the set comprising effective compliances S^* of the form

$$S^* = s^* \otimes s^* + tT, \tag{4.22}$$

where s^* is a symmetric, positive definite matrix satisfying the constraints:

$$\begin{aligned} &\mathbf{Tr} s^* \le \mathbf{Tr} s_0 \\ &\det s^* \ge \det s_0, \end{aligned} \tag{4.23}$$

as sketched in figure 1,

4.3 Elastic percolation.

Our results in section 3 could be interpreted as "elastic percolation" results. To this end we consider the equivalent (in the sense of [8], see also [17]) problem, where

$$S(x) = s(x) \otimes s(x) \tag{4.24}$$

is degenerate. Physically it means that locally the material is rigid with respect to all local stresses $\sigma(x)$, such that $(s(x), \sigma(x)) = 0$. Then our results from section 3 say that if an applied stress produces a non-zero strain, then this "percolating" strain field must be of the form

$$\varepsilon(x) = \alpha(x)s(x), \tag{4.25}$$

for some scalar field $\alpha(x)$.

Now, we describe a related result that has some similarities with a model problem from [6] for shape memory polycrystals. Consider an elasticity tensor $C(x)$ that is assumed to be degenerate "along" a *positive definite* eigenstrain $\varepsilon^0(x)$:

$$\mathrm{Nul}(C(x)) = \mathrm{Span}(\{\varepsilon^0(x)\}). \tag{4.26}$$

Thus, if

$$e(u) = \alpha(x)\varepsilon^0(x), \quad x \in Q, \tag{4.27}$$

for some scalar filed $\alpha(x)$ then $\sigma(x) = C(x)e(u) = 0$. In other words the "easy" strain $\fint_{\varepsilon^0(x)}$ would "percolate" if it satisfies (4.27), which is actually the same equation as (4.25). We want to know if for a given degenerate $C(x)$ the "easy" strain $\varepsilon^0(x)$ "percolates", i.e. whether there is an elastic strain $e(u)$ such that (4.27) holds almost everywhere. We will answer this question a little later. But first let us compare (4.27) to a model problem for shape memory polycrystals from [6].

A pure shape memory crystal has a set $\mathcal{S}$ of recoverable strains. The stress-strain law in [6]

$$\sigma = \overline{\phi}(e) \tag{4.28}$$

has the property that $\overline{\phi}(e) = 0$ whenever $e \in \mathcal{S}$. In some examples in [6, section 5.3]

$$\mathcal{S} = \mathrm{Span}(\{\varepsilon_0\}), \tag{4.29}$$

where ε_0 is a constant 2x2 strain tensor. A polycrystal would exhibit a shape memory behavior if there exists a displacement field $u(x)$ such that

$$e(u(x)) \in \mathcal{S}(x) \tag{4.30}$$

for almost all x. The set $\mathcal{S}(x)$ is the set of stress-free strains at the point x:

$$\mathcal{S}(x) = R(x)\mathcal{S}R^t(x), \tag{4.31}$$

where $R(x)$ is the rotation field defining the microstructure of the polycrystal. The notation in (4.31) means that every element in $\mathcal{S}(x)$ is obtained from an element of $\mathcal{S}$ according to (4.31). In the case when $\mathcal{S}$ is given by (4.29) the shape memory behavior will be present if there is a displacement field $u(x)$ such that

$$e(u(x)) = \alpha(x)\varepsilon_0(x), \tag{4.32}$$

where

$$\varepsilon_0(x) = R(x)\varepsilon_0 R^t(x). \tag{4.33}$$

It remains to notice that (4.32) has the form of (4.27). The two problems are not identical, however. According to our assumption $\varepsilon^0(x)$ in (4.27) is positive definite, while in (4.32) the stress-free strain ε_0 has eigenvalues of opposite sign, according to [6]. The reason for the latter is that ε_0 comes from the kinematic compatibility condition between austenite and martensite variants in a pure shape memory crystal.

Now it is the time to address the question of existence of the strain field satisfying (4.27). In two space dimensions the differential condition on a tensor field to be a strain, coupled with (4.27) gives:

$$\frac{\partial^2}{\partial x_1^2}(\alpha(x)\varepsilon^0_{22}(x)) + \frac{\partial^2}{\partial x_2^2}(\alpha(x)\varepsilon^0_{11}(x)) = 2\frac{\partial^2}{\partial x_1 \partial x_2}(\alpha(x)\varepsilon^0_{12}(x)). \tag{4.34}$$

We may rewrite the above equations as

$$\mathbf{div}\ \mathbf{div}\ (\widehat{\varepsilon^0}(x)\alpha(x)) = 0, \quad \alpha(x) \in L^2(Q), \tag{4.35}$$

which coincides with (3.10). The tensor $\widehat{\varepsilon^0}(x)$ is obtained from $\varepsilon^0(x)$ the same way $\hat{s}(x)$ is obtained from $s(x)$, i.e. according to (3.7). As we showed in the previous section, (4.35) has a unique solution up to a constant multiple even in the case of a nonsmooth field $\varepsilon^0(x)$. Then the set of "easy" macro-strains is a one-dimensional subspace spanned by a constant strain e_0,

$$e_0 = \int_Q \alpha(x)\varepsilon^0(x)dx. \tag{4.36}$$

Thus for every degenerate Hooke's law $C(x)$ with a uniformly positive definite tensor spanning the null-space at each point x, there is a one-dimensional subspace of "easy" macro-strains spanned by e_0 given by (4.35) and (4.36).

It is curious that if ε_0 has eigenvalues of opposite signs then the dimension of the set of “easy” macro-strains is microstructure-dependent, as shown in [6]. We call this situation “hyperbolic elastic percolation” because (4.34) becomes a hyperbolic PDE. By contrast, we call our case “elliptic elastic percolation” as (4.34) is then elliptic, and the dimension of the set of “easy” macro-strains is microstructure-independent.

Acknowledgements. The authors are thankful to Professors R. V. Kohn and L. Gibiansky for many helpful remarks. We also wish to thank our referee for carefully reading the paper and forcing us to improve the exposition. GWM gratefully acknowledges the support of the National Science Foundation through grants DMS-9501025 and DMS-9402763.

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