**ELASTIC ENERGY MINIMIZATION AND THE RECOVERABLE
STRAINS OF POLYCRYSTALLINE SHAPE-MEMORY MATERIALS**

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IMA Preprint Series # 1366

November 1995

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Elastic Energy Minimization and the Recoverable Strains of Polycrystalline Shape–Memory Materials

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October, 1995

SUBMITTED TO THE ARCHIVE FOR RATIONAL MECHANICS AND ANALYSIS

Abstract

Shape–memory behavior is the ability of certain materials to recover, on heating, apparently plastic deformation sustained below a critical temperature. Some materials have good shape–memory behavior as single crystals but little or none as polycrystals, while others have good shape–memory behavior even as polycrystals. We propose a method for explaining the difference.

Our approach is based on elastic energy minimization. It leads to a special class of nonlinear homogenization problems, involving integrands that are degenerate near the origin. We explore the behavior of these problems through various examples and bounds. The elementary “Taylor bound” and the newer “translation method” are central to our analysis.

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1 Introduction

Much work has been done on the modelling of polycrystalline composites, i.e. composites made from a single material mixed with itself in different orientations. Separately, much work has been done on the modelling of martensitic transformation in crystalline solids. This paper combines the two themes: we address certain properties of a polycrystalline composite whose basic crystal undergoes a martensitic transformation.

The physical context of our work is the modelling of shape-memory alloys. These materials have the ability to recover, on heating, apparently plastic deformation sustained below a critical temperature. Some materials exhibit good shape-memory as single crystals but

little or none as polycrystals, while others exhibit good shape-memory even as polycrystals. Our goal is to explain the difference, through a model based on elastic energy minimization.

The mathematical setting of our work is nonlinear homogenization. Indeed, energy minimization leads us to consider a certain class of physically nonlinear polycrystals. The “basic crystal” energy is degenerate near the origin, i.e. its graph is flat in some directions. The polycrystal is described by an “effective energy,” and our task is say whether or not it is similarly degenerate. We do not solve this problem in general. Rather, we formulate some principles, mainly at the level of conjecture. Then we explore the validity of these principles through rigorous analyses of special cases and dimensionally-reduced model problems.

The mathematical heart of this paper is our treatment of the models. We use bounds to show that our principles are correct, and examples to show they are sharp. Our main techniques are translation bounds, elastic comparison bounds, lamination, and spatially periodic homogenization. None of these methods is conceptually new: in various forms and combinations they have been used to study martensitic transformation, (e.g. [6, 7]), linear composites (e.g. [4, 5, 31, 54, 82]), and ductile composites (e.g. [14, 61, 69]). But along with the work just cited on plasticity, ours is among the first applications of these techniques to the analysis of nonlinear composites. There are other useful approaches to nonlinear homogenization besides those employed herein; see for example [17, 53, 80, 81].

Our goals are an amorphous mixture of mechanics and mathematics. Therefore it is not a simple matter to list our main results, and we shall not attempt to do so in this introduction. Instead, we begin each section of the paper with a summary of *its* results. A central issue is the accuracy of the “Taylor estimate;” Section 2.4 explains what this means and summarizes our relevant results. Readers primarily interested in the mechanics of shape-memory behavior will want to concentrate on Sections 2 and 3, which justify the use of energy minimization and explore the implications of the Taylor estimate. Readers primarily interested in nonlinear homogenization will want to concentrate instead on Sections 4 and 5, which explore the accuracy of the Taylor estimate using methods from homogenization.

We mention some related work. Our article [11] can be seen as an extension of Section 3: it summarizes the experimental literature on recoverable strain, and compares it to the predictions of the Taylor estimate.¹ Our article [12] can be viewed as a supplement to Section 4.2: it gives additional examples of polycrystals with explicitly computable effective behavior. And the article [45] applies similar methods to some model problems of polycrystal plasticity.

We are naturally not the first to address the micromechanics of shape-memory polycrystals. Saburi and Nenno gave a qualitative but very insightful discussion in [74]; our work can be viewed as an attempt to make their ideas more quantitative. The papers of Ono et al. [62, 63, 64, 65] on stress-induced martensite use a constant-strain hypothesis analogous to our Taylor estimate; Bruno, Leo, and Reitich have developed a different model which permits non-constant strain [17]. Several authors have developed approaches based on some type of mean field theory, including [15, 25, 66, 67, 77, 78]. There is also a lot of work on phenomenological models for specific shape-memory devices such as TiNi wires.

¹We take this opportunity to correct a misstatement in [11]. Section 3 of that paper says we can prove with mathematical rigor that polycrystals with sufficient symmetry made from a cubic-tetragonal material have no recoverable strain. That announcement was unfortunately premature. The results in Section 5 of this article are consistent with such a conclusion but they fall short of demonstrating it.

see e.g. [32] and many of the articles in [16, 36, 47].

The rest of this introduction gives a brief and non-technical explanation of our viewpoint. Saburi and Nenno gave a qualitative but very insightful discussion in [74]; our work can be viewed as an attempt to make their ideas more quantitative. The source of the shape-memory effect is a martensitic phase transformation: deformation is recoverable because it is due not to slip, but rather to rearrangement of martensite variants, see e.g. [57, 74, 79, 84]. Suppose one begins with a single crystal of the high temperature phase, *austenite*. As it is cooled the transformation takes place, creating a mixture of variants of the low temperature phase, *martensite*. The macroscopic effect of the transformation is negligible due to self-accommodation: the different variants of martensite have different stress-free strains, but they can arrange themselves so that each is essentially stress-free [8].

Now deform the sample. The variants will rearrange themselves, if they can, so as to remain stress-free. The resulting deformation appears macroscopically plastic: there is no restoring force, since the variants in their new configurations are not stressed. But it is in fact *recoverable*: heating the crystal above its transformation temperature turns each variant of martensite back to austenite and the crystal springs back to its original shape. Notice, however, that only certain strains can be recovered: those that can be accommodated by rearrangement of the martensite variants. Larger strains will introduce stress, leading to lattice defects and nonrecoverability. We are thus led to the following modelling hypothesis:

Hypothesis 1. *The recoverable strains for a single crystal can be identified with the strains achievable by stress-free mixtures of martensite variants.*

Next consider a polycrystal, consisting (in the austenite phase) of a large number of grains with different orientations. On cooling, each grain transforms to a self-accommodated mixture of martensite variants. As the polycrystal is deformed, each grain tries to accommodate the strain by adjusting its microstructure of stress-free variants. The deformation is recoverable if they succeed. We are thus led to a second modelling hypothesis, the polycrystalline extension of Hypothesis 1:

Hypothesis 2. *The recoverable strains for a polycrystal are the macroscopic averages of locally varying strain fields which can be accommodated within each grain by rearrangement of the martensite variants.*

Our goal is to understand the potential shape-memory effect inherent in a given polycrystal, by calculating the set of recoverable strains using Hypotheses 1 and 2. These hypotheses are abstractions of generally accepted principles. They will be restated mathematically in Section 2. We dwell on them a bit, since they provide the mechanical justification for all that follows.

Implicit in these hypotheses is the idea that if a deformation *can* be accommodated by a stress-free microstructure then it *will* be. This requires that the martensite domain structure be sufficiently mobile, and the slip systems sufficiently rigid; otherwise plastic deformation would occur instead of rearrangement. Also implicit in Hypothesis 2 is an assumption that the length scale of martensite microstructure is small compared to the grain size. This is reflected in our mathematical model by the fact that we minimize elastic energy, without accounting for surface energy.

Our hypotheses reduce the task of estimating recoverable strain to a problem of kinematics. We shall explain this in detail in Section 2, but briefly the story is as follows. A shape-memory single crystal has an associated set $\mathcal{S}$ of recoverable strains, determined by the crystallography of the phase transformation via Hypothesis 1. In a polycrystal made from this material, each grain has its own set $\mathcal{S}(x)$ of recoverable strains, obtained by rotation from $\mathcal{S}$. When the polycrystal is deformed, each grain tries to accommodate the deformation by a stress-free arrangement of martensite variants, and this corresponds to achieving a (mesoscopic) strain $e(x) \in \mathcal{S}(x)$. But the grains are not free to deform independently: each is constrained by its neighbors. If $\mathcal{S}$ is too small then the rotated sets $\mathcal{S}(x)$ may be elastically incompatible, i.e. there may not exist local strain fields $e = \frac{1}{2}(\nabla u + \nabla u^T)$ satisfying $e(x) \in \mathcal{S}(x)$. Such a polycrystal has no recoverable strain, in other words it is a poor shape-memory material. If $\mathcal{S}$ is big enough then the rotated sets $\mathcal{S}(x)$ will be elastically compatible, i.e. there will exist strains satisfying $e(x) \in \mathcal{S}(x)$. Such a polycrystal will display shape-memory behavior. We would then like to estimate the magnitude and direction of the recoverable strains, taking proper account of the interactions between grains.

As our discussion suggests, the essence of the matter is kinematic compatibility: the fact that not every second-order tensor field is the strain of a deformation. Compatibility has played a major role in recent work on the effective behavior of polycrystalline composites, through bounds based on compensated compactness and the translation method. Compatibility has also been crucial to recent work on the modelling of martensitic transformation using elastic energy minimization and the minors relations. So it is natural that we borrow ideas and tools from these areas.

Our analysis of recoverable strain is in some ways parallel to the theory of polycrystal plasticity. Both topics lead to problems of nonlinear homogenization. The specific nonlinearities are different, but in each case there is an elementary “Taylor bound,” proved using a constant-strain test function. In polycrystalline plasticity, the Taylor bound is widely believed to provide a good estimate for the yield stress of a polycrystal. We shall show in various examples that the Taylor bound is also surprisingly reliable as a predictor of recoverable strain.

Hypotheses 1 and 2 are of course merely approximations to the truth. They correctly capture many trends but they also have some deficiencies. One issue concerns how literally to take the phrase “stress-free”. Real microstructures are not exactly stress-free since phase boundary motion requires nonzero driving traction. Therefore it might be better to identify recoverable strains with microstructures which are in some sense low-stress rather than stress-free. An advantage of our approach based on elastic energy minimization is that it considers the existence of “low-energy” as well as stress-free microstructures.

The essence of Hypotheses 1 and 2 is the idea that a deformation of the martensite which can not be accommodated by a stress-free mixture of martensite will damage the crystalline lattice. This viewpoint is useful for predicting recoverable strain, however it says nothing about the actual failure modes of a polycrystal when deformed beyond its recoverable strain. For example, our viewpoint can not explain why CuAlNi polycrystals are brittle while TiNi polycrystals are ductile.

Finally we note that this paper only attempts to estimate the set of recoverable strains. We do not try to obtain a constitutive description for the polycrystal based on some constitutive description of the single crystal. Such an analysis would require different methods,

and would have to consider the energy dissipated by the motion of phase boundaries as well as the elastic energy stored in the polycrystal. Constitutive modelling has been addressed by some of the authors cited above, without however focusing on the roles of crystallography and texture as we do here.

2 Elastic energy minimization and recoverable strain

This section develops our variational approach to the analysis of recoverable strain. We shall discuss the *microscopic* energy φ , the *mesoscopic* energy $\hat{\varphi}$, and the *macroscopic* energy $\bar{\varphi}$ of a shape-memory polycrystal. They describe its behavior on three different length scales: smaller than, comparable to, and larger than the grain size. Mathematically, φ has multi-well structure; $\hat{\varphi}$ is obtained by relaxation; and $\bar{\varphi}$ is obtained by homogenization. The set of recoverable strains for a single crystal, which we denote by $\mathcal{S}$, is determined by the mesoscopic energy — it is the set where $\hat{\varphi}$ is minimized. The set of recoverable strains for a polycrystal, which we denote by $\mathcal{P}$, is determined by the macroscopic energy — it is the set where $\bar{\varphi}$ is minimized.

Our goal is to assess the recoverable strain, i.e. to estimate the size of $\mathcal{P}$. This is a difficult problem, and we are far from a complete solution. But there is one easy result, the *Taylor bound*, based on the use of a constant-strain test field. It says that $\mathcal{P}$ contains a certain set $\mathcal{T}$. We call $\mathcal{T}$ the *Taylor estimate*, because we believe it correctly estimates the dimension of $\mathcal{P}$ (though not necessarily its size) in most cases.

This paper uses geometrically linear rather than nonlinear elasticity. We do so as a matter of necessity, not choice. Some shape-memory materials recover as much as 10% strain, so the adequacy of a small-strain theory is unclear. There is no conceptual obstacle to the development of a similar theory using nonlinear elasticity: our microscopic, mesoscopic, and macroscopic energies all have natural analogues. However we do not know the nonlinear analogue of $\mathcal{S}$, because we lack a nonlinear version of Proposition 2.1.

2.1 Martensitic transformation

The source of the shape-memory effect is a martensitic phase transformation. We therefore begin with a brief discussion of this phenomenon. For the moment our attention is on single crystals, not polycrystals.

A material which undergoes a martensitic phase transformation has two distinct crystalline structures: the parent or *austenite* phase, preferred at high temperatures; and the product or *martensite* phase, preferred at low temperatures. The austenite lattice is more symmetric; in all known shape-memory materials it has cubic symmetry. The martensite lattice is less symmetric; it may have tetragonal, trigonal, orthorhombic, or monoclinic symmetry. We may discuss all these cases simultaneously by supposing that the symmetry group of the martensite has index k in that of the austenite.

Because of the change of symmetry, the martensite phase occurs in k different symmetry-related *variants*. They have the same crystalline structure, but bear different relations to the austenite lattice. There are 3 variants for a cubic-tetragonal transformation, 4 for cubic-trigonal, 6 for cubic-orthorhombic, and 12 for cubic-monoclinic. (Our use of the word “variant” is standard but not universal. Some authors use this term for the different

possible structures of austenite/twinned-martensite interfaces; that usage is different from ours. See [11, 74] for further discussion of this point.)

Martensitic transformation is coherent, i.e. it does not damage the crystalline lattice. It may therefore be modelled by means of elasticity, see e.g. [6, 7, 40, 72]. We use the austenite phase at the transition temperature as our reference configuration. The transformation from austenite to the i th variant of martensite has an associated transformation strain $e^{(i)}$, which can be determined from lattice parameters. Since the austenite lattice is our reference state, $e^{(i)}$ is also the stress-free strain of the i th variant of martensite. The stress-free strain of the austenite is $e^{(0)} = 0$.

Some materials undergo a sequence of martensitic transformations at different temperatures. For example, TiNi transforms from cubic to trigonal (the R-phase) at one temperature, then to monoclinic (the martensite phase) at a lower one. In such a case our reference configuration is the highest-temperature phase, and our “variants” are the thermodynamically stable phases at the temperature of deformation. This choice is appropriate for the modelling of recoverable strain, which is fundamentally a stress-free phenomenon. A study of stress-induced martensite would have to proceed differently, considering also the thermodynamically unstable phases which may be stabilized by stress.

2.2 The recoverable strain of a single crystal

Thus far we have identified each variant of martensite with an associated transformation strain. This is adequate at the smallest length scale, but the effects which interest us are more complicated. When a single crystal of austenite is transformed by cooling to martensite the result is usually not a single variant, but rather a mixture of martensite variants. The geometry of the mixture is far from arbitrary, but it is also far from determined. Moreover, the ability to form such mixtures lies at the foundation of shape-memory behavior. We therefore need a means of identifying and discussing stress-free mixtures of martensite variants.

The language of energy minimization provides a convenient tool. The main idea is that the stress-free states of the crystal minimize an elastic energy functional

$$\int_{\Omega} \varphi(e(u), \theta) dx . \quad (2.1)$$

Here Ω is the region occupied by the crystal; $e(u) = \frac{1}{2}(\nabla u + \nabla u^T)$ is the linear strain associated with displacement u ; and θ is the temperature, assumed constant and controlled.

We shall refer to the integrand φ as the *microscopic* elastic energy. It is nonconvex, with multiwell structure — one well for each phase or variant. If we treat the austenite and each variant of martensite as linearly elastic materials, then φ has the form

$$\varphi(e, \theta) = \min_{i=0,1,\dots,k} \left\{ \frac{1}{2}(e - e^{(i)}) \cdot A^{(i)}(e - e^{(i)}) + \varpi^{(i)}(\theta) \right\} , \quad (2.2)$$

in which we take the convention that $i = 0$ refers to austenite, and $i = 1, \dots, k$ to the martensite variants. The i th phase or variant has stress-free strain $e^{(i)}$ and Hooke’s law $A^{(i)}$; they may depend on θ , but that is not essential. The crucial temperature dependence is that of $\varpi^{(i)}$, the energy of the stress-free state: it controls the relative stability of the phases.

The variants are symmetry-related, so $\varpi^{(1)} = \dots = \varpi^{(k)}$. The transition temperature θ_0 is characterized by an exchange of stability between austenite and martensite: above θ_0 the austenite state is preferred, i.e. $\varpi^{(0)} < \varpi^{(1)}$; below θ_0 the martensite state is preferred, i.e. $\varpi^{(1)} < \varpi^{(0)}$.

The connection between energy minimization and recoverable strain is provided by Hypothesis 1. According to it, the recoverable strains are those achieved by stress-free mixtures of martensite variants *at the temperature of deformation*. Therefore we only have to consider behavior at a fixed temperature θ_1 , well below the transition temperature. We claim that the stress-free mixtures of martensite variants at temperature θ_1 are in one-to-one correspondence with the minimizers of (2.1). Indeed, viewed as a function of strain the microscopic energy $\varphi(e, \theta_1)$ is minimized precisely at $e^{(1)}, \dots, e^{(k)}$. The minimum value of (2.1) is therefore $\varpi^{(1)}|\Omega|$, and it is achieved precisely when $e(u) \in \{e^{(1)}, \dots, e^{(k)}\}$ a.e. in Ω . We identify such deformations with stress-free mixtures, viewing the set where $e(u) = e^{(i)}$ as being occupied by the i th variant.

The preceding discussion applies to elastic energy minimizers. Since the integrand φ is nonconvex, it is also important to consider minimizing sequences, i.e. sequences $\{u_n\}$ such that $\int_{\Omega} \varphi(e(u_n), \theta_1) dx \rightarrow \varpi^1|\Omega|$ as $n \rightarrow \infty$. Such a sequence does not, in general, converge to an energy minimizer. But it nevertheless determines an “essentially stress-free mixture” of martensite variants (technically: a minimizing Young measure), see e.g. [6, 7, 43]. The reason is that if $\int_{\Omega} \varphi(e(u), \theta_1) dx \approx \varpi^1|\Omega|$ then $e(u)(x)$ must be close to one of the stress-free strains $e^{(1)}, \dots, e^{(k)}$ except on a subset of Ω of small measure. We will not distinguish in what follows between minimizers and minimizing sequences. In other words, we shall assume that the recoverable deformations include essentially stress-free mixtures of martensite variants as well as exactly stress-free mixtures.

The arguments just presented do not use the full form of φ as defined by (2.2). In truth, all we shall really use in this paper are the following three properties of the microscopic elastic energy below the transition temperature: (a) it is minimized precisely at the stress-free strains of the martensite variants $e^{(1)}, \dots, e^{(k)}$; (b) it departs from each $e^{(i)}$ quadratically; and (c) it has quadratic growth at infinity. Its dependence on temperature is irrelevant, since we only consider the behavior at a fixed temperature θ_1 . The specific form of the Hooke’s laws $A^{(i)}$ in (2.2) is also irrelevant; all we use is their positive definiteness. And the austenite well plays no role, since its energy is higher than that of the martensite. Such details would be important for modelling other phenomena such as pseudoelastic behavior and stress-induced martensite. But according to Hypothesis 1 they are unimportant for the modelling of recoverable strain. As a practical matter, we may therefore work with the simpler microscopic energy

$$\varphi(e) = \min_{i=1, \dots, k} \left\{ \frac{1}{2} |e - e^{(i)}|^2 \right\} \quad (2.3)$$

rather than (2.2).

Hypothesis 1 links recoverable strain with stress-free mixtures of martensite variants. We have connected these in turn to elastic energy minimization. But we have yet to address the main issue: which overall strains are recoverable? This question involves large-scale rather than microscopic behavior, i.e. it concerns the functional $\int \varphi(e(u)) dx$ rather than its integrand $\varphi(e)$. Hence the answer involves a new object, the *mesoscopic* elastic energy $\hat{\varphi}$.

Physically, $\hat{\varphi}(e)$ is the average stored energy when the average strain is e . Mathematically, it is defined by

$$\hat{\varphi}(e) = \min_{u=e \cdot x \text{ at } \partial\Omega} \int_{\Omega} \varphi(e(u)) \, dx , \quad (2.4)$$

in which the slashed integral denotes spatial averaging:

$$\int_{\Omega} f \, dx = \frac{1}{|\Omega|} \int_{\Omega} f \, dx . \quad (2.5)$$

We note the elementary but important fact that the minimum value of $\hat{\varphi}$ is the same as that of φ .

The mesoscopic energy $\hat{\varphi}$ is known as the *relaxation* of φ . There is an extensive literature on relaxation. Our favorite expository treatment is Section 2 of [46]; further details and references can be found in [1, 19, 20, 43]. The theory contains many results justifying our viewpoint that $\hat{\varphi}$ represents the overall behavior of a system with microscopic energy φ . In particular, the definition (2.4) does not really depend on the choice of domain Ω ; there are equivalent definitions using periodic rather than affine boundary conditions, or Young measures rather than spatial averages; minimizing $\int_{\Omega} \varphi(e(u)) \, dx$ with specified boundary conditions is equivalent to minimizing the relaxed problem $\int_{\Omega} \hat{\varphi}(e(u)) \, dx$ with the same boundary conditions; and the relaxed problem is lower semicontinuous.

We are now able to give Hypothesis 1 a mathematically precise formulation.

Hypothesis 1 revisited. *The recoverable strains for a single crystal are the minimizers of its mesoscopic energy $\hat{\varphi}$.*

In summary: to predict the recoverable strains of a shape-memory single crystal, we start from the stress-free strains of its martensite variants, $e^{(1)}, \dots, e^{(k)}$. We first form the (simplified) microscopic elastic energy φ , defined by (2.3). Then we pass to its relaxation, the mesoscopic energy $\hat{\varphi}$ defined by (2.4). Finally we look at the set where $\hat{\varphi}$ achieves its minimum value:

$$\mathcal{S} = \{e : \hat{\varphi}(e) = 0\} . \quad (2.6)$$

According to our model, the elements of $\mathcal{S}$ are the overall strains which are recoverable for this crystal.

To make use of this model, we must be able to evaluate the set $\mathcal{S}$. Viewed as a general mathematical problem — starting from k arbitrarily chosen symmetric matrices $e^{(1)}, \dots, e^{(k)}$ — the evaluation of $\mathcal{S}$ is quite subtle; see [10] for some recent developments. But the goal of this paper is more specific, namely the modelling of recoverable strain. Therefore the matrices $e^{(1)}, \dots, e^{(k)}$ are not at all arbitrary; rather, they are determined by the symmetry of the transformation. For most types of phase transformations actually observed in shape-memory materials they lie in a class we know how to handle. Specifically, the stress-free strains associated with a cubic-tetragonal, cubic-trigonal, or cubic-orthorhombic transformation fall within the scope of the following result from [9]:

Proposition 2.1 *Let us call two linear strains f and g “elastically compatible” if they satisfy $f - g = \frac{1}{2}(a \otimes n + n \otimes a)$ for some vectors a and n . Suppose the stress-free strains $e^{(1)}, \dots, e^{(k)}$ are pairwise elastically compatible. Then the associated set $\mathcal{S}$, defined by (2.6), is simply their convex hull.*

The cubic–monoclinic case is different: its stress–free strains are not pairwise compatible, and the associated set $\mathcal{S}$ is *not* the convex hull. We shall prove this in Section 3.6.

The number of variants turns out to be crucially important. To see why, note that the convexification of φ is always a lower bound for $\hat{\varphi}$. Therefore $\mathcal{S}$ is always *contained in* the convex hull of $\{e^{(i)}\}_{i=1}^k$. Since the martensite variants are symmetry related, they all have the same trace, i.e. $\text{tr } e^{(1)} = \dots = \text{tr } e^{(k)}$. Thus $\mathcal{S}$ lies in a $(k - 1)$ -dimensional subset of the 5-dimensional “deviatoric hyperplane” $\text{tr } e = \text{tr } e^{(i)}$. When $k < 6$, e.g. when the phase transformation is cubic–tetragonal or cubic–trigonal, $\mathcal{S}$ is *dimensionally deficient*: its dimension is strictly smaller than that of the deviatoric hyperplane. When $k \geq 6$, on the other hand, counting suggests that $\mathcal{S}$ should be a set with interior in the deviatoric hyperplane. We shall confirm this conclusion in Section 3 for the cases of a cubic–orthorhombic or cubic–monoclinic phase transformation.

Another important fact is that when the austenite is cubic and the martensite is tetragonal, trigonal, orthorhombic, or monoclinic, $\mathcal{S}$ contains the isotropic strain

$$\mathcal{I} = \frac{1}{3} \text{tr } e^{(i)} I . \quad (2.7)$$

This follows from the characterizations of $\mathcal{S}$ given in Section 3. It is linked to the phenomenon of self–accommodation [8].

The availability of Proposition 2.1 is the main reason we work with geometrically linear rather than nonlinear elasticity. The central ideas of this section extend straightforwardly to the geometrically nonlinear context, see e.g. [7, 28, 18]. However, in the geometrically nonlinear setting we know rather little about the set where $\hat{\varphi} = 0$. It has only been characterized for the special case of *two* elastically compatible variants [7].

It is instructive to compare our approach with that of Saburi and Nenno [74]. To estimate the recoverable deformations of a single crystal, they determine, for each direction in deformation space, the variant with the largest transformation strain in that direction. This is done using a geometrically nonlinear approach closer to that of [6, 7] than to the one adopted here. In essence, this calculation determines the *extreme points* of the nonlinear analogue of $\mathcal{S}$. It certainly provides an estimate for the recoverable deformations: they must lie within the convex hull of the extreme points. However, this calculation does not fully determine the set of recoverable deformations, since we expect this set to be nonconvex. (In the geometrically nonlinear setting it is nonconvex even for the case of two variants [7].)

2.3 The recoverable strain of a polycrystal

A polycrystal is an assemblage of grains, each composed of the same shape–memory material in a different orientation. We assume there are no residual stresses, so the grains are all stress–free when the polycrystal is in its austenite state. We also assume the grains are perfectly bonded, so the elastic displacement is continuous.

To describe a polycrystal we must specify its *texture*, i.e. the shapes of the grains and their orientations. The texture can be represented by a rotation–valued function $R(x)$, constant on each grain, giving the crystalline orientation relative to a fixed, reference crystal. The function $R(x)$ is discontinuous at grain boundaries, so it implicitly determines the shape

of each grain as well as its orientation. If $e^{(1)}, \dots, e^{(k)}$ are the stress-free strains of the reference crystal, then a grain with orientation R has stress-free strains $Re^{(1)}R^T, \dots, Re^{(k)}R^T$.

We began our discussion of single crystals by drawing a correspondence between minimizers of the functional (2.1) and stress-free mixtures of martensite variants. The same argument works for polycrystals, using

$$\int_{\Omega} \varphi(R^T(x)e(u)R(x)) dx \quad (2.8)$$

in place of (2.1). In particular, minimizers of (2.8) determine stress-free configurations of the polycrystal with texture $R(x)$.

Consider now the mesoscopic analogue of (2.8):

$$\int_{\Omega} \hat{\varphi}(R^T(x)e(u)R(x)) dx . \quad (2.9)$$

The theory of relaxation says that (2.8) and (2.9) are in a certain sense equivalent: minimizing sequences for the former converge weakly to minimizers of the latter, and minimizers of the latter give rise to minimizing sequences for the former [1]. We do not wish to distinguish between minimizers and minimizing sequences. Hence for the purpose of identifying stress-free configurations we may use the relaxed problem (2.9) instead of (2.8).

Let us dwell a bit on the relation between (2.8) and (2.9). The essential difference is the interpretation of the strain field. In (2.8), $e(u)$ represents the microscopic strain, which must take values $R(x)e^{(1)}R^T(x), \dots, R(x)e^{(k)}R^T(x)$ to describe a stress-free configuration of the polycrystal. In (2.9), by contrast, $e(u)$ represents the mesoscopic strain — the average (technically: weak limit) of a spatially oscillatory strain field associated with a mixture of martensite variants. Because the mesoscopic strain is an average quantity, it has more freedom than its microscopic analogue: the integrand of (2.9) is minimized whenever $R^T(x)e(u)R(x) \in \mathcal{S}$.

Hypothesis 2 makes reference to “locally varying strain fields which can be accommodated within each grain by rearrangement of martensite variants.” We now have a concise description of such fields: they are the (mesoscopic) strains satisfying $R^T(x)e(u)R(x) \in \mathcal{S}$ almost everywhere. Equivalently, within each grain $e(u)$ must remain in the set of *recoverable strains for that grain*,

$$\mathcal{S}(x) = R(x)\mathcal{S}R^T(x) . \quad (2.10)$$

We remark that though $R(x)$ is piecewise constant, $e(u)$ need not be. It has only to remain in the set $\mathcal{S}(x)$. This reflects the fact that we do not expect the microstructure of each grain to be uniform. Rather, the mixture of martensite variants may differ from point to point, due to the influence of neighboring grains.

As presented, our passage from (2.8) to (2.9) depends on the absence of a surface energy or strain gradient term. With more effort, however, one can actually include surface energy and still arrive at (2.9), provided that the surface energy density is small compared to the grain size [29]. The essential physical hypothesis is that the martensite variants can form mixtures on a length scale much smaller than the grain size.

We have linked recoverable strain in polycrystals to mesoscopic strain fields minimizing (2.9), or equivalently to strains such that $e(u) \in \mathcal{S}(x)$ for every x . Now we address the

central question: which overall strains are recoverable for a polycrystal? This is a problem of *nonlinear homogenization*. The functional (2.9) can be viewed as describing a nonlinear polycrystal with reference energy $\hat{\varphi}$. Our question concerns its behavior on a length scale much larger than the grain size. The answer therefore involves the effective or *macroscopic* energy $\bar{\varphi}$, see e.g. [20, 37, 51, 73]. We shall discuss the definition of $\bar{\varphi}$ presently. But roughly speaking, $\bar{\varphi}(e)$ is the average stored energy when the average strain is e . The passage from $\hat{\varphi}$ to $\bar{\varphi}$ is formally similar to that from φ to $\hat{\varphi}$, except that the averaging is done on a different length scale. The passage from φ to $\hat{\varphi}$ is associated with the multiwell character of φ , and it involves averaging over mixtures of martensite variants on a subgrain length scale. The passage from $\hat{\varphi}$ to $\bar{\varphi}$, by contrast, is associated with the polycrystalline texture, and it involves averaging over many grains.

We thus arrive at our mathematically precise version of Hypothesis 2.

Hypothesis 2 revisited. *The recoverable strains for a polycrystal are the minimizers of its macroscopic energy $\bar{\varphi}$.*

In summary: to predict the recoverable strains for a shape-memory polycrystal, we start from the mesoscopic energy of the reference crystal, $\hat{\varphi}$, discussed in Section 2.2. It has minimum value 0, and this minimum is degenerate since $\hat{\varphi} = 0$ on $\mathcal{S}$. To incorporate the effects of texture, we use nonlinear homogenization to pass to the macroscopic energy $\bar{\varphi}$. Then we look at the set

$$\mathcal{P} = \{e : \bar{\varphi}(e) = 0\} . \quad (2.11)$$

Its elements are the macroscopic strains consistent with the pointwise constraint $e(u)(x) \in \mathcal{S}(x)$. Put differently, they are the macroscopic strains which can be produced by microscopic mixtures of stress-free variants. According to our model, these are the recoverable strains for the polycrystal.

Actually, we are interested in more than just the set $\mathcal{P}$. We are also interested in the set where $\bar{\varphi}$ is small, say

$$\mathcal{P}_\delta = \{e : \bar{\varphi}(e) \leq \delta\} \quad (2.12)$$

with δ close to 0. These are the macroscopic strains consistent with microscopic mixtures of *nearly* stress-free variants. Notice that $\mathcal{P}_\delta$ may be considerably larger than $\mathcal{P}$ if $\bar{\varphi}$ is degenerate near $\mathcal{P}$, for example if $\bar{\varphi}(e) \sim [\text{dist}(e, \mathcal{P})]^3$ as e departs from $\mathcal{P}$. One might argue that Hypothesis 2 should not be taken too literally, and the true set of recoverable strains should resemble $\mathcal{P}_\delta$ more than $\mathcal{P}$. We shall discuss this idea in Section 6.1.

In passing from Hypothesis 2 to (2.11), we have implicitly assumed that $\bar{\varphi}$ has minimum value 0. This is a consequence of (2.7). The isotropic tensor $\mathcal{I}$ is in $\mathcal{S}$, so $\hat{\varphi}(R^T(x)\mathcal{I}R(x)) = \hat{\varphi}(\mathcal{I}) = 0$ for every x . It follows that $\bar{\varphi}(\mathcal{I}) = 0$.

It remains to discuss the definition of $\bar{\varphi}$. For general polycrystals — neither random nor periodic — a convenient definition is based on affine boundary conditions:

$$\bar{\varphi}(\bar{e}) = \min_{u=\bar{e} \cdot x \text{ at } \partial\Omega} \int_{\Omega} \hat{\varphi}(R^T(x)e(u)R(x)) dx . \quad (2.13)$$

This has the advantage of being easy to use, however the resulting $\bar{\varphi}$ depends on the details of the domain Ω and the texture $R(x)$. One might say that it describes a “specific sample” of polycrystal.

When the texture $R(x)$ is spatially periodic and $\hat{\varphi}$ is convex, a better definition is

$$\bar{\varphi}(\bar{\epsilon}) = \min_{f^{e(u)=\bar{\epsilon}}} \int \hat{\varphi}(R^T(x)e(u)R(x)) dx, \quad (2.14)$$

in which the averages are over the period cell, and the minimization is over spatially periodic strain fields. When $R(x)$ is random rather than periodic, there is an analogous definition using ensemble averaging. The advantage of (2.14) is that it does not depend on the shape of the sample. In other words, it describes the polycrystal as a material in its own right.

The two definitions (2.13) and (2.14) are consistent in the following sense. Let $R(\cdot)$ be a spatially periodic, rotation-valued function, and let Ω be a given domain. For any $\epsilon > 0$, we can consider the polycrystal with shape Ω and texture $R(x/\epsilon)$. Let $\bar{\varphi}_\epsilon$ be its macroscopic energy defined via (2.13). Then

$$\lim_{\epsilon \rightarrow 0} \bar{\varphi}_\epsilon \text{ is the macroscopic energy given by (2.14),} \quad (2.15)$$

see e.g. [51]. An analogous assertion holds in the random case too, see e.g. [35].

This result has the following important corollary: for proving texture-independent bounds on $\bar{\varphi}$, it is sufficient to work with (2.13). There is no need to argue separately for (2.14). Once a texture-independent bound has been proved using affine boundary conditions, it extends to the periodic case automatically via (2.15).

The definitions (2.13) and (2.14) are the simplest ones, and they are sufficient for our purposes. There is another, more general approach based on the theory of Γ -convergence, see e.g. [20, 37]. It defines a polycrystal through a *sequence* of textures, which need not be random or periodic or have any other special structure. The definition of $\bar{\varphi}$ is analogous to (2.14), but with spatial averages replaced by weak limits. This viewpoint is superior to the periodic and random theories, since it gives a sample-independent effective energy without any structural hypothesis on the texture. For the purposes of the present paper, however, there is no need to address the definition via Γ -convergence separately. Bounds proved using (2.13) extend automatically to effective energies defined via Γ -convergence as well, by an argument similar to (2.15). (Alternatively, our proofs can easily be reformulated in the language of Γ -convergence.)

The mesoscopic energy $\hat{\varphi}$ is always quasiconvex, but it need not be convex. The analysis of effective behavior becomes more subtle when the reference energy is quasiconvex but not convex, see e.g. [33]. This complication can be ignored for tetragonal, trigonal, or orthorhombic martensite, since in those cases $\mathcal{S}$ is also the zero-set of the convexification of φ . It might be important for monoclinic martensite, since in that case $\mathcal{S}$ is smaller than the zero-set of the convexification of φ . However the difference between quasiconvexity and convexity will play no role in the present work.

2.4 The Taylor bound and the Taylor estimate

Our task is now clear. To assess the recoverable strain of a shape-memory polycrystal we must consider the associated macroscopic energy $\bar{\varphi}$, and estimate the set $\mathcal{P}$ where $\bar{\varphi} = 0$.

This task might at first appear hopeless. We certainly cannot expect a formula for $\bar{\varphi}$, since this would amount to solving the nonlinear homogenization problem (2.13) analytically. But our goal is more limited: we are mainly interested in the set $\mathcal{P}$, not the whole

function $\bar{\varphi}$. We shall argue that while $\mathcal{P}$ is in general texture-dependent, its dimension is more or less universal.

To explain, let's start with the elementary but fundamental *Taylor bound*, based on the use of a constant-strain test field:

Proposition 2.2 *The set $\mathcal{P}$ of recoverable strains contains at least the set*

$$\mathcal{T} = \bigcap_{x \in \Omega} \mathcal{S}(x) = \{e : R^T(x)eR(x) \in \mathcal{S} \text{ for each } x \in \Omega\} , \quad (2.16)$$

Proof. If $e \in \mathcal{T}$ then the constant-strain test field $u = e \cdot x$ has $\hat{\varphi}(R^T(x)eR(x)) \equiv 0$. Therefore $\bar{\varphi}(e) = 0$ from the definition (2.13). $\square$

We call this the “Taylor bound” to highlight the analogy with Taylor’s uniform-strain hypothesis from polycrystal plasticity [13, 83].

Proposition 2.2 says only that $\mathcal{P} \supset \mathcal{T}$. It is silent concerning how much bigger $\mathcal{P}$ might be. We believe, however, that $\mathcal{T}$ is usually a good indicator for $\mathcal{P}$. More precisely, we conjecture that for polycrystals with sufficient symmetry, $\mathcal{P}$ has the *same dimension* as $\mathcal{T}$. We therefore like to call $\mathcal{T}$ the *Taylor estimate*.

The set $\mathcal{T}$ is never empty: it always contains at least the strain $\mathcal{I}$, by (2.7). We say the Taylor bound is *trivial* if $\mathcal{T}$ consists of just this one point. For such polycrystals Proposition 2.2 says only that $\mathcal{I} \in \mathcal{P}$, but our conjecture says that $\mathcal{P} = \{\mathcal{I}\}$. In other words, such polycrystals should have no recoverable strain.

Sections 4 and 5 are largely devoted to justifying our conjecture. Here is a summary of the results in its favor.

- We consider two cases in which the Taylor model is trivial, and show that for polycrystals with sufficient symmetry $\mathcal{P}$ is also trivial. We do this for the “scalar two-variant material” (Section 4.3), and for the “2D diagonal, trace-free material” (Section 5.3).
- We consider one case when the Taylor estimate is one dimensional, and show that for polycrystals with sufficient symmetry $\mathcal{P}$ is also one dimensional. This is done for “cubic-tetragonal polycrystals with $\langle 001 \rangle$ texture” (Section 5.4).
- We consider one case when the Taylor estimate is full-dimensional, and show that the set $\mathcal{P}$ can easily be larger than $\mathcal{T}$. We also give an example, however, in which $\mathcal{P}$ is equal to $\mathcal{T}$. This is done for the “scalar four-variant material” (Section 4.5).

There is also one result running contrary. For our “2D diagonal elastic material” the Taylor estimate is one-dimensional, however there are polycrystals, even isotropic ones, for which $\mathcal{P}$ is three-dimensional (Section 5.2). Thus our conjecture is false in this case. In particular, it cannot be taken as a universally valid assertion about nonlinear homogenization. Rather, it must reflect some (as yet undetermined) feature of the set $\mathcal{S}$.

Our conjecture provides the essential link between the symmetry of the phase transition and the recoverable strains of polycrystals. When there are fewer than 6 variants (tetragonal or trigonal martensite) the set $\mathcal{S}$ is dimensionally deficient, and $\mathcal{T}$ is trivial. We conjecture that $\mathcal{P}$ is also trivial. Therefore such materials lose their shape-memory behavior when formed into unstructured polycrystals. When there are 6 or more variants (orthorhombic or

monoclinic martensite) the set $\mathcal{S}$ contains a neighborhood of $\mathcal{I}$ in the deviatoric hyperplane $\text{tr } e = \text{constant}$, so the same is true of $\mathcal{T}$ and $\mathcal{P}$. Polycrystals made from such materials can recover some strain in any deviatoric direction. The maximum recoverable strain is unclear, but we expect it to exceed the conservative estimate $\mathcal{T}$.

We dwell for a moment on the physical meaning of the Taylor estimate. It describes the strains which can be accommodated *without making use of cooperative effects* between grains. Indeed, if the constant strain $e(u) = \bar{e}$ suffices to achieve $\bar{\varphi}(\bar{e}) = 0$, then there is no need for any grain to take into account what its neighbor is doing. Rather, each grain may simply adjust its own microstructure to be consistent with mesoscopic strain $\bar{e}$.

Let us explain heuristically why $\mathcal{P}$ should be trivial if $\mathcal{T}$ is. We start with the observation that for $\mathcal{T}$ to be trivial, $\mathcal{S}$ must be dimensionally deficient, i.e. it must not span the entire deviatoric strain space. So the constraint $e(x) \in \mathcal{S}(x)$ restricts the mesoscopic strain to lie in a lower dimensional set, varying from grain to grain. This is a severe algebraic restriction. We expect it to be inconsistent with the linear differential constraints $e_{ij,kl} + e_{kl,ij} = e_{ik,jl} + e_{jl,ik}$ which must be satisfied if $e(x)$ is to come from a deformation.

The opposite extreme occurs when the Taylor estimate is full-dimensional, i.e. $\mathcal{T}$ contains a neighborhood of $\mathcal{I}$ in the hyperplane $\text{tr } e = \text{constant}$. In this case $\mathcal{T}$ and $\mathcal{P}$ will have the same dimension, but we expect $\mathcal{P}$ to be larger in most cases. Indeed, when $\mathcal{T}$ is full-dimensional the constraint $e \in \mathcal{S}(x)$ permits deviatoric strains in a neighborhood of $\mathcal{I}$ in each grain. If $\bar{e} \in \mathcal{T}$ then the constant strain $e(x) \equiv \bar{e}$ will be at the boundary of $\mathcal{S}(x)$ only in selected grains with special orientations. So this restriction is only active on a sparse set. We therefore expect considerable freedom in finding nonconstant, kinematically admissible perturbations of $\bar{e}$.

The Taylor estimate depends on texture, but the dependence is rather weak. It takes into account the list of orientations present in the polycrystal, but not their volume fractions. In some cases further information may be available, for example the two-point statistics of the orientation distribution. The question of how to use such information is difficult and largely open. Our main technique, the translation method, seems not to have room for such extra information.

2.5 Universal bounds and sums of energies

Much of Sections 4 and 5 are devoted to “universal results,” i.e. statements valid for all polycrystals. This might seem somewhat strange. We expect polycrystals to be different from single crystals. But a single crystal is a trivial example of a polycrystal. So how can a universal statement be of any value?

The answer lies in considering *sums of energies*. For example, in analyzing the scalar, two-variant material we shall show that

$$\bar{\varphi}(f) + \bar{\varphi}(f^\perp) \geq C|f|^4 \quad (2.17)$$

when f is close to 0. (For this model problem $\bar{\varphi}$ is a function of vectors in $\mathbb{R}^2$; $f^\perp$ is the rotation of f by 90 degrees.) The estimate (2.17) is valid for both single crystals and polycrystals, without any hypothesis on the texture. But if $\bar{\varphi}(f) = \bar{\varphi}(f^\perp)$ then (2.17) becomes $2\bar{\varphi}(f) \geq C|f|^4$. This shows that for polycrystals with square symmetry, $\bar{\varphi} = 0$ only at $f = 0$.

In short: rather than focus on polycrystals with sufficient symmetry, we may look instead for universal bounds coupling the effective behavior at several symmetry-related macroscopic fields. This idea is not new; it is standard procedure when using the translation method to bound the effective moduli of linear composites, see e.g. [4, 5, 30, 54, 82].

3 Implications for shape-memory behavior

We have argued that energy minimization can predict the shape-memory behavior of polycrystals. We have furthermore conjectured that the Taylor estimate $\mathcal{T}$ provides a good indicator for the set of recoverable strains $\mathcal{P}$ predicted by energy minimization.

This section evaluates the Taylor estimate, and compares its predictions with the actual behavior of selected materials. For alloys with tetragonal or trigonal martensite the Taylor estimate is trivial; as expected, such materials make poor shape-memory polycrystals. For alloys with orthorhombic or monoclinic martensite the Taylor estimate is nontrivial; as expected, such materials retain some shape-memory behavior in polycrystalline form. There is, however, an important distinction which lies beyond the scope of our approach: when the Taylor estimate is trivial our model predicts damage to the crystalline lattice, but it does not differentiate between ductile failure and brittle fracture.

An extensive discussion of the Taylor estimate is given in [11], along with a survey of the experimental literature. The goal of this section is different and more limited. We mainly aim to demonstrate our model's validity, and its shortcomings. Therefore we shall be brief, discussing only a few representative materials and omitting many details.

3.1 Some representative materials

Here is some information about the behavior of four particular alloys:

Ni-37Al (at.%) This material undergoes a cubic-tetragonal transformation. Enami *et al.* [23] report that single crystals recover tensile strains ranging from 0 to 13% depending on orientation. Polycrystals are very poor shape-memory materials, being greatly susceptible to intergranular fracture in tension. With specially-designed specimens and a special bending device, Potapov *et al.* [71] obtained partial recovery of 0.7% bending strain; larger bending strains caused fracture. In compression, Kim and Wayman [42] report recovery of only about 0.2% strain.

Fe-27Ni-0.8C (wt.%) This material undergoes a cubic-tetragonal transformation. Kajiwara and Kikuchi [38] report that polycrystalline cold rolled plates do not fully recover their strain on heating. However they do recover part of the strain: roughly 75–95% of a 1–2% bending strain, and about 50% of a 5–7% tensile strain.

Cu-14Al-4Ni (wt.%) This material undergoes both cubic-orthorhombic and cubic-monoclinic transformations, depending on experimental conditions. Single crystals recover tensile strains ranging from 2 to 9% depending on orientation. Eucken and Hirsch [24] report that polycrystalline ribbons with uncontrolled texture recover only about 2.5% tensile strain, but specially textured polycrystalline ribbons fully recover about 6.5% tensile strain.

Ti-50.6Ni (at.%) This material is widely used commercially. It undergoes a cubic–monoclinic transformation. Single crystals recover tensile strains ranging from 3 to 10% depending on orientation [56, 74, 76]. Ling and Kaplow report that drawn polycrystalline wires fully recover from 4 to 8% strain depending on deformation mode, processing and manufacturer [48, 49]. Similar observations have been published by others including [55, 68, 75, 76].

3.2 Implications of the Taylor estimate

All known shape–memory alloys have cubic symmetry in the austenite phase. Most of them have tetragonal, trigonal, orthorhombic, or monoclinic symmetry in the martensite phase. We therefore confine our attention to materials which undergo a cubic–tetragonal, cubic–trigonal, cubic–orthorhombic, or cubic–monoclinic transformation. The analysis of [11], summarized in part in Sections 3.3–3.6, shows that:

- (1) The Taylor estimate is trivial for polycrystals with general texture when the martensite is tetragonal or trigonal.
- (2) The Taylor estimate is never trivial when the martensite is orthorhombic or monoclinic.
- (3) The Taylor estimate can be nontrivial when the martensite is tetragonal or trigonal, for polycrystals with special texture.
- (4) When the martensite is orthorhombic or monoclinic, the Taylor estimate can be significantly larger for polycrystals with special texture than it is for unstructured polycrystals.

These predictions are consistent with the experimental data cited above. The materials with a trivial Taylor estimate (NiAl and FeNiC) lose most or all of their shape–memory behavior when taken in polycrystalline form, while those with a nontrivial Taylor estimate (CuAlNi and TiNi) retain their shape–memory behavior in polycrystalline form. And polycrystals with special textures can have larger recoverable strains than unstructured polycrystals (CuAlNi). Our model does not, however, explain the partial recovery observed in FeNiC, nor does it explain why NiAl and FeNiC have very different failure modes. It also falls short of explaining why TiNi is such an exceptionally good polycrystalline shape–memory material.

The remainder of this section elaborates upon the conclusions (1)–(4) listed above. All calculations are done in an orthonormal basis, with axes parallel to the sides of the cubic unit cell of the austenite reference crystal.

3.3 Tetragonal martensite

There are 3 variants of martensite in this case. The stress–free strains are obtained from

$$\begin{pmatrix} \alpha & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & \beta \end{pmatrix}$$

by permuting the coordinates. The variants are pairwise elastically compatible, i.e. the hypothesis of Proposition 2.1 is valid in this case. So $\mathcal{S}$ is the convex hull of the stress-free strains. Some calculation gives

$$\mathcal{S} = \left\{ e \left\| \begin{array}{l} e_{12} = e_{13} = e_{23} = 0, \\ e_{11} + e_{22} + e_{33} = 2\alpha + \beta, \\ \min\{\alpha, \beta\} \leq e_{11}, e_{22}, e_{33} \leq \max\{\alpha, \beta\} \end{array} \right. \right\}. \quad (3.1)$$

This is a two dimensional set in the five dimensional space of “deviatoric” strains (those satisfying $\text{tr } e = 2\alpha + \beta$). Therefore the Taylor estimate is trivial for polycrystals with general texture. In fact, the Taylor estimate is trivial unless the orientation function satisfies $R(x)e = e$ for every x , with $e = (1, 0, 0)$ or $(0, 1, 0)$ or $(0, 0, 1)$.

Let us consider in more detail the exceptional case when the Taylor estimate is nontrivial. We may suppose without loss of generality that $e = (0, 0, 1)$, so each $R(x)$ is a rotation about the x_3 axis. We say such a polycrystal has $\langle 001 \rangle$ texture. Some calculation shows that for such polycrystals, the Taylor estimate consists of uniaxial extension or contraction along $(0, 0, 1)$ accompanied by uniform lateral compression or extension:

$$\mathcal{T} = \left\{ e \left\| \begin{array}{l} e_{12} = e_{13} = e_{23} = 0, \\ e_{11} = e_{22}, \\ e_{11} + e_{22} + e_{33} = 2\alpha + \beta, \\ \min\{\alpha, \beta\} \leq e_{11}, e_{22}, e_{33} \leq \max\{\alpha, \beta\} \end{array} \right. \right\}.$$

Our conjectured relation between $\mathcal{T}$ and $\mathcal{P}$ suggests that $\mathcal{P}$ should be one-dimensional for polycrystals with $\langle 001 \rangle$ texture, and $\mathcal{P}$ should be trivial for polycrystals with general texture, assuming sufficient symmetry in each case. We shall prove the first statement (but not the second) in Section 5.4.

3.4 Trigonal martensite

There are 4 variants of martensite in this case. The stress-free strains are obtained from

$$\begin{pmatrix} \beta & \alpha & \alpha \\ \alpha & \beta & \alpha \\ \alpha & \alpha & \beta \end{pmatrix}$$

by replacing four of the six α 's with $-\alpha$ and permuting the basis. (The four transformation strains are listed explicitly in [11].)

Concerning the Taylor estimate, the situation is similar to the tetragonal case. The transformation strains are pairwise elastically compatible, so $\mathcal{S}$ is their convex hull. It is a three-dimensional set in the five-dimensional space of deviatoric strains. Therefore $\mathcal{T}$ is trivial for polycrystals with general texture. However one can get a nontrivial Taylor estimate by imposing some restrictions on the texture.

3.5 Orthorhombic martensite

There are 6 variants of martensite in this case. There are in principle two different types of cubic to orthorhombic transformation. In the first type the stress-free strains are obtained

from

$$\begin{pmatrix} \alpha & 0 & 0 \\ 0 & \beta & 0 \\ 0 & 0 & \gamma \end{pmatrix}$$

by permuting the coordinates. We are not aware of any material that undergoes this type of transformation. Therefore we shall not consider it further.

In the second type of cubic–orthorhombic transformation the stress–free strains are obtained from

$$\begin{pmatrix} \alpha & \delta & 0 \\ \delta & \alpha & 0 \\ 0 & 0 & \beta \end{pmatrix}$$

by replacing δ with $-\delta$ and permuting the coordinates. The $\beta_1 \rightarrow \gamma'_1$ transformation in CuAlNi is of this type. The stress–free strains are pairwise compatible, so $\mathcal{S}$ is their convex hull. Some calculation gives

$$\mathcal{S} = \left\{ e \left\| \begin{array}{l} e_{11} + e_{22} + e_{33} = 2\alpha + \beta, \\ \min\{\alpha, \beta\} \leq e_{11}, e_{22}, e_{33} \leq \max\{\alpha, \beta\}, \\ -\left(\frac{e_{ii}-\alpha}{\beta-\alpha}\right)\delta \leq e_{jk} \leq \left(\frac{e_{ii}-\alpha}{\beta-\alpha}\right)\delta \quad \text{for each } \{ijk\} = \text{perm}\{123\} \end{array} \right. \right\},$$

in which $\text{perm}\{123\}$ denotes an arbitrary permutation of $\{1, 2, 3\}$. This set spans the deviatoric subspace, so the Taylor estimate is always nontrivial. For polycrystals in which all orientations occur we get

$$\mathcal{T} = \left\{ e \left\| \begin{array}{l} e \text{ has eigenvalues } \lambda_1, \lambda_2, \lambda_3 \text{ which satisfy} \\ \lambda_1 + \lambda_2 + \lambda_3 = 2\alpha + \beta, \\ \min\{\alpha, \beta\} \leq \lambda_1, \lambda_2, \lambda_3 \leq \max\{\alpha, \beta\}, \\ \frac{\lambda_i - \lambda_j}{2} \leq \frac{\lambda_k - \alpha}{\beta - \alpha} \delta \quad \text{for all } \{ijk\} = \text{perm}\{123\} \end{array} \right. \right\}. \quad (3.2)$$

One can show that this set contains a ball of radius roughly $\frac{1}{2} \min\{\frac{|\alpha-\beta|}{2}, \delta\}$ around $\mathcal{I}$ in the deviatoric subspace.

For textured polycrystals — specifically those which use only selected orientations — the Taylor estimate can be significantly larger. See [11] for an analysis of textured ribbons of the type studied by Eucken and Hirsch in [24].

3.6 Monoclinic martensite

There are 12 variants of martensite in this case. There are two different types of cubic–monoclinic transformation; we address them separately.

MONOCLINIC-I

The transformation strains of the 12 variants of martensite are shown in Table 1. The transformation in TiNi is of this type. The stress–free strains are *not* pairwise compatible in this case, i.e. the hypothesis of Proposition 2.1 is not satisfied. Indeed, unless the lattice parameters take very special values we have $\det(e^{(1)} - e^{(8)}) \neq 0$, so $e^{(1)} - e^{(8)}$ has rank 3

Table 1: The transformation strains of the 12 variants of monoclinic-I martensite

Variant number	Transformation strain	Variant number	Transformation strain
1	$\begin{pmatrix} \alpha & \delta & \epsilon \\ \delta & \alpha & \epsilon \\ \epsilon & \epsilon & \beta \end{pmatrix}$	2	$\begin{pmatrix} \alpha & \delta & -\epsilon \\ \delta & \alpha & -\epsilon \\ -\epsilon & -\epsilon & \beta \end{pmatrix}$
3	$\begin{pmatrix} \alpha & -\delta & -\epsilon \\ -\delta & \alpha & \epsilon \\ -\epsilon & \epsilon & \beta \end{pmatrix}$	4	$\begin{pmatrix} \alpha & -\delta & \epsilon \\ -\delta & \alpha & -\epsilon \\ \epsilon & -\epsilon & \beta \end{pmatrix}$
5	$\begin{pmatrix} \alpha & \epsilon & \delta \\ \epsilon & \beta & \epsilon \\ \delta & \epsilon & \alpha \end{pmatrix}$	6	$\begin{pmatrix} \alpha & -\epsilon & \delta \\ -\epsilon & \beta & -\epsilon \\ \delta & -\epsilon & \alpha \end{pmatrix}$
7	$\begin{pmatrix} \alpha & -\epsilon & -\delta \\ -\epsilon & \beta & \epsilon \\ -\delta & \epsilon & \alpha \end{pmatrix}$	8	$\begin{pmatrix} \alpha & \epsilon & -\delta \\ \epsilon & \beta & -\epsilon \\ -\delta & -\epsilon & \alpha \end{pmatrix}$
9	$\begin{pmatrix} \beta & \epsilon & \epsilon \\ \epsilon & \alpha & \delta \\ \epsilon & \delta & \alpha \end{pmatrix}$	10	$\begin{pmatrix} \beta & -\epsilon & -\epsilon \\ -\epsilon & \alpha & \delta \\ -\epsilon & \delta & \alpha \end{pmatrix}$
11	$\begin{pmatrix} \beta & -\epsilon & \epsilon \\ -\epsilon & \alpha & -\delta \\ \epsilon & -\delta & \alpha \end{pmatrix}$	12	$\begin{pmatrix} \beta & \epsilon & -\epsilon \\ \epsilon & \alpha & -\delta \\ -\epsilon & -\delta & \alpha \end{pmatrix}$
We number the variants so that $\delta > 0$ and $\epsilon > 0$.			

and it cannot have the form $\frac{1}{2}(a \otimes n + n \otimes a)$. Thus variants 1 and 8 are not compatible, and we cannot use Proposition 2.1 to calculate $\mathcal{S}$.

In fact, $\mathcal{S}$ is *not* the convex hull of the transformation strains when the martensite has monoclinic-I symmetry. To demonstrate this assertion, consider the matrix

$$e_0 = \frac{1}{2} \{e^{(1)} + e^{(8)}\} = \frac{1}{2} \begin{pmatrix} 2\alpha & \delta + \epsilon & -\delta + \epsilon \\ \delta + \epsilon & \alpha + \beta & 0 \\ -\delta + \epsilon & 0 & \alpha + \beta \end{pmatrix}, \quad (3.3)$$

which is obviously in the convex hull of the transformation strains. We claim that $e_0 \notin \mathcal{S}$. The crucial observation is that $\frac{1}{2}(e^{(1)} + e^{(8)})$ is the *only* way to express e_0 as a convex combination of the transformation strains. Now, if e_0 were in $\mathcal{S}$ then there would exist an (essentially) stress-free mixture of martensite variants with average strain e_0 . Our observation implies that such a mixture can only involve the two variants $e^{(1)}$ and $e^{(8)}$. More precisely, the Young measure limit of strains associated with such a microstructure would have to be the sum of two Dirac measures, one at $e^{(1)}$ and the other $e^{(8)}$, each with weight 1/2. But there is no such Young measure, since $e^{(1)}$ and $e^{(8)}$ are incompatible [21]. Therefore e_0 does not belong to $\mathcal{S}$.

We do not know the precise form of the set $\mathcal{S}$ in this case, but we have an inner estimate:

$$\mathcal{S} \supset \left\{ e \left\| \begin{array}{l} e_{11} + e_{22} + e_{33} = 2\alpha + \beta, \\ \min\{\alpha, \beta\} \leq e_{11}, e_{22}, e_{33} \leq \max\{\alpha, \beta\}, \\ -\left(\frac{e_{ii}-\alpha}{\beta-\alpha}\right) \delta \leq e_{jk} \leq \left(\frac{e_{ii}-\alpha}{\beta-\alpha}\right) \delta \quad \text{for each } \{ijk\} = \text{perm}\{123\} \end{array} \right. \right\}. \quad (3.4)$$

This is proved by comparison with the case the orthorhombic case (see [11]). In particular, $\mathcal{S}$ spans the space of deviatoric strains.

There is a corresponding inner estimate for $\mathcal{T}$: for general polycrystals, in which all orientations occur,

$$\mathcal{T}_{\text{monoclinic-I}} \supset \mathcal{T}_{\text{orthorhombic}} \quad (3.5)$$

where $\mathcal{T}_{\text{orthorhombic}}$ is defined by (3.2).

MONOCLINIC-II

In the other type of cubic-monoclinic transformation the 12 stress-free strains are obtained from

$$\begin{pmatrix} \alpha + \epsilon & \delta & 0 \\ \delta & \alpha - \epsilon & 0 \\ 0 & 0 & \beta \end{pmatrix} \quad (3.6)$$

by replacing δ with $-\delta$ and permuting the coordinates. The $\beta_1 \rightarrow \beta'_1$ transformation in CuAlNi is of this type.

Once again the variants are not pairwise compatible, and Proposition 2.1 cannot be used to evaluate $\mathcal{S}$. We believe that $\mathcal{S}$ is strictly smaller than the convex hull in this case too, though we have no rigorous proof.

We can again obtain inner estimates for $\mathcal{S}$ and $\mathcal{T}$ by comparing with the orthorhombic case: assertions (3.4) and (3.5) hold for monoclinic-II as well as for monoclinic-I martensite.

3.7 Discussion

The Taylor estimate distinguishes clearly between alloys with tetragonal or trigonal martensite on the one hand and those with orthorhombic or monoclinic martensite on the other. In the former case a general polycrystal should not recover any strain; in the latter case every polycrystal should recover some strain. This is consistent with the trends shown by experimental data.

We have not been able to distinguish significantly between the effect of orthorhombic and monoclinic martensite. This is because our estimates for $\mathcal{T}_{monoclinic}$ are obtained by comparison with $\mathcal{T}_{orthorhombic}$. We know that $\mathcal{T}_{monoclinic-II}$ is strictly larger than $\mathcal{T}_{orthorhombic}$ (see [11]), and we believe the same is true for $\mathcal{T}_{monoclinic-I}$. But we don't have a good estimate of how much larger. It is natural to guess that the size of the parameter ϵ in Table 1 and (3.6) should be relevant. This discussion may be purely academic, however, since we believe that $\mathcal{P}$ is strictly larger than $\mathcal{T}$ for polycrystals with orthorhombic or monoclinic martensite. (See Section 4.5 for an argument supporting this belief.)

Our analysis does not fully explain the large recoverable strain of drawn polycrystalline wires made from TiNi. Single-crystal TiNi recovers only about 3% tensile strain in some directions, yet such wires recover tensile strains as high as 8%. We doubt that the explanation lies in the Taylor estimate alone. Perhaps these wires have special textures, giving them larger recoverable strains than general polycrystals. Or perhaps this is a case where $\mathcal{P}$ is significantly larger than $\mathcal{T}$.

Our viewpoint has one significant shortcoming: it does not predict the consequences of nonrecoverable deformation. The behavior of CuAlNi is a case in point. Polycrystals made from this material are observed to recover some strain, consistent with our analysis. However, CuAlNi polycrystals fail very easily at grain boundaries, making this a poor shape-memory material for practical applications. Our analysis does not explain why such failure occurs in CuAlNi but not, say, in TiNi. (It is not always clear whether the martensite in a CuAlNi polycrystal is γ'_1 (orthorhombic) or β'_1 (monoclinic-II); usually γ'_1 is thermally induced while β'_1 is stress-induced. However the preceding remarks apply in either case.)

4 Scalar model problems

We want to assess the accuracy of the Taylor estimate, and to know how $\bar{\varphi}$ behaves as it departs from 0. This section examines analogous questions in a dimensionally-reduced setting, where the basic unknown is a scalar valued function $\eta : \mathbb{R}^2 \rightarrow \mathbb{R}$ rather than an elastic displacement u . The microscopic energy is a multi-well function of the vector $\nabla\eta$. Our model problems can be viewed as describing polycrystals with special textures, deformed in antiplane shear. We shall consider two different cases: the *two-variant material* and the *four-variant material*.

For the two-variant material the Taylor estimate is trivial. We shall show that for polycrystals with sufficient symmetry $\mathcal{P}$ is also trivial, i.e. $\bar{\varphi}(f) = 0$ only at $f = 0$. We also have information on how $\bar{\varphi}$ departs from 0: for polycrystals with sufficient symmetry its graph is flatter than quadratic at $f = 0$.

For the four-variant material the Taylor estimate is nontrivial. We shall show by example that the Taylor estimate can be sharp. But we shall argue that such behavior is the

exception rather than the rule.

A more detailed summary of results appears in Section 4.1. Our analysis, presented in Sections 4.2–4.6, uses various tools including elementary bounds, the translation method, and a linear comparison bound. Section 4.7 discusses some features of these methods.

4.1 Formulation of the models and summary of results

In our scalar analogy the “microscopic energy” of a “single crystal” has the form $\varphi(\nabla\eta)$, where $\eta : \mathbb{R}^2 \rightarrow \mathbb{R}$. By analogy with (2.3), a material with “ k variants” having “stress-free strains” $\{f^{(i)}\}_{i=1}^k$ corresponds to a microscopic energy of the form

$$\varphi(f) = \min_{i=1,\dots,k} \left\{ \frac{1}{2} |f - f^{(i)}|^2 \right\} . \quad (4.1)$$

The “mesoscopic energy” is the relaxation of φ , defined by the analogue of (2.4):

$$\hat{\varphi}(f) = \min_{\eta=f \cdot x \text{ at } \partial\Omega} \int_{\Omega} \varphi(\nabla\eta(x)) \, dx .$$

In this scalar setting relaxation is the same as convexification, see e.g. [19]. Therefore $\hat{\varphi} = \varphi^{**}$, i.e. the graph of $\hat{\varphi}$ is the convex envelope of the graph of φ . In particular, the set of “recoverable strains for the single crystal”

$$\mathcal{S} = \{f : \hat{\varphi}(f) = 0\}$$

is the convex hull of the preferred gradients $\{f^{(i)}\}_{i=1}^k$.

A “polycrystal with texture $R(x)$ ” is described by a function $R(x)$ taking values in the two-dimensional rotation group $\text{SO}(2)$. The associated energy is the analogue of (2.9):

$$\int_{\Omega} \hat{\varphi}(R(x)\nabla\eta) \, dx .$$

The “macroscopic energy of the polycrystal” $\bar{\varphi}$ is determined by nonlinear homogenization. We need not repeat the discussion accompanying (2.13)–(2.15); suffice it to say that the definition via affine boundary conditions is

$$\bar{\varphi}(f) = \min_{\eta=f \cdot x \text{ at } \partial\Omega} \int_{\Omega} \hat{\varphi}(R(x)\nabla\eta) \, dx . \quad (4.2)$$

We are interested in the “set of recoverable strains for the polycrystal,”

$$\mathcal{P} = \{f : \bar{\varphi}(f) = 0\} ,$$

and in the behavior of $\bar{\varphi}$ in a neighborhood of $\mathcal{P}$.

The “Taylor estimate” is the analogue of (2.16):

$$\mathcal{T} = \bigcap_{x \in \Omega} R^T(x)\mathcal{S} ,$$

where the intersection is over all rotations occurring in the polycrystal. The “Taylor bound,” proved using constant-gradient test fields, says

$$\mathcal{P} \supset \mathcal{T} .$$

We shall consider two different examples of φ : the “two-variant material,” which has $k = 2$ variants of “martensite;” and the “four-variant material,” which has $k = 4$ variants. The martensite variants should be symmetry-related, so the following choices seem natural.

The two-variant material. We take the “martensite variants” to be centered at $f^{(1)} = (-1, 0)$ and $f^{(2)} = (1, 0)$. Then the microscopic energy (4.1) becomes

$$\varphi(f) = \min \left\{ \frac{1}{2} [(f_1 - 1)^2 + f_2^2], \frac{1}{2} [(f_1 + 1)^2 + f_2^2] \right\}, \quad (4.3)$$

and the mesoscopic energy is easily seen to be

$$\hat{\varphi}(f) = \frac{1}{2} [(|f_1| - 1)_+^2 + f_2^2] \quad (4.4)$$

with the convention that $\alpha_+ = \max\{\alpha, 0\}$. The set of “recoverable strains for the single crystal” is just a line segment in the two-dimensional space of gradients:

$$\mathcal{S} = \{(f_1, f_2) : |f_1| \leq 1, f_2 = 0\}.$$

Since $\mathcal{S}$ is dimensionally deficient, the Taylor estimate is trivial. In fact

$$\mathcal{T} = \{0\}$$

for any polycrystal which makes use of at least two distinct rotations, since $R_1^T \mathcal{S} \cap R_2^T \mathcal{S} = \{0\}$ unless $R_2 = \pm R_1$. (We identify the orientations R and $-R$, since $\hat{\varphi}(f) = \hat{\varphi}(-f)$.)

The four-variant material. We take the “martensite variants” to be centered at $f^{(1)} = (-1, -1)$, $f^{(2)} = (-1, 1)$, $f^{(3)} = (1, -1)$ and $f^{(4)} = (1, 1)$. Then the microscopic energy (4.1) becomes

$$\varphi(f) = \min \left\{ \frac{1}{2} [(f_1 \pm 1)^2 + (f_2 \pm 1)^2] \right\} \quad (4.5)$$

and the mesoscopic energy is easily seen to be

$$\hat{\varphi}(f) = \frac{1}{2} [(|f_1| - 1)_+^2 + (|f_2| - 1)_+^2]. \quad (4.6)$$

The set of “recoverable strains for the single crystal” is now a set with interior, namely a square in the two-dimensional space of gradients:

$$\mathcal{S} = \{(f_1, f_2) : |f_1| \leq 1, |f_2| \leq 1\}.$$

Since $\mathcal{S}$ is full-dimensional, the Taylor estimate is nontrivial. The smallest possible Taylor estimate occurs when the polycrystal makes use of every orientation; then $\mathcal{T}$ is just the inscribed circle:

$$\mathcal{T} = \{f : |f| \leq 1\}.$$

Summary of results. We are interested in the two-variant material because it serves as an example in which the Taylor bound is trivial. Our results for this material are as follows:

- For any polycrystal, $\mathcal{P}$ is either $\{0\}$ or else a line segment passing through the origin (Theorem 4.4). We call polycrystals for which $\mathcal{P}$ is a line segment *degenerate*, and those for which $\mathcal{P} = \{0\}$ *nondegenerate*.
- A polycrystal with sufficient symmetry is necessarily nondegenerate (Theorem 4.3). The symmetry required to assure nondegeneracy is quite weak: the conclusion holds if (i) $\bar{\varphi}$ is isotropic, i.e. $\bar{\varphi}(f)$ depends only on $|f|$; or if (ii) $\bar{\varphi}$ has square symmetry, i.e. $\bar{\varphi}(f) = \bar{\varphi}(f^\perp)$; or even if (iii) $\bar{\varphi}$ has “bounded eccentricity,” i.e. $\bar{\varphi}(f) \leq \alpha \bar{\varphi}(g)$ whenever $|f| = |g|$, for some fixed $\alpha > 0$. These assertions follow from the more quantitative result that for any polycrystal, with no symmetry requirement,

$$\bar{\varphi}(f) + \bar{\varphi}(f^\perp) \geq C|f|^4$$

for f near 0. This estimate is in a certain sense sharp (Theorem 4.5).

- The preceding estimate shows that for polycrystals with square symmetry, $\bar{\varphi}(f) \geq C|f|^4$ near 0. For such polycrystals we also have an upper bound: $\bar{\varphi}$ is flatter than quadratic at $f = 0$, i.e.

$$|f|^{-2}\bar{\varphi}(f) \rightarrow 0 \quad \text{as } f \rightarrow 0$$

(Theorem 4.9). Thus, although $\bar{\varphi}$ is “nondegenerate” its quadratic approximation at 0 is nevertheless degenerate. The symmetry required for this conclusion is not that $\bar{\varphi}(f) = \bar{\varphi}(f^\perp)$, but rather that a certain “linear comparison material” be isotropic.

- For a degenerate polycrystal, $\bar{\varphi}$ grows quadratically in the direction normal to $\mathcal{P}$ (Theorem 4.6). Thus a degenerate polycrystal behaves a lot like the single crystal.
- We shall give some examples for which $\mathcal{P}$ can be computed exactly, and $\bar{\varphi}$ estimated within a constant (Examples 4.1 and 4.2). They suggest that finding $\bar{\varphi}$ for a polycrystal made of the two-variant material is something like a percolation problem.

We are interested in the four-variant material because it serves as an example in which the Taylor bound is nontrivial. Our results for this material are as follows:

- The Taylor bound can be sharp, i.e. there are nontrivial polycrystals for which $\mathcal{P} = \mathcal{T}$ (Example 4.10).
- The Taylor bound is not necessarily sharp, i.e. there are many polycrystals for which $\mathcal{P}$ is bigger than $\mathcal{T}$ (Example 4.11). We shall argue, moreover, that such behavior is typical.
- There is an outer estimate for $\mathcal{P}$, complementing the inner estimate from the Taylor bound. In general, with no hypothesis on the texture,

$$\{|f| \leq 1\} \subset \mathcal{P} \subset \{|f| \leq \sqrt{2}\}$$

(equation 4.49). When the orientations are “equidistributed” the outer estimate is smaller: a ball of radius $4/\pi$ rather than $\sqrt{2}$ (equation 4.52).

We conjectured in Section 2.4 that $\mathcal{T}$ correctly estimates the dimension of $\mathcal{P}$, though not necessarily its size, for polycrystals with sufficient symmetry. The results in this section support that conjecture. For polycrystals made from the two-variant material $\mathcal{T}$ is a single point and so is $\mathcal{P}$ (assuming some symmetry). For polycrystals made from the four-variant material $\mathcal{T}$ is two-dimensional and so is $\mathcal{P}$, but the latter can be larger.

Our results on the two-variant material suggest, however, that in concentrating on the set where $\bar{\varphi} = 0$ we may be asking a somewhat unstable question. Since $\bar{\varphi}$ is flatter than quadratic near 0, the set where $\bar{\varphi} < \delta^2$ is *larger than* a ball of radius $C\delta$ — though no bigger than a ball of radius $C\sqrt{\delta}$.

We devote the rest of this subsection to some observations and bounds which will be needed in the sequel.

Basic properties of $\hat{\varphi}$ and $\bar{\varphi}$. In this scalar setting relaxation is the same as convexification, so the mesoscopic energy $\hat{\varphi}$ is convex. It follows that the macroscopic energy $\bar{\varphi}$ is also convex. Our two-variant and four-variant energies φ have the further properties that $\varphi(-f) = \varphi(f)$, $\varphi \geq 0$, and $\varphi(0) = 0$. It is easy to see that $\hat{\varphi}$ and $\bar{\varphi}$ inherit these properties.

The elementary upper bound. We may obtain an upper bound on $\bar{\varphi}$ by choosing any test field which satisfies the boundary conditions of the defining variational principle (4.2). The constant-strain test field $\eta(x) = f \cdot x$ gives the *elementary upper bound*

$$\bar{\varphi}(f) \leq \int_{\Omega} \hat{\varphi}(R(x)f) dx . \quad (4.7)$$

The Taylor bound is an immediate consequence, since $\hat{\varphi} \geq 0$ and $\hat{\varphi}(f) = 0$ for $f \in \mathcal{S}$.

The elementary lower bound and the dual variational principle. We may obtain a lower bound by “dropping the constraint of kinematic admissibility” in the defining variational principle (4.2), i.e. by replacing the curl-free vector field $\nabla\eta$ with an arbitrary vector field ξ such that $\int \xi = f$. This gives the *elementary lower bound*

$$\bar{\varphi}(f) \geq \min_{\int_{\Omega} \xi(x) dx = f} \int_{\Omega} \hat{\varphi}(R(x)\xi(x)) dx . \quad (4.8)$$

There is an alternative approach to the elementary lower bound which is easier to calculate. We shall use the notation

$$\psi^*(g) = \max_f \{f \cdot g - \psi(f)\}$$

for the Fenchel transform of a function ψ . To get a lower bound for $\bar{\varphi}(f)$, let η be any test field admissible for (4.2), and consider any vector field $g : \Omega \rightarrow \mathbb{R}^2$. We start from the pointwise inequality

$$\hat{\varphi}^*(Rg) \geq (R\nabla\eta) \cdot (Rg) - \hat{\varphi}(R\nabla\eta) .$$

If we restrict g to satisfy $\nabla \cdot g = 0$, then integration yields

$$\int_{\Omega} \hat{\varphi}^*(Rg) \geq \int_{\Omega} f \cdot g - \int_{\Omega} \hat{\varphi}(R\nabla\eta) .$$

Optimization over η and g gives the *dual variational principle* for $\bar{\varphi}$:

$$\bar{\varphi}(f) \geq \max_{\nabla \cdot g = 0} \int_{\Omega} \{f \cdot g(x) - \hat{\varphi}^*(R(x)g(x))\} dx . \quad (4.9)$$

We call this the dual variational principle for $\bar{\varphi}$, because if $\hat{\varphi}$ satisfies some minor continuity and growth hypotheses (which hold in our examples) then the relation (4.9) is actually valid with the inequality replaced by equality. All we shall need, however, is the more elementary inequality (4.9).

We get a lower bound for $\bar{\varphi}$ by choosing a specific test field for (4.9). The simplest choices are the constant fields. One can show that maximizing (4.9) over all *constant* g leads precisely to the elementary lower bound (4.8).

For our purposes it will sometimes not be necessary to maximize over all constant g . Instead we shall use just $g = \alpha f$ with $\alpha \in \mathbb{R}$. The resulting bound is

$$\bar{\varphi}(f) \geq \alpha |f|^2 - \int_{\Omega} \hat{\varphi}^*(\alpha R(x)f) dx \quad (4.10)$$

for any $\alpha \in \mathbb{R}$.

Explicit evaluation of the Fenchel transforms. To make use of (4.9) or (4.10) we need to know $\hat{\varphi}^*$. In the present scalar context the relaxation $\hat{\varphi}$ is the convexification φ^{**} , so $\hat{\varphi}^* = \varphi^{***} = \varphi^*$. An elementary calculation gives

$$\hat{\varphi}^*(f) = \begin{cases} \frac{1}{2}|f|^2 + |f_1| & \text{for the two-variant material (4.3)} \\ \frac{1}{2}|f|^2 + |f_1| + |f_2| & \text{for the four-variant material (4.5).} \end{cases} \quad (4.11)$$

4.2 The two-variant material: examples

We shall discuss two specific examples. The first is degenerate, in other words $\mathcal{P}$ is a line segment and $\bar{\varphi}$ resembles the energy of the basic crystal. The second is nondegenerate, in other words $\mathcal{P} = \{0\}$ and $\bar{\varphi}$ is strictly convex at 0. After presenting the examples we discuss the sense in which they are typical of polycrystals made from the two-variant material. We also discuss some connections between this problem and percolation or turbulent transport.

Both our examples are spatially periodic polycrystals made using just two orientations in a checkerboard geometry. We shall therefore use the periodic definition of $\bar{\varphi}$,

$$\bar{\varphi}(f) = \min_{\nabla \eta = f} \int \hat{\varphi}(R(x)\nabla \eta) dx , \quad (4.12)$$

rather than (4.2). The admissible test functions for (4.12) are those for which $\nabla \eta$ is periodic with the same period cell as $R(x)$. The dual variational principle (4.9) remains valid in this setting, with the restriction that the test field g be periodic as well as divergence-free. The elementary upper and lower bounds remain valid without qualification.

In thinking about polycrystals made from the two-variant material, we sometimes find it easier to visualize the divergence-free flow $\sigma = (\nabla \eta)^\perp$ rather than $\nabla \eta$. Each grain has a direction in which flow is “free” (provided that its magnitude stays less than 1); flow in the orthogonal direction is not prohibited, but it costs energy. In Example 4.1 the flow goes in rivers up and down the columns. In Example 4.2 it trickles through the corners.

Figure 1: The microstructure for Example 4.1. The double arrow in each square shows the direction of f such that $\hat{\varphi}(Rf) = 0$.

Example 4.1 The checkerboard polycrystal with rotations θ and $-\theta$, $0 < \theta < \pi/4$.

Consider the checkerboard polycrystal obtained by taking

$$R(x) = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}$$

in the “grey” and “white” squares, respectively (see Figure 1). We assert that in this case

$$\mathcal{P} = \{(s, 0) : |s| \leq \cos \theta - \sin \theta\} .$$

To show that $(s, 0) \in \mathcal{P}$ when $|s| \leq \cos \theta - \sin \theta$, we must construct a suitable test function η . It should have $\nabla \eta$ periodic, $f \nabla \eta = (s, 0)$, and $\hat{\varphi}(R(x) \nabla \eta) \equiv 0$. The last condition will be satisfied exactly if

$$\begin{aligned} \nabla \eta & \parallel (\cos \theta, \sin \theta) && \text{in the grey squares, and} \\ \nabla \eta & \parallel (\cos \theta, -\sin \theta) && \text{in the white squares, and} \\ |\nabla \eta| & \leq 1 && \text{pointwise.} \end{aligned}$$

For $\theta < \pi/4$ and s sufficiently small it is easy to construct test fields with these properties: the level lines of η zigzag down the “columns” (see Figure 2). The main constraint is the requirement that each zigzag stay within its column. An elementary calculation shows that this constraint is equivalent to $|s| \leq \cos \theta - \sin \theta$.

Now let us show that $\mathcal{P}$ contains no other points. We will show in Theorem 4.4 that when $\mathcal{P}$ is nontrivial it must be a line segment. Hence the $\mathcal{P}$ of this example is a subset of the horizontal axis, and our task is to show that $\bar{\varphi}(s, 0) > 0$ for $|s| > \cos \theta - \sin \theta$. It is possible to argue geometrically, showing in essence that the construction considered above is the only possibility. But let us argue variationally instead. Consider the periodic, divergence-free vector field g sketched in Figure 3: it is supported in thin strips that zig-zag across the rows, almost but not quite parallel to the diagonals. Taking the slopes of the

Figure 2: *The construction of $\nabla\eta$ for Example 4.1. The darkly shaded regions form the support of $\nabla\eta$. The lines within them are level sets of η .*

Figure 3: *The construction of g for Example 4.1. The darkly shaded regions form the support of g . The arrows within them give its direction.*

Figure 4: The microstructure for Example 4.2. The double arrow in each square shows the direction of f such that $\hat{\varphi}(Rf) = 0$.

strips to be $\pm(1 - \mu)/(1 + \mu)$ with $\mu > 0$, we have

$$\begin{aligned} g &= (1 + \mu, -1 + \mu) \quad \text{or} \quad 0 \quad \text{in the grey squares,} \\ g &= (1 + \mu, 1 - \mu) \quad \text{or} \quad 0 \quad \text{in the white squares.} \end{aligned}$$

Let us evaluate the lower bound (4.9) at τg . Using the formula (4.11) for $\hat{\varphi}^*$ and writing $h = h(\mu)$ for the area fraction of the strips, we get

$$\begin{aligned} \bar{\varphi}(s, 0) &\geq \tau \int g \cdot (s, 0) - \frac{1}{2} \tau^2 \int |g|^2 - |\tau| \int |(R(x)g) \cdot e_1| \\ &= \tau h(1 + \mu)s - \tau^2 h(1 + \mu^2) - |\tau| h(\cos \theta - \sin \theta + c_0 \mu) \end{aligned} \quad (4.13)$$

with $c_0 = (\cos \theta + \sin \theta)$. To get the best bound we should maximize with respect to τ . The result will be positive exactly if

$$(1 + \mu)|s| > \cos \theta - \sin \theta + c_0 \mu.$$

If $|s| > \cos \theta - \sin \theta$ then this inequality holds for sufficiently small μ , demonstrating that $(s, 0) \notin \mathcal{P}$. $\square$

Example 4.2 The checkerboard polycrystal with rotations $\pi/4$ and $-\pi/4$.

This microstructure is the limit of those considered in Example (4.1) as $\theta \rightarrow \pi/4$ (see Figure 4). We assert that in this case $\mathcal{P} = \{0\}$ and

$$c|f|^3 \leq \bar{\varphi}(f) \leq C|f|^3 \quad \text{for } f \text{ near } 0.$$

We begin with the upper bound. It will suffice to show that

$$\bar{\varphi}(t, 0) \leq C|t|^3, \quad (4.14)$$

Figure 5: *The construction of $\nabla\eta$ for Example 4.2. The darkly shaded regions form the support of $\nabla\eta$. The lines within them are level sets of η .*

for then symmetry implies $\bar{\varphi}(0,t) \leq C|t|^3$, and a simple argument using convexity yields $\bar{\varphi}(f) \leq C'|f|^3$ for all f . To prove (4.14) we shall construct a test function η with $\nabla\eta$ periodic, such that $\oint \nabla\eta = (t, 0)$ and $\oint \hat{\varphi}(R(x)\nabla\eta) \leq Ct^3$. The successful construction resembles that of Example 4.1: once again the support of $\nabla\eta$ zigzags down the columns. But we can no longer keep $\hat{\varphi}(R(x)\nabla\eta) = 0$: that would restrict the support of $\nabla\eta$ to the diagonals, a set of measure zero. Instead we take the slopes of the zigzag to be slightly more vertical than the diagonals, so the direction of $\nabla\eta$ deviates slightly from the preferred ones (see Figure 5). Note the resemblance between Figures 3 and 5: $(\nabla\eta)^\perp$ is similar to our vector field g , except that it flows down the columns instead of across the rows. Quantitatively, our choice is:

$$\begin{aligned} \nabla\eta &= \frac{1}{\sqrt{2}}(1+\mu, 1-\mu) & \text{or } 0 & \text{ in the grey squares,} \\ \nabla\eta &= \frac{1}{\sqrt{2}}(1+\mu, -1+\mu) & \text{or } 0 & \text{ in the white squares,} \end{aligned}$$

with $\mu > 0$ small. Euclidean geometry gives $h = 2\mu/(1+\mu)$ for the area fraction of $\text{supp } \nabla\eta$, and it follows that

$$\oint \nabla\eta = (\sqrt{2}\mu, 0).$$

The local energy is

$$\hat{\varphi}(R(x)\nabla\eta) = \frac{1}{2}\mu^2$$

wherever $\nabla\eta \neq 0$, so this test field shows that

$$\bar{\varphi}(\sqrt{2}\mu, 0) \leq \frac{1}{2}\mu^2 h = \frac{\mu^3}{1+\mu}.$$

The substitution $t = \sqrt{2}\mu$ gives the desired bound (4.14).

We turn now to the lower bound. It will suffice to show that

$$\bar{\varphi}(f) \geq c|f_1|^3 \tag{4.15}$$

for f near 0; then symmetry implies $\bar{\varphi}(f) \geq c|f_2|^3$, and it follows that $\bar{\varphi}(f) \geq c'|f|^3$ for any f near 0. To prove (4.15) we apply the dual variational principle, with the same test field $\tau g(x)$ used in Example 4.1. The result is still estimated by (4.13), but the last term is now

$$|\tau| \int |R(x)g \cdot e_1| = \sqrt{2}|\tau|\mu h ,$$

where $h = 2\mu/(1 + \mu)$ is the volume fraction of $\text{supp } g$. Our conclusion is therefore

$$\bar{\varphi}(f) \geq \max_{\tau} \left[\tau h(1 + \mu)f_1 - \tau^2 h(1 + \mu^2) - \sqrt{2}|\tau|h\mu \right] .$$

This bound is positive when $(1 + \mu)|f_1| > \sqrt{2}\mu$, i.e. when

$$\mu < \frac{|f_1|}{\sqrt{2} - |f_1|} .$$

So it is natural to choose $\mu = a|f_1|$, with $a < 1/\sqrt{2}$ a suitable constant. The optimal value of the bound becomes

$$\frac{h \left[(1 + \mu)|f_1| - \sqrt{2}\mu \right]^2}{4(1 + \mu^2)} = \frac{a(1 - \sqrt{2}a)^2}{2} |f_1|^3 + O(f_1^4) ,$$

which has the desired form (4.15) when f is near 0. $\square$

Discussion

These examples are in some sense representative. Indeed, Theorem 4.4 says that for any polycrystal made from the two-variant material, either $\mathcal{P}$ is a line segment as in Example 4.1, or $\mathcal{P} = \{0\}$ as in Example 4.2. Moreover, Theorems 4.3 and 4.7 show that for polycrystals with square symmetry, $\bar{\varphi}$ is flatter than quadratic but no flatter than quartic; the cubic behavior of Example 4.2 lies between these two extremes.

An important feature of our examples is the highly nonuniform and texture-dependent character of the test fields. Even in Example 4.2, where $\mathcal{P}$ is correctly predicted by the Taylor bound, the fields associated to $f \neq 0$ are nowhere near constant within the grains. Moreover, multi-grain junctions (corners) play a major role. Some authors have modelled the response of shape-memory polycrystals to stress by applying mean field theory, assuming implicitly that the strain is constant within each grain. Our examples make us wonder about the adequacy of this approximation.

We do not mean to suggest that our examples are in any sense universal. Actually, the nondegenerate Example 4.2 is somewhat special because its highly ordered structure makes percolation relatively easy (via corners). Our paper [12] discusses other examples, still highly ordered, in which percolation is more difficult and $\bar{\varphi}$ behaves like $|f|^2/(-\log |f|)$ rather than $|f|^3$. It would be interesting to consider some disordered cases, such as a random checkerboard. Our intuition is that the “percolating paths” (level sets of η) should be quite complicated in the disordered setting, leading to macroscopic behavior $\bar{\varphi}$ that is very nearly quadratic.

However, complexity alone does not preclude degeneracy: it is easy to give examples of polycrystals with complicated textures which are nevertheless degenerate. Indeed, given any function η_0 with $|\nabla\eta_0| \leq 1$, $\nabla\eta_0$ periodic, and $f\nabla\eta_0 = g_0 \neq 0$, there is a rotation-valued function $R(x)$ such that $R(x)\nabla\eta_0 \parallel (1, 0)$ for all x . The associated polycrystal is clearly degenerate, since $g_0 \in \mathcal{P}$. If η_0 is piecewise linear then the rotation field $R(x)$ is piecewise constant, and the polycrystal has distinct “grains.” One can easily arrange that $\nabla\eta_0$ take just three values, and then the polycrystal makes use of just three orientations. To construct such examples, and to see how complex they can be, suppose g_0 lies in the interior of the convex hull of three vectors g_1, g_2 and g_3 , with $|g_i| \leq 1$. Then there exists a triangle $\mathcal{D}$ which is the union of three disjoint subtriangles $\{\mathcal{D}_i\}_{i=1}^3$, and a function $\eta : \mathcal{D} \rightarrow \mathbb{R}$ which satisfies $\eta = g_0 \cdot x$ at $\partial\mathcal{D}$ and $\nabla\eta = g_i$ on each $\mathcal{D}_i$, $i = 1, 2, 3$. Now consider any packing of the period cell by scaled copies of $\mathcal{D}$. Using scaled versions of η on each scaled copy of $\mathcal{D}$, we obtain a test function η_0 on the entire period cell such that $f\nabla\eta_0 = g_0$ and $\nabla\eta_0 \in \{g_1, g_2, g_3\}$ except for a set of measure 0. The associated polycrystal is degenerate no matter how complex the packing. (We thank Vladimir Sverak for this observation.)

We have already mentioned that it is sometimes convenient to visualize the divergence-free flow $(\nabla\eta)^\perp$ rather than the gradient field $\nabla\eta$. Viewed this way, the task of evaluating $\mathcal{P}$ for a polycrystal made from the two-variant material is something like a problem of percolation. In Example 4.1 the directions of free flow percolate vertically on a set of positive measure, so $\mathcal{P}$ consists of an interval along the horizontal axis. In Example 4.2 the directions of free flow still percolate, but they do so only on a set of measure zero, so $\mathcal{P}$ is trivial.

The percolation problem that determines $\mathcal{P}$ is similar to one which arises in connection with 2D models of turbulent transport, see e.g. [26]. But there are some differences: for example, our directions of free flow have no preferred sign. When percolation doesn’t occur, or if it occurs only on a set of measure zero, then the two problems become quite different: ours achieves the required net flow by deviating from the free directions, while turbulent transport is dominated by diffusion across streamlines.

4.3 The two-variant material: lower bounds

We turn to the task of bounding $\bar{\varphi}$ from below, for polycrystals made from the two-variant material. Our main result is the quartic lower bound $\bar{\varphi}(f) + \bar{\varphi}(f^\perp) \geq C|f|^4$ (Theorem 4.3). A closely related argument shows that $\mathcal{P}$ can be no bigger than a line segment through 0 (Theorem 4.4). The quartic lower bound is in general sharp (Theorem 4.5). But we can say more if the polycrystal is known to be degenerate: then $\bar{\varphi}$ behaves quadratically in the direction normal to $\mathcal{P}$ (Theorem 4.6).

We shall present our lower bounds assuming that $\bar{\varphi}$ is defined using affine boundary conditions (4.2). But the results and proofs are also valid for the periodic definition (4.12).

It might seem natural to start with the elementary lower bound discussed at the end of Section 4.1. We don’t do so, because it doesn’t give a very good bound. See Section 4.7 for a discussion of this point, and an explanation of how Theorem 4.3 arises from a combination of the translation method and an elementary lower bound.

To warm up, and to motivate the proof of Theorem 4.3, we begin with a simple proof

that

$$\bar{\varphi}(f) + \bar{\varphi}(f^\perp) = 0 \implies f = 0 \quad (4.16)$$

for any polycrystal made from the two-variant material. Indeed, if $\bar{\varphi}(f) + \bar{\varphi}(f^\perp) = 0$ then each term must vanish separately, since $\bar{\varphi} \geq 0$. So $\bar{\varphi}(f) = 0$, and the extremal η in the definition of $\bar{\varphi}(f)$ satisfies $\hat{\varphi}(R(x)\nabla\eta) \equiv 0$. Similarly, $\bar{\varphi}(f^\perp) = 0$ and the associated extremal ζ satisfies $\hat{\varphi}(R(x)\nabla\zeta) \equiv 0$. We thus conclude the existence of two functions η and ζ such that

$$\begin{aligned} \eta &= f \cdot x \text{ at } \partial\Omega, & R(x)\nabla\eta \parallel e_1 \text{ in } \Omega; \\ \zeta &= f^\perp \cdot x \text{ at } \partial\Omega, & R(x)\nabla\zeta \parallel e_1 \text{ in } \Omega. \end{aligned} \quad (4.17)$$

This is a severe constraint: the two gradient fields $\nabla\eta$ and $\nabla\zeta$ have orthogonal average values $\int \nabla\eta = f$ and $\int \nabla\zeta = f^\perp$, yet they are pointwise parallel in every grain. We claim this is impossible, except in the trivial case $f = 0$. To see why, consider the null-Lagrangian

$$\det(\nabla\eta, \nabla\zeta) = \eta_{,1}\zeta_{,2} - \eta_{,2}\zeta_{,1} = (\eta\zeta_{,2})_{,1} - (\eta\zeta_{,1})_{,2} . \quad (4.18)$$

Integration by parts shows that if $\eta = f \cdot x$ and $\zeta = g \cdot x$ at $\partial\Omega$ then

$$\int_{\Omega} \det(\nabla\eta, \nabla\zeta) = \det(f, g) . \quad (4.19)$$

We apply this with η and ζ from (4.17) to get

$$0 = \int_{\Omega} \det(\nabla\eta, \nabla\zeta) = \det(f, f^\perp) . \quad (4.20)$$

But

$$\det(f, f^\perp) = |f|^2 , \quad (4.21)$$

and it follows that $f = 0$.

The argument just presented is perfectly rigorous. But its conclusion (4.16) is unsatisfactory. The problem is that (4.16) gives no positive lower bound for $\bar{\varphi}(f) + \bar{\varphi}(f^\perp)$. As a result, it does not preclude the existence of a *sequence* of polycrystals, with different textures $R_j(x)$, whose macroscopic energies $\bar{\varphi}_j$ might tend to zero uniformly in a neighborhood of 0. We want to consider homogenization-limits of polycrystals as being polycrystals themselves. This is essential, because it is only in the limit (grain size)/(sample size) $\rightarrow 0$ that our working definition (4.2) for the macroscopic energy coalesces with the other standard definitions based on spatial periodicity, randomness, or Γ -convergence. But after passage to such a limit our conclusion disappears: we are left with nothing but the trivial result $\bar{\varphi}(f) + \bar{\varphi}(f^\perp) \geq 0$.

The solution, of course, is to use the determinant null-Lagrangian more effectively. Related techniques have been used by many authors to bound the effective moduli of linear composites (e.g. [4, 5, 30, 54, 82]) and to give lower bounds for relaxed energies (e.g. [7, 44]).

Theorem 4.3 *For any polycrystal made from the two-variant material, the macroscopic energy satisfies*

$$\bar{\varphi}(f) + \bar{\varphi}(f^\perp) \geq \max_{|\lambda| < 1} \left[\lambda |f|^2 - \frac{\lambda^2}{1 - \lambda^2} \right] \quad (4.22)$$

for every $f \in \mathbb{R}^2$. Taking $\lambda = |f|^2/2$ gives the more explicit bound

$$\bar{\varphi}(f) + \bar{\varphi}(f^\perp) \geq \frac{1}{2}|f|^4 \left[1 - \frac{2}{(4 - |f|^4)} \right], \quad (4.23)$$

which is asymptotic to $|f|^4/4$ as $f \rightarrow 0$. Finally,

$$\bar{\varphi}(f) + \bar{\varphi}(f^\perp) \geq \frac{1}{6}|f|^4 \quad \text{for } |f| \leq 1 \quad (4.24)$$

as an immediate consequence of (4.23).

Proof. Combining the definition (4.2) of $\bar{\varphi}$ with the properties of the determinant (4.19), (4.21) we see that

$$\bar{\varphi}(f) + \bar{\varphi}(f^\perp) - \lambda|f|^2 = \min_{\substack{\eta=f \cdot x \text{ at } \partial\Omega \\ \zeta=f^\perp \cdot x \text{ at } \partial\Omega}} \int_{\Omega} [\hat{\varphi}(R\nabla\eta) + \hat{\varphi}(R\nabla\zeta) - \lambda \det(\nabla\eta, \nabla\zeta)] dx \quad (4.25)$$

for any $\lambda \in \mathbb{R}$. To estimate the integrand on the right hand side, we first use the rotational invariance of the determinant:

$$\hat{\varphi}(R\nabla\eta) + \hat{\varphi}(R\nabla\zeta) - \lambda \det(\nabla\eta, \nabla\zeta) = \hat{\varphi}(R\nabla\eta) + \hat{\varphi}(R\nabla\zeta) - \lambda \det(R\nabla\eta, R\nabla\zeta).$$

Next we use the fact that for every $s, t \in \mathbb{R}^2$ and every $|\lambda| < 1$,

$$\hat{\varphi}(s) + \hat{\varphi}(t) - \lambda \det(s, t) \geq -\frac{\lambda^2}{1 - \lambda^2}. \quad (4.26)$$

This elementary inequality is proved by direct calculation, starting from the formula (4.4) for $\hat{\varphi}$. Applying (4.26) pointwise with $s = R\nabla\eta$ and $t = R\nabla\zeta$ gives

$$\hat{\varphi}(R\nabla\eta) + \hat{\varphi}(R\nabla\zeta) - \lambda \det(R\nabla\eta, R\nabla\zeta) \geq -\frac{\lambda^2}{1 - \lambda^2}$$

for any $|\lambda| < 1$. Optimization over λ gives the desired assertion (4.22). $\square$

The main point of Theorem 4.3 is the quartic lower bound $\bar{\varphi}(f) + \bar{\varphi}(f^\perp) \geq C|f|^4$. We shall give a different proof of this bound in Section 4.7.

We have focussed on correlating $\bar{\varphi}(f)$ and $\bar{\varphi}(f^\perp)$, but the same argument can be used to correlate $\bar{\varphi}(f)$ and $\bar{\varphi}(g)$ for any f and g . This leads to the following result.

Theorem 4.4 *For any polycrystal made from the two-variant material, the macroscopic energy satisfies*

$$\bar{\varphi}(f) + \bar{\varphi}(R_\theta f) \geq \frac{1}{6}|f|^4 \sin^2 \theta \quad (4.27)$$

for every θ , $0 \leq \theta \leq \pi/2$, and every $|f| \leq 1$. Here R_θ denotes rotation by angle θ . We also have

$$\bar{\varphi}(f) \geq \frac{1}{2}(|f| - 1)_+^2 \quad (4.28)$$

for every $f \in \mathbb{R}^2$. It follows that $\mathcal{P}$ is either $\{0\}$ or else a line segment centered at 0 of length at most 2.

Proof. To prove (4.27) we argue as for Theorem 4.3, with $R_\theta f$ in place of $f^\perp$. This gives

$$\bar{\varphi}(f) + \bar{\varphi}(R_\theta f) \geq \lambda |f|^2 \sin \theta - \frac{\lambda^2}{1 - \lambda^2} .$$

since $\det(f, R_\theta f) = |f|^2 \sin \theta$. Taking $\lambda = \frac{1}{2}|f|^2 \sin \theta$, we conclude that

$$\bar{\varphi}(f) + \bar{\varphi}(R_\theta f) \geq \frac{1}{2}|f|^4 \sin^2 \theta \left[1 - \frac{2}{4 - |f|^4 \sin^2 \theta} \right] ,$$

which leads immediately to (4.27) when $|f| \leq 1$.

The second assertion (4.28) is even easier. We start from the fact that

$$\hat{\varphi}(f) \geq \frac{1}{2}(|f| - 1)_+^2 \quad (4.29)$$

for every $f \in \mathbb{R}^2$. This is easy to verify by direct calculation, starting from the definition (4.4). The expression on the right is rotationally invariant and convex, so (4.29) and Jensen's inequality give

$$\int_{\Omega} \hat{\varphi}(R(x)\nabla \eta) dx \geq \frac{1}{2} \int_{\Omega} (|\nabla \eta| - 1)_+^2 dx \geq \frac{1}{2}(|f| - 1)_+^2$$

whenever $\eta = f \cdot x$ at $\partial\Omega$. Minimization over η gives (4.28). We note in passing that (4.28) is actually the texture-independent elementary lower bound, c.f. Section 4.7.

Finally we draw conclusions about the form of $\mathcal{P}$. This set always contains 0 since $\bar{\varphi}(0) = 0$. Suppose it contains a nonzero vector f_0 . Then it contains $-f_0$, since $\bar{\varphi}(f) = \bar{\varphi}(-f)$; so it contains $[-f_0, f_0]$, by convexity. Applying (4.27) with $f \in [-f_0, f_0]$, we see that $\mathcal{P}$ is restricted to the line through f_0 ; and applying (4.28), we see that $\mathcal{P}$ is restricted to the intersection of this line with $\{|f| \leq 1\}$. Remembering that $\mathcal{P}$ is convex and symmetric about 0, we conclude that the only possibilities are $\{0\}$ or a line segment centered at 0 of length at most 2. $\square$

The final assertion of Theorem 4.4 says that the dimension of $\mathcal{P}$ is less than or equal to that of $\mathcal{S}$. It seems reasonable to conjecture that this is always the case in physically relevant examples. However the analogous assertion is false for our “2D diagonal elastic material” (see Section 5.2).

The preceding results are geometry-independent. They even apply to single crystals, which may be viewed as special examples of polycrystals. But they are most interesting for polycrystals with a certain amount of symmetry. If, for example, $\bar{\varphi}$ has “bounded eccentricity” in the sense that

$$\bar{\varphi}(R_\theta f) \leq \alpha \bar{\varphi}(f) \text{ for all } f \in \mathbb{R}^2 \text{ and all } \theta \in [0, 2\pi] \quad (4.30)$$

then we immediately conclude that $\mathcal{P} = \{0\}$ and $\bar{\varphi}(f) \geq C|f|^4$ for $|f| \leq 1$. A condition like (4.30) is rarely easy to verify except as a consequence of symmetry. We may consider polycrystals with square symmetry, i.e. such that

$$\bar{\varphi}(f^\perp) = \bar{\varphi}(f) \text{ for all } f \in \mathbb{R} ;$$

Example 4.2 falls in this category. Or we may consider random polycrystals in which the grain shapes and orientations have no preferred direction, leading to isotropy:

$$\bar{\varphi}(f) \text{ depends only on } |f|.$$

Either symmetry hypothesis implies once again that $\mathcal{P} = \{0\}$ and $\bar{\varphi} \geq C|f|^4$.

We turn now to the sharpness of our quartic lower bound. It is important to distinguish between two different questions:

- (a) Given f near 0, does there exist a polycrystal such that $\bar{\varphi}(f) + \bar{\varphi}(f^\perp) \leq C|f|^4$?
- (b) Does there exist a polycrystal such that $\bar{\varphi}(f) + \bar{\varphi}(f^\perp) \leq C|f|^4$ for all f near 0?

The difference, of course, is in the placement of the quantifiers. Question (a) permits the texture of the polycrystal to depend upon f , whereas (b) does not. We shall give an affirmative answer to (a), but (b) remains open. Since the geometry-independent bound (4.24) amounts to an estimate for $\min_{\text{textures}}[\bar{\varphi}(f) + \bar{\varphi}(f^\perp)]$, our affirmative answer to (a) shows that Theorem 4.3 is within a constant of being optimal near $f = 0$.

Theorem 4.5 *For any f near 0 there is a polycrystal made from the two-variant material such that*

$$\bar{\varphi}(f) + \bar{\varphi}(f^\perp) \leq C|f|^4. \quad (4.31)$$

The constant C is independent of f , though the polycrystal depends on $|f|$.

Proof. We shall construct the desired polycrystal as a rank-one laminate, using the periodic definition of $\bar{\varphi}$ to define its macroscopic energy. It is convenient to give the orientation of a grain by specifying the “easy direction.” For example, the standard orientation has easy direction e_1 , and a grain with energy $\hat{\varphi}(R\nabla\eta)$ has easy direction $R^T e_1$.

Consider the layered polycrystal obtained as follows: fixing $\beta > 0$, we mix the two-variant material in its standard orientation with a rotated version having easy direction parallel to $(1, 4\beta)$, using area fraction 1/2 of each, with layer normal parallel to $(1, 2\beta)$. To estimate the macroscopic energy of this polycrystal, we use the test functions

$$\nabla\eta = \begin{cases} (-1 + 2\beta, 4\beta^2) & \text{in the standard layers} \\ (1, 4\beta) & \text{in the rotated layers} \end{cases}$$

and

$$\nabla\zeta = \begin{cases} (1, 0) & \text{in the standard layers} \\ (-1, -4\beta) & \text{in the rotated layers.} \end{cases}$$

These choices are admissible (i.e. η and ζ are continuous) because in each case the discontinuity of the gradient is parallel to the layer normal. They show that

$$\bar{\varphi}(\beta, 2\beta + 2\beta^2) \leq \frac{1}{4} \cdot 16\beta^4 + \frac{1}{4} \left[(1 + 16\beta^2)^{1/2} - 1 \right]^2 \leq C_1\beta^4$$

and

$$\bar{\varphi}(0, -2\beta) \leq 0 + \frac{1}{4} \left[(1 + 16\beta^2)^{1/2} - 1 \right]^2 \leq C_1\beta^4$$

for a suitable constant C_1 and sufficiently small β . So the convex set $\{f : \bar{\varphi}(f) \leq C_1\beta^4\}$ contains $(\beta, 2\beta + 2\beta^2)$ and $(0, -2\beta)$. But then it also contains $(-\beta, -2\beta - 2\beta^2)$ and $(0, 2\beta)$, and all convex combinations of these points. If β is sufficiently small then the convex hull contains a ball of radius $c_0\beta$ about 0. We conclude that this polycrystal satisfies

$$\bar{\varphi}(f) \leq C_1\beta^4 \text{ for all } |f| \leq c_0\beta.$$

Writing $\gamma = c_0\beta$, we have shown the existence of a polycrystal such that

$$\bar{\varphi}(f) \leq C_1c_0^{-4}\gamma^4 \text{ for all } |f| \leq \gamma. \quad (4.32)$$

The proposition now follows easily: given f , consider the polycrystal constructed as above with $\gamma = |f|$. It satisfies $\bar{\varphi}(f) + \bar{\varphi}(f^\perp) \leq C|f|^4$ with $C = 2C_1c_0^{-4}$, as an immediate consequence of (4.32). $\square$

The preceding result shows that our quartic lower bound is within a constant of being optimal. There is another approach, a little more complicated, which gives a sharper result: for any f near 0 and any $\varepsilon > 0$ there is a polycrystal such that

$$\bar{\varphi}(f) + \bar{\varphi}(f^\perp) \leq \frac{1+\varepsilon}{4}|f|^4. \quad (4.33)$$

Thus (4.23) even gets the constant right in the limit $f \rightarrow 0$. Besides giving a sharper result the proof of (4.33) is also of conceptual interest, because it provides a direct link between our work on shape-memory polycrystals and that of Ball and James on shape-memory single crystals. We therefore sketch this alternative argument.

Theorem 4.3 amounts to a lower bound for

$$\min_{R(x) \in SO(2)} \min_{\substack{\eta=f \cdot x \text{ at } \partial\Omega \\ \zeta=f^\perp \cdot x \text{ at } \partial\Omega}} \int_{\Omega} [\hat{\varphi}(R(x)\nabla\eta) + \hat{\varphi}(R(x)\nabla\zeta)] dx.$$

The value does not depend on the order of minimization, so we may switch the order and pass the minimization over $R(x)$ inside the integral. This yields a problem of the form

$$\min_{\substack{\eta=f \cdot x \text{ at } \partial\Omega \\ \zeta=f^\perp \cdot x \text{ at } \partial\Omega}} \int_{\Omega} W(\nabla\eta, \nabla\zeta) dx \quad (4.34)$$

with integrand

$$W(f, g) = \min_{R \in SO(2)} [\hat{\varphi}(Rf) + \hat{\varphi}(Rg)].$$

If we view f and g as the columns of a 2×2 matrix F , then W becomes a map from $\mathbb{R}^{2 \times 2}$ to $\mathbb{R}$, and it obviously satisfies $W(RF) = W(F)$ for any $R \in SO(2)$. This looks like the condition of frame indifference in hyperelasticity, so (4.34) resembles a problem of elastic energy minimization. The analogy is not perfect: in nonlinear elasticity when we minimize $\int W(Du) dx$, it is the rows of Du , not the columns, that are gradients. But this difference turns out not to be very important.

To justify (4.33) with $f = (\beta, 0)$ and $f^\perp = (0, \beta)$, it would suffice to find test functions η and ζ and a rotation field $R(x)$ such that $\eta = \beta x_1$ and $\zeta = \beta x_2$ at $\partial\Omega$, and

$$\{\nabla\eta, \nabla\zeta\} = R(x)A \text{ or } R(x)B \text{ almost everywhere in } \Omega, \quad (4.35)$$

where A and B are the matrices

$$A = \frac{1}{2} \begin{pmatrix} 2 & 2 \\ -\beta^2 & \beta^2 \end{pmatrix}, \quad B = \frac{1}{2} \begin{pmatrix} -2 & 2 \\ -\beta^2 & -\beta^2 \end{pmatrix}.$$

The point, of course, is that the columns of A and B satisfy

$$\hat{\varphi}(\pm 1, \pm \frac{1}{2}\beta^2) = \frac{1}{8}\beta^4.$$

So the polycrystal with orientation $R(x)$ would have $\bar{\varphi}(\beta, 0) \leq \int \hat{\varphi}(R(x)\nabla\eta) = \beta^4/8$ and $\bar{\varphi}(0, \beta) \leq \int \hat{\varphi}(R(x)\nabla\zeta) = \beta^4/8$, giving (4.33) with $\varepsilon = 0$.

Property (4.35) demands that $\{\nabla\eta, \nabla\zeta\}$ take only values on the two “wells” $SO(2)A$ and $SO(2)B$. Perhaps this can actually be achieved using methods from [58]. But it is easier to achieve it “approximately,” in the sense of Young measures. This can be done using second-rank lamination, by an argument parallel to that of [7]. Omitting the details (which are somewhat tedious), we summarize the result of this construction: it gives a sequence of (η_j, ζ_j) , $j = 1, 2, \dots$, with affine boundary data $\eta_j = \beta x_1$, $\zeta_j = \beta x_2$ at $\partial\Omega$ and satisfying a uniform Lipschitz bound $|\nabla\eta_j| + |\nabla\zeta_j| < M$, such that

$$\{\nabla\eta_j, \nabla\zeta_j\} \in SO(2)A \cup SO(2)B \text{ except on a set of measure } \leq 1/j.$$

Arguing as before, we conclude the existence of a polycrystal such that

$$\bar{\varphi}_j(f) + \bar{\varphi}_j(f^\perp) \leq \frac{1}{4}|f|^4 + C/j.$$

The desired estimate (4.33) follows, by taking j so large that $C/j \leq \frac{\varepsilon}{4}|f|^4$.

Our last task is an improved lower bound for degenerate polycrystals. Theorem 4.4 shows that if $\bar{\varphi}$ is zero in some direction, then it grows quartically in every other direction. We shall improve on this by showing that it must actually grow quadratically. The proof uses the degenerate $\nabla\eta$ to construct a convenient test field for the dual variational principle (4.9).

Theorem 4.6 *Consider a degenerate polycrystal made from the two-variant material, and suppose without loss of generality that $\mathcal{P}$ is a line segment of length 2μ on the f_1 axis. Then*

$$\bar{\varphi}(f) \geq \frac{1}{2}\mu^2 f_2^2.$$

Proof. Our hypothesis is that $\bar{\varphi}(\mu, 0) = 0$. If η achieves the minimum in the definition of $\bar{\varphi}(\mu, 0)$ then

$$\int_{\Omega} \hat{\varphi}(R(x)\nabla\eta(x)) dx = 0 \quad \text{and} \quad \int_{\Omega} \nabla\eta dx = (\mu, 0).$$

Evidently, $R(x)\nabla\eta(x)|e_1$ and $|\nabla\eta(x)| \leq 1$ almost everywhere in Ω . Since we are in two space dimensions, $(\nabla\eta)^\perp$ is divergence free, and we may consider $g = \tau(\nabla\eta)^\perp$ as a test field for the dual variational principle for any $\tau > 0$. It satisfies $R(x)g(x)|e_2$, $|g| < \tau$ almost everywhere, and $\int_{\Omega} g(x) dx = \tau(0, \mu)$. Therefore the dual variational principle gives

$$\bar{\varphi}(f) \geq \max_{\tau} \left\{ f \cdot \tau\mu e_2 - \int_{\Omega} \hat{\varphi}^*(R(x)g(x)) dx \right\}.$$

Recall from (4.11) that $\hat{\varphi}^*(f) = \frac{1}{2}|f|^2 + |f_1|$. Since the e_1 component of $R(x)g$ vanishes, we get

$$\int_{\Omega} \hat{\varphi}^*(R(x)g(x)) dx = \frac{1}{2} \int_{\Omega} |g|^2 dx \leq \frac{\tau^2}{2}.$$

Thus $\bar{\varphi}(f) \geq \max_{\tau} \{\tau \mu f_2 - \tau^2/2\} = \frac{1}{2} \mu^2 f_2^2$. $\square$

4.4 The two-variant material: upper bounds

We turn to the task of bounding $\bar{\varphi}$ above. Our main conclusion is Theorem 4.9, which asserts that for polycrystals with sufficient symmetry $\bar{\varphi}$ is flatter than quadratic at $f = 0$. The argument combines two tools: a “linear comparison bound,” Theorem 4.7, quite general in concept; and Dykhne–Keller duality, Lemma 4.8, which is special to the 2D scalar case.

The linear comparison bound is insensitive to the precise definition of $\bar{\varphi}$. But Dykhne–Keller duality is somewhat sensitive: it does not work for affine boundary conditions. So this part of our analysis requires $\bar{\varphi}$ to be defined via spatial periodicity, randomness, or G-convergence.

We begin with a heuristic explanation why $\bar{\varphi}$ should be flatter than quadratic for polycrystals with sufficient symmetry. The essence of the matter is that *linearization and homogenization should commute*. To explain what this means, we note that the quadratic approximation of the two-variant basic crystal energy near 0 is

$$\hat{\varphi}_{lin}(f) = \frac{1}{2} f_2^2.$$

Hence the linearized problem is one of “degenerate conductivity,” with a basic crystal whose principal conductivities are 0 and 1.

“Linearization then homogenization” means starting with the linear polycrystal whose local energy is $\hat{\varphi}_{lin}(R(x)f)$, then passing in the usual way to its effective energy $\bar{\varphi}_{lin}(f)$. “Homogenization then linearization” means considering our nonlinear macroscopic energy $\bar{\varphi}$, then taking its quadratic approximation near $f = 0$. If the two operations commute then we should have

$$\bar{\varphi}(f) = \bar{\varphi}_{lin}(f) + o(|f|^2).$$

Dykhne–Keller duality gives restrictions on the form of $\bar{\varphi}_{lin}$. Assuming square symmetry, so that $\bar{\varphi}_{lin}$ is isotropic, duality gives $\bar{\varphi}_{lin}(f) = c|f|^2$ with $c^2 = 0 \cdot 1$ the product of the principal conductivities of $\hat{\varphi}_{lin}$. Evidently $c = 0$, so we conclude (heuristically) that $\bar{\varphi}$ is flatter than quadratic.

The problem with this argument is the degenerate character of $\hat{\varphi}$. The assertion that linearization commutes with homogenization has been proved for spatially periodic polycrystals made from a basic crystal that is strictly convex [2, 33]. But our $\hat{\varphi}$ is not strictly convex, since it arises as a relaxation. Therefore $\hat{\varphi}_{lin}$ is a degenerate quadratic form, and linear homogenization theory does not apply. It is not even clear that $\bar{\varphi}_{lin}$ is well-defined.

The resolution of this difficulty involves perturbing $\hat{\varphi}_{lin}$ to make it slightly nondegenerate. We shall actually use not $\hat{\varphi}_{lin}$ but

$$\hat{\varphi}_{\varepsilon}(f) = \frac{1}{2} [\varepsilon f_1^2 + f_2^2] \tag{4.36}$$

with $\varepsilon > 0$.

Theorem 4.7 *Consider a polycrystal made from the two-variant material, with texture function $R(x)$ and macroscopic energy $\bar{\varphi}(f)$. For $\varepsilon > 0$ let $\bar{\varphi}_\varepsilon(f)$ be the effective energy of the linear polycrystal made from the basic crystal $\hat{\varphi}_\varepsilon$ using the same texture $R(x)$. Then we have the estimate*

$$\bar{\varphi}(f) \leq \bar{\varphi}_\varepsilon(f) + C|f|^{2+\delta} \quad (4.37)$$

for every $f \in \mathbb{R}^2$. The constants C and δ depend on ε , but they are positive and finite and they do not depend on f or the polycrystalline texture.

Proof. Our goal is an upper bound for $\bar{\varphi}$, and our plan is to use the linear comparison material $\hat{\varphi}_\varepsilon$. We cannot expect an inequality of the form $\bar{\varphi}(f) \leq \bar{\varphi}_\varepsilon(f)$, because the local fields are not necessarily bounded and the local energies are ordered only when f is near 0. But we shall use elliptic theory to control the local fields, leading to the extra term $C|f|^{2+\delta}$.

It suffices to work with the definition of $\bar{\varphi}$ based on affine boundary conditions (4.2). The corresponding assertions for other definitions follow as corollaries, as explained in Section 2. Because the argument makes use of elliptic regularity, it requires $\partial\Omega$ to have some minimal regularity; we shall assume without further mention that this hypothesis is satisfied.

Our starting point is the following global relation between $\hat{\varphi}$ and $\hat{\varphi}_\varepsilon$:

$$\hat{\varphi}(f) \leq \hat{\varphi}_\varepsilon(f) + \begin{cases} 0 & \text{if } |f_1| < 1 \\ \frac{1}{2}f_1^2 & \text{if } |f_1| \geq 1 \end{cases}.$$

This is clear from the fact that $(|f_1| - 1)^2 \leq f_1^2$ when $|f_1| \geq 1$. Using it, we easily see that

$$\int_{\Omega} \hat{\varphi}(R(x)\nabla\eta) dx \leq \int_{\Omega} \hat{\varphi}_\varepsilon(R(x)\nabla\eta) dx + \frac{1}{2} \int_{\{|\nabla\eta| \geq 1\}} |\nabla\eta|^2 dx \quad (4.38)$$

for any $\eta : \mathbb{R}^2 \rightarrow \mathbb{R}$. Now let us choose $\eta = \eta_\varepsilon^f$ to be the solution of the linear polycrystal problem

$$\min_{\eta=f \cdot x \text{ at } \partial\Omega} \int_{\Omega} \hat{\varphi}_\varepsilon(R(x)\nabla\eta) dx.$$

Use of this test function in (4.38) gives

$$\bar{\varphi}(f) \leq \bar{\varphi}_\varepsilon(f) + \frac{1}{2|\Omega|} \int_{\{|\nabla\eta_\varepsilon^f| \geq 1\}} |\nabla\eta_\varepsilon^f|^2 dx. \quad (4.39)$$

It remains to estimate the integral on the right hand side of (4.39). We do this using Meyers' theorem, which says that $\nabla\eta_\varepsilon^f$ is actually in L^p for some p slightly larger than 2. To get a quantitative estimate, consider $\tilde{\eta} = \eta_\varepsilon^f - f \cdot x$. It solves an equation of the form

$$\nabla \cdot (a_\varepsilon(x)\nabla\tilde{\eta}) = \nabla \cdot F, \quad \tilde{\eta} = 0 \text{ at } \partial\Omega,$$

with $a_\varepsilon(x) = \varepsilon R^T(x)e_1 \otimes R^T(x)e_1 + R^T(x)e_2 \otimes R^T(x)e_2$ and $F = -a_\varepsilon(x)f$. The crucial information for Meyers' theorem is that

$$\varepsilon|\xi|^2 \leq \langle a_\varepsilon(x)\xi, \xi \rangle \leq |\xi|^2 \quad \text{and} \quad \|F\|_{L^\infty} \leq |f|.$$

We deduce from Theorem 1 of [52] that $\tilde{\eta}$ satisfies

$$\left(\int_{\Omega} |\nabla\tilde{\eta}|^{2+\delta} dx \right)^{1/(2+\delta)} \leq C_1 |f| \quad (4.40)$$

for some $\delta, C_1 > 0$. The constants depend on ε , with $\delta \rightarrow 0$ and $C_1 \rightarrow \infty$ as $\varepsilon \rightarrow 0$. But they are independent of f and $R(x)$, and that is what matters to us.

The rest of the argument is easy. By (4.40) and the triangle inequality, $\|\nabla \eta_\varepsilon^f\|_{L^{2+\delta}} \leq C_2|f|$. Therefore

$$\int_{\{|\nabla \eta_\varepsilon^f| \geq 1\}} |\nabla \eta|^2 dx \leq \int_{\Omega} |\nabla \eta_\varepsilon^f|^{2+\delta} \leq C_2^{2+\delta} |f|^{2+\delta}.$$

Combining this with (4.39) gives the desired estimate (4.37). $\square$

Our comments motivating Theorem 4.7 concentrated on the relationship between linearization and homogenization. But there is also a different way to view this result. Several authors have considered “linear comparison bounds,” which estimate the behavior of a nonlinear composite by comparison with a suitably chosen linear composite [14, 61, 69]. Theorem 4.7 is clearly a bound of this type. We note in passing that this theorem and its proof generalize easily to the 3D elastic setting.

Having estimated $\bar{\varphi}$ by comparison with a linear composite, we are left with the task of estimating $\bar{\varphi}_\varepsilon$. In the 3D elastic case we expect the analogue of $\bar{\varphi}_\varepsilon$ to depend on the texture. But in the 2D scalar setting it is sharply restricted by duality. The following result has its roots in the work of Dykhne and Keller [22, 39], see also [30, 37, 41].

Lemma 4.8 *Consider a linear conducting polycrystal in two space dimensions, made from a basic crystal with principal conductivities a_1 and a_2 . Let $\bar{a}$ be its effective conductivity, defined using either (i) spatially periodic homogenization, (ii) the theory of random composites, or (iii) the theory of G -convergence. Then $\det \bar{a} = a_1 a_2$. If the polycrystal has square symmetry — which means $\bar{a} = R_{\pi/2}^T \bar{a} R_{\pi/2}$, implying isotropy since $\bar{a}$ is a second-order tensor — then it follows that $\bar{a} = \sqrt{a_1 a_2} I$.*

We apply this, of course, with $a_1 = \varepsilon$, $a_2 = 1$, and $\bar{\varphi}_\varepsilon(f) = \frac{1}{2}(\bar{a}f, f)$. The square symmetry of $\bar{a}$ is typically a consequence of microstructural symmetry; this is the case, for example, for the “diagonal checkerboard” microstructure of Example 4.2.

Theorem 4.9 *Consider a polycrystal made from the two-variant material. Suppose (for example, as a consequence of symmetry) that the linear comparison polycrystal has square symmetry, so $\bar{\varphi}_\varepsilon(f) = \frac{1}{2}\sqrt{\varepsilon}|f|^2$ for every $\varepsilon > 0$. Then $\bar{\varphi}(f) = o(|f|^2)$ in the sense that*

$$|f|^{-2}\bar{\varphi}(f) \rightarrow 0 \quad \text{as} \quad |f| \rightarrow 0. \quad (4.41)$$

Proof. Theorem 4.7 gives

$$\bar{\varphi}(f) \leq \frac{1}{2}\sqrt{\varepsilon}|f|^2 + C_\varepsilon|f|^{2+\delta(\varepsilon)}.$$

Therefore $\lim_{f \rightarrow 0} |f|^{-2}\bar{\varphi}(f) \leq \sqrt{\varepsilon}/2$ for every $\varepsilon > 0$, and (4.41) follows by passage to the limit $\varepsilon \rightarrow 0$. $\square$

This completes our treatment of the two-variant material, aside from some methodological issues to be addressed in Section 4.7. We therefore turn to the four-variant model.

Figure 6: *The microstructure for Example 4.10. The box in each square indicates the set of f such that $\hat{\varphi}(Rf) = 0$.*

4.5 The four-variant material: examples

This material has $\hat{\varphi} = 0$ on the square $\mathcal{S} = \{|f_1| \leq 1, |f_2| \leq 1\}$, a set with interior. So its Taylor estimate $\mathcal{T}$ is nontrivial, and $\mathcal{P} = \{\bar{\varphi} = 0\}$ contains a neighborhood of 0. We are interested in the size of $\mathcal{P}$, and particularly in the accuracy of the Taylor estimate. We believe that for this material, $\mathcal{T}$ usually underestimates $\mathcal{P}$.

This section presents two examples. In the first the Taylor estimate turns out to be sharp. In the second the Taylor estimate is not sharp. After presenting the examples we discuss our view that the first is exceptional, and the second typical.

Our examples are spatially periodic, so it is natural to use the definition of $\bar{\varphi}$ via periodic homogenization, (4.12).

Example 4.10 *The checkerboard polycrystal with rotations 0 and $\pi/4$.*

Consider the checkerboard polycrystal obtained by taking

$$R(x) = I \quad \text{and} \quad R_{\pi/4}$$

in the grey and white squares respectively (see Figure 6). Since there are only two rotations, the Taylor estimate $\mathcal{T} = \mathcal{S} \cap R_{\pi/4}^T \mathcal{S}$ is a regular octagon centered at the origin (Figure 7). We shall show that the Taylor estimate is sharp for this polycrystal, i.e.

$$\mathcal{P} = \mathcal{T}.$$

We know from the Taylor bound that $\mathcal{P} \supset \mathcal{T}$, so our task is to show that

$$\bar{\varphi}(f) = 0 \implies \begin{cases} |f_1| \leq 1, & |f_1 + f_2| \leq \sqrt{2}, \\ |f_2| \leq 1, & |f_1 - f_2| \leq \sqrt{2}. \end{cases} \quad (4.42)$$

There are two approaches. The first makes use of the elementary lower bound, much as we did in Example 4.1. Each of the inequalities in (4.42) requires the use of a different test field

Figure 7: *The Taylor estimate for Example 4.10.*

g — supported near the horizontal and vertical lines of the lattice (to show $|f_1|, |f_2| \leq 1$) and near the diagonals (to show $|f_1 \pm f_2| \leq 1$). The second is more geometric, and perhaps more intuitive, so we prefer to present it instead.

If $\bar{\varphi}(f) = 0$, then there exists a function η with $\nabla\eta = (\eta_1, \eta_2)$ periodic such that $f \nabla\eta = f$ and $\hat{\varphi}(R(x)\nabla\eta) \equiv 0$. The last condition is equivalent to

$$\begin{aligned} |\eta_1| \leq 1, |\eta_2| \leq 1 & \text{ in the grey squares,} \\ |\eta_1 \pm \eta_2| \leq \sqrt{2} & \text{ in the white squares.} \end{aligned}$$

To show that $|f_1| \leq 1$, we observe that the restriction of η to any horizontal line segment in a grey grain is Lipschitz continuous with Lipschitz constant 1. (The restriction of η is meaningful, since η is Lipschitz continuous.) The horizontal lines of the lattice are unions of such segments, so it follows that

$$|\eta(x_1, x_2) - \eta(x'_1, x_2)| \leq |x_1 - x'_1|$$

along such lines. Now, η can be written as $f \cdot x + \tilde{\eta}$ with $\tilde{\eta}$ periodic. So the choice $|x_1 - x'_1| = 1$ yields $|f_1| \leq 1$. A similar argument using vertical rather than horizontal lines shows that $|f_2| \leq 1$.

To prove the remaining inequalities we argue similarly using the white grains. In these regions it is the restriction of η to lines of slope ± 1 that have Lipschitz constant 1. As luck would have it, the white grains percolate along selected lines of slope ± 1 , namely the alternate diagonals. Arguing as above, we conclude that $|f_1 + f_2| \leq \sqrt{2}$ (using diagonals of slope 1) and $|f_1 - f_2| \leq \sqrt{2}$ (using diagonals of slope -1). Thus $\bar{\varphi}(f) = 0$ implies $f \in \mathcal{T}$. $\square$

Example 4.11 *The checkerboard polycrystal with rotations θ and $\pi/4$, with $\theta > 0$.*

Now consider the checkerboard polycrystal with

$$R(x) = R_\theta \quad \text{and} \quad R_{\pi/4}$$

in the grey and white squares respectively. We restrict our attention to θ near 0, so this microstructure can be viewed as a perturbation of the one considered above. The Taylor

Figure 8: The Taylor estimate for Example 4.11. Its boundary intersects the x_1 axis at $(\alpha_{Taylor}, 0)$.

bound $T = R_\theta^T \mathcal{S} \cap R_{\pi/4}^T \mathcal{S}$ is still an octagon, but no longer a regular one (see Figure 8). We claim that the Taylor bound is not sharp in this case. In fact, we shall show that

$$\max\{\alpha : \bar{\varphi}(\alpha, 0) = 0\} \text{ is larger than predicted by the Taylor bound.} \quad (4.43)$$

To prove (4.43) we need simply display a test function η satisfying $\nabla \eta$ periodic, $\oint \nabla \eta = (\alpha, 0)$, and $\bar{\varphi}(R(x)\nabla \eta) \equiv 0$, with $\alpha > \alpha_{Taylor}$, where $\alpha_{Taylor} = 1/\cos \theta$ is the maximal value predicted by the Taylor bound. We know that the constant-gradient test function $\alpha_{Taylor} x_1$ has energy zero. So it is natural to work perturbatively, seeking η in the form

$$\eta = \alpha_{Taylor} x_1 + \varepsilon \psi(x) .$$

The conditions that $\varepsilon \psi$ must satisfy are quite different in the two types of grains, since $(\alpha_{Taylor}, 0)$ is on the boundary of $R_\theta^T \mathcal{S}$ but in the interior of $R_{\pi/4}^T \mathcal{S}$. In fact, if

$$\begin{aligned} |\nabla \psi| &\leq 1 && \text{everywhere, and} \\ (R_\theta \nabla \psi) \cdot e_1 &\leq 0 && \text{in the grey grains} \end{aligned}$$

then the corresponding η has energy zero for sufficiently small $\varepsilon > 0$. To obtain (4.43) we need to satisfy these conditions, and also

$$\oint \psi_{,1} > 0, \quad \oint \psi_{,2} = 0 .$$

Such a function ψ is easily constructed; one choice is indicated by Figure 9. Our construction actually has $(R_\theta \nabla \psi) \cdot e_1 \equiv 0$ in the grey squares. This fixes the slope of the level lines of ψ in every alternate grain. Because we have complete freedom in the remaining grains, it is easy to meet this constraint.

What is the form of $\mathcal{S}$ for this microstructure? Our best guess is shown in Figure 10. The Taylor estimate remains sharp at the faces attributable to the white grains, by the argument of Example 4.10. But it cannot be sharp anywhere on the faces attributable to the grey grains, by (4.43) and convexity.

Figure 9: *The construction of $\nabla\psi$ for Example 4.11. The darkly shaded regions form the support of $\nabla\psi$.*

Figure 10: *Conjectured form of the set $\mathcal{P}$ for Example 4.11.*

It is easy to modify the example so that the Taylor bound is not sharp along any of its eight faces: we need only rotate by an angle different from $\pi/4$ in the white grains. $\square$

Discussion.

We think Example 4.10 is the result of a coincidence, and Example 4.11 is more typical. Indeed, consider any polycrystal made from the four-gradient material using finitely many rotations. Points in $\mathcal{P}$ correspond to test functions satisfying $\hat{\varphi}(R(x)\nabla\eta) = 0$. In a grain with (constant) rotation R , the restriction of η to certain lines – those in direction $R^T e_1$ and $R^T e_2$ – will be Lipschitz continuous with Lipschitz constant 1. Example 4.10 is special because some of these lines connect, traversing the entire microstructure (with constant direction). Example 4.11 eliminates some of these connections by rotating the material in the grey grains. It appears that the existence of such connections should be quite exceptional.

The perturbative argument of Example 4.11 seems very robust. It should extend easily to other classes of microstructures, and to polycrystals involving more than two rotations. In fact, the more rotations there are the easier it should become to violate the Taylor bound, because the perturbation ψ is constrained only at grains with special orientations. For a random polycrystal with equidistributed rotations, it seems natural to guess that $\mathcal{P}$ is strictly larger than the Taylor estimate.

4.6 The four-variant material: bounds

We have relatively little to say concerning bounds for the four-variant material. Basically, we know no useful results aside from those which follow from the elementary upper and lower bounds.

We already used the elementary upper bound: it was the source of the Taylor bound. It says

$$\bar{\varphi}(f) \leq \int_{\Omega} \hat{\varphi}(R(x)f) dx \quad (4.44)$$

with

$$\hat{\varphi}(f) = \frac{1}{2}(|f_1| - 1)_+^2 + \frac{1}{2}(|f_2| - 1)_+^2 .$$

If we know nothing of the texture, then the only possible estimate is

$$\int_{\Omega} \hat{\varphi}(R(x)f) dx \leq \max_{R \in SO(2)} \hat{\varphi}(Rf) ,$$

leading to

$$\bar{\varphi}(f) \leq \frac{1}{2}(|f| - 1)_+^2 . \quad (4.45)$$

This is consistent with the texture-independent version of the Taylor bound, which says $\mathcal{P} \supset \cap_{R \in SO(2)} R^T \mathcal{S} = \{|f| \leq 1\}$ for any polycrystal made from the four-variant material.

With some information on the texture we can get a better bound. For example, the Taylor bound involves only those rotations that actually occur in the polycrystal. It is natural to consider the case of a polycrystal with *equidistributed* rotations, i.e. one in which

$$\int_{\Omega} \hat{\varphi}(R(x)f) dx = \int_{SO(2)} \hat{\varphi}(Rf) dR . \quad (4.46)$$

In this case direct evaluation of the integral gives

$$\bar{\varphi}(f) \leq \begin{cases} 0 & \text{if } |f| \leq 1 \\ \frac{2}{\pi}(\frac{|f|^2}{2} + 1) \arccos(1/|f|) - \frac{3}{\pi}(|f|^2 - 1)^{1/2} & \text{if } |f| \geq 1. \end{cases} \quad (4.47)$$

Although (4.47) lies below (4.45), it gives no new information on $\mathcal{P}$. We argued in Section 4.5 that $\mathcal{P}$ should be bigger than $\mathcal{T}$ in most cases. Alas, the elementary upper bound is too crude to capture the considerations of that argument.

Section 4.4 derived an upper bound for the two-variant material by means of a “linear comparison bound.” It is natural to wonder whether one can improve on (4.44) by a similar technique. We were not able to do so. The four-variant material seems less well suited to linear comparison because it vanishes in a neighborhood of $f = 0$, and the questions of interest don’t relate to behavior near 0.

We turn now to the elementary lower bound. One verifies that $\min_{R \in SO(2)} \hat{\varphi}(Rf) = \frac{1}{2}(|f| - \sqrt{2})_+^2$, so (4.8) leads easily to

$$\bar{\varphi}(f) \geq \frac{1}{2}(|f| - \sqrt{2})_+^2. \quad (4.48)$$

This is the texture-independent version of the elementary lower bound. We conclude as a corollary that

$$\mathcal{P} \subset \{f : |f| \leq \sqrt{2}\}. \quad (4.49)$$

When textural information is available, it is more convenient to use the other version of the bound:

$$\bar{\varphi}(f) \geq \alpha|f|^2 - \int_{\Omega} \hat{\varphi}^*(\alpha R(x)f) dx$$

for every $\alpha \in \mathbb{R}$, with

$$\hat{\varphi}^*(f) = \frac{1}{2}|f|^2 + |f_1| + |f_2|.$$

Writing $R(x)f = (|f| \cos \theta(x), |f| \sin \theta(x))$, we get

$$\bar{\varphi}(f) \geq \alpha|f|^2 - \frac{1}{2}\alpha^2|f|^2 - |\alpha||f| \int_{\Omega} |\cos \theta(x)| + |\sin \theta(x)| dx.$$

Optimization over α gives the texture-dependent version of the elementary lower bound:

$$\bar{\varphi}(f) \geq \frac{1}{2} \left(|f| - \int_{\Omega} |\cos \theta(x)| + |\sin \theta(x)| dx \right)_+^2. \quad (4.50)$$

Using only the fact that $|\cos \theta| + |\sin \theta| \leq \sqrt{2}$ we recover (4.48). Using the rotations in the polycrystal and their area fractions, we can clearly get a better bound. When the rotations are equidistributed (4.50) becomes

$$\bar{\varphi}(f) \geq \frac{1}{2} \left(|f| - \frac{4}{\pi} \right)_+^2, \quad (4.51)$$

and we get an improvement of (4.49):

$$\mathcal{P} \subset \{f : |f| \leq 4/\pi\}. \quad (4.52)$$

Our analysis of the two-variant material relied on the translation method rather than the elementary lower bound. However, translation gives nothing new for the four-variant material. We shall explain why not in Section 4.7.

4.7 Discussion of bounding techniques

Of our various upper and lower bounds, the quartic lower bound of Theorem 4.3 is perhaps the most interesting. The treatment in Section 4.3 is efficient — but maybe too efficient. This section aims to put that argument in context, and to share some things we learned while investigating it.

The elementary lower bound for the two-variant material. We summarize briefly the consequences of the elementary lower bound, to demonstrate the need for a better method. Everything is parallel to the analysis done in Section 4.6 for the four-variant material. Remembering that $\hat{\varphi}(f) = \frac{1}{2} [(|f_1| - 1)_+^2 + f_2^2]$, we get $\min_{R \in SO(2)} \hat{\varphi}(Rf) = \frac{1}{2} (|f| - 1)_+^2$, so the texture-independent bound analogous to (4.48) is

$$\bar{\varphi}(f) \geq \frac{1}{2} (|f| - 1)_+^2 . \quad (4.53)$$

It is sharp, since equality is achieved (for any fixed f) by an appropriately oriented single crystal. But it tells us nothing about the accuracy of the Taylor estimate. (Remember, $\mathcal{T} = \{0\}$ for the two-variant material.)

When textural information is available we may argue instead as for (4.50) to get

$$\bar{\varphi}(f) \geq \frac{1}{2} \left(|f| - \int_{\Omega} |\cos \theta(x)| dx \right)_+^2 .$$

If, for example, the rotations are equidistributed then $\int |\cos \theta| = 2/\pi$ and we get

$$\bar{\varphi}(f) \geq \frac{1}{2} (|f| - 2/\pi)_+^2 .$$

Though tighter than (4.53), this bound still vanishes near 0, so it still tells us nothing about the Taylor estimate.

The translation method. To do better, we should bound a sum of energies rather than a single energy. The translation method gives a convenient way to do this.

We considered the sum of two energies in Section 4.3, but one can just as easily consider any number k . The sum of k energies is characterized by adding k copies of the defining variational principle:

$$\sum_{i=1}^k \bar{\varphi}(f^i) = \min_{\eta^i = f^i \cdot x \text{ at } \partial\Omega} \int_{\Omega} \left\{ \sum_{i=1}^k \hat{\varphi}(R(x) \nabla \eta^i) \right\} dx . \quad (4.54)$$

The elementary lower bound for this sum of energies gives nothing new; just a sum of elementary lower bounds. The essence of the translation method is the observation that one can do better. Here is the basic idea, in its simplest and most general form, applied to the sum of energies (4.54). (Our treatment is somewhat similar to that of [70].) The “translation” τ can be any function of $x \in \Omega$ and $\nabla \eta^1, \dots, \nabla \eta^k$, i.e. any function $\tau : \Omega \times \mathbb{R}^{2k} \rightarrow \mathbb{R}$. It is convenient to write $\tau = \tau(x, \{\nabla \eta^i\})$, where $\{\nabla \eta^i\}$ is the $2 \times k$ matrix with columns $\nabla \eta^i$. For any $2 \times k$ matrix $F = \{f^i\}$ we may define $\bar{\tau}(F)$ by

$$\bar{\tau}(F) = \min_{\eta^i = f^i \cdot x \text{ at } \partial\Omega} \int_{\Omega} \tau(x, \{\nabla \eta^i\}) dx . \quad (4.55)$$

The notation $\bar{\tau}$ has been chosen to emphasize the analogy with the effective energy (4.2). Combining (4.54) and (4.55) we obtain

$$\int_{\Omega} \left\{ \sum_{i=1}^k \hat{\varphi}(R(x) \nabla \eta^i) \right\} dx - \bar{\tau}(\{f^i\}) \geq \int_{\Omega} \left\{ \sum_{i=1}^k \hat{\varphi}(R(x) \nabla \eta^i) - \tau(x, \{\nabla \eta^i\}) \right\} dx$$

whenever $\eta^1, \dots, \eta^k$ satisfy $\eta^i = f^i \cdot x$ at $\partial\Omega$. Minimization over η^i yields the *translated variational inequality*:

$$\sum_{i=1}^k \bar{\varphi}(f^i) \geq \bar{\tau}(\{f^i\}) + \min_{\eta^i = f^i \cdot x \text{ at } \partial\Omega} \int_{\Omega} \left\{ \sum_{i=1}^k \hat{\varphi}(R(x) \nabla \eta^i) - \tau(x, \{\nabla \eta^i\}) \right\} dx. \quad (4.56)$$

The name reflects the analogy between (4.2) and (4.56): the minimum on the right hand side of (4.56) is the “macroscopic energy” of the fictitious “material” obtained by vectorization (considering several energies at once) and translation (subtracting $\tau(x, \{\nabla \eta^i\})$).

The right hand side of (4.56) is as difficult to evaluate as the original effective energy. So it is natural to estimate it using the elementary lower bound (4.8). This gives the *translation bound*

$$\sum_{i=1}^k \bar{\varphi}(f^i) \geq \bar{\tau}(\{f^i\}) + \min_{f_{\Omega} \xi^i = f^i} \int_{\Omega} \left\{ \sum_{i=1}^k \hat{\varphi}(R(x) \xi^i) - \tau(x, \{\xi^i\}) \right\} dx. \quad (4.57)$$

in which each ξ^i ranges over arbitrary vector fields on Ω .

For this bound to be of use, we must be able to evaluate $\bar{\tau}$. Most of the literature on linear composites uses homogeneous, quadratic translations, i.e. functions $\tau = \tau(\{f^i\})$ which are independent of x and quadratic in $\{f^i\}$. The useful choices are those which are *quasiconvex*, i.e. for which $\bar{\tau}(F) = \tau(F)$; they are easily characterized using compensated compactness or Fourier analysis. One finds a different choice in the recent literature on plasticity: the linear comparison bounds exploited in [14, 61, 69] can be viewed as examples of (4.57) with $k = 1$, and $\tau(x, f)$ the energy of an appropriately chosen linear composite.

We must also be able to evaluate the right hand side of (4.57). When considering linear composites it is natural to insist that the integrand be a nonnegative quadratic form, i.e. that $\sum \hat{\varphi}(Rf^i) - \tau(\{f^i\})$ be a convex function of the matrix $\{f^i\}$ for every $R \in SO(2)$. Then the elementary bound is easy to compute, using standard methods from the theory of effective moduli. When considering nonlinear composites, however, it is not natural to impose either positivity or convexity. If $\sum \hat{\varphi}(Rf^i) - \tau(\{f^i\})$ is nonconvex then the minimum in (4.56) might not be achieved, but that doesn't matter – we care only about the minimum value. It is estimated by (4.57), which can be evaluated using convex duality as we did for the elementary lower bound in (4.10).

Let us connect this discussion with the proof of Theorem 4.3. Our estimate (4.25) is clearly a special case of the translated variational inequality (4.56) with $f^1 = f$, $f^2 = f^\perp$ and $\tau = \lambda \det$. The analogue of (4.10) in this setting is

$$\bar{\varphi}(f) + \bar{\varphi}(f^\perp) \geq \lambda |f|^2 + 2\alpha |f|^2 - \int_{\Omega} \Psi_{\lambda}(\alpha R(x)f, \alpha R(x)f^\perp) dx \quad (4.58)$$

for any $\alpha \in \mathbb{R}$, where

$$\Psi_{\lambda}(s, t) = \max_{f, g \in \mathbb{R}^2} \{s \cdot f + t \cdot g - \hat{\varphi}(f) - \hat{\varphi}(g) + \lambda \det(f, g)\} \quad (4.59)$$

is the Fenchel transform of the translated integrand. The elementary inequality (4.26) used in the proof of Theorem 4.3 is precisely the assertion that $\Psi_\lambda(0,0) \leq \lambda^2/(1-\lambda^2)$ when $|\lambda| < 1$. Thus our proof of the theorem was based on (4.58) with $\alpha = 0$.

One might wonder whether a different choice of α would give a better bound. The answer is no. To explain why not, we must evaluate $\Psi_\lambda(\alpha R(x)f, \alpha R(x)f^\perp)$. A calculation based on the definitions (4.4) and (4.59) shows that when $|\lambda| \geq 1$, $\Psi_\lambda(g, g^\perp) = +\infty$ for any $g \neq 0$. We may therefore restrict our attention to $|\lambda| < 1$. Writing the 2×2 matrix $\{\alpha R(x)f, \alpha R(x)f^\perp\}$ as

$$\alpha|f| \begin{pmatrix} \cos \theta(x) & \sin \theta(x) \\ -\sin \theta(x) & \cos \theta(x) \end{pmatrix} = \begin{pmatrix} \gamma(x) & \delta(x) \\ -\delta(x) & \gamma(x) \end{pmatrix},$$

we find after some calculation that

$$\Psi_\lambda \begin{pmatrix} \gamma & \delta \\ -\delta & \gamma \end{pmatrix} = \frac{\lambda^2}{1-\lambda^2} + \frac{\gamma^2 + \delta^2}{1-\lambda} + \frac{|\gamma| + |\delta|}{1-\lambda}.$$

Thus

$$\Psi_\lambda(\alpha R(x)f, \alpha R(x)f^\perp) = \frac{\lambda^2}{1-\lambda^2} + \frac{\alpha^2|f|^2}{1-\lambda} + |\alpha||f| \frac{|\cos \theta(x)| + |\sin \theta(x)|}{1-\lambda},$$

and (4.58) asserts that

$$\bar{\varphi}(f) + \bar{\varphi}(f^\perp) \geq \lambda|f|^2 + 2\alpha|f|^2 - \frac{\lambda^2}{1-\lambda^2} - \frac{\alpha^2|f|^2}{1-\lambda} - \frac{|\alpha||f|}{1-\lambda} \int_\Omega |\cos \theta(x)| + |\sin \theta(x)| dx \quad (4.60)$$

for every $\alpha \in \mathbb{R}$. We claim that the optimal choice is $\alpha = 0$ when $|f|$ is small. This is easily seen by reorganizing the right hand side of (4.60) as

$$\lambda|f|^2 - \frac{\lambda^2}{1-\lambda^2} - \frac{\alpha^2|f|^2}{1-\lambda} + |\alpha||f| \left\{ 2\operatorname{sgn}(\alpha)|f| - \frac{1}{1-\lambda} \int_\Omega |\cos \theta(x)| + |\sin \theta(x)| dx \right\}.$$

Only the last two terms involve α . Each vanishes when $\alpha = 0$, and each is negative for $\alpha \neq 0$ and $|f|$ sufficiently small. So the bound is optimized at $\alpha = 0$.

We explained above that the translated energy does not have to be convex. In the present setting it is *necessarily* nonconvex, on account of the degeneracy of $\hat{\varphi}$. Indeed, for f and g near 0 the translated two-variant energy is $\hat{\varphi}(f) + \hat{\varphi}(g) - \lambda \det(f, g) = \frac{1}{2}f_2^2 + \frac{1}{2}g_2^2 - \lambda f_1 g_2 + \lambda f_2 g_1$, which is nonconvex for every $\lambda \neq 0$. Fortunately, the correct restriction is not convexity, but rather the boundedness of the Fenchel transform Ψ_λ . In our example this becomes the restriction $|\lambda| < 1$; in general, it is sufficient that the translated energy be strictly convex at infinity.

We mentioned in Section 4.6 that translation by $\lambda \det$ doesn't give anything new for the four-variant material. To explain why not, we recall that in this case $\hat{\varphi}$ vanishes in a neighborhood of 0. So

$$\Psi_\lambda(0,0) = \max_{f,g \in \mathbb{R}^2} \{-\hat{\varphi}(f) - \hat{\varphi}(g) + \lambda \det(f, g)\} \geq c_0|\lambda|$$

for a suitable $c_0 > 0$. Therefore the translation bound at $\alpha = 0$ says

$$\bar{\varphi}(f) + \bar{\varphi}(f^\perp) \geq \lambda|f|^2 - c_0|\lambda| .$$

If f is near 0 then optimization in λ chooses $\lambda = 0$, and the argument reduces to the elementary lower bound. A more laborious calculation shows that for larger $|f|$ and for $\alpha \neq 0$ the situation is similar: the optimal λ is always 0, bringing us back to the elementary lower bound.

The translation bound is better than the (untranslated) elementary bound because it incorporates the information implicit in (4.55). Thoughtful readers might wonder whether (4.57) makes optimal use of that information. We believe it does. A different approach, which might seem to carry more information, would be to drop the constraint of kinematic admissibility in (4.54) while keeping as a constraint the relation $\int \tau(x, \{\nabla \eta^i\}) \geq \bar{\tau}(\{f^i\})$. In other words, we could consider the bound

$$\sum_{i=1}^k \bar{\varphi}(f^i) \geq \min_{\substack{\int \xi^i(x) = f^i, \\ \int \tau(x, \{\xi^i\}) \geq \bar{\tau}(\{f^i\})}} \int_{\Omega} \sum_{i=1}^k \hat{\varphi}(R(x)\xi^i) dx , \quad (4.61)$$

which follows easily from (4.2) and (4.55) by proving it for $\xi^i = \nabla \eta^i$ then dropping the constraint that ξ^i be a gradient. However, the apparently more general (4.61) is operationally equivalent to our translation bound (4.57). The reason is that (4.61) is equivalent to a convex optimization over the Young measures associated with $\{\xi^i\}$ (see e.g. [27]). The minimum of the constrained problem is also the minimum of a suitable unconstrained problem, by convex duality or equivalently the method of Lagrange multipliers. The resulting bound is identical to our translation bound (4.57) with τ replaced by $\lambda\tau$ for some Lagrange multiplier λ .

An alternative proof of Theorem 4.3. The translation method estimates the minimum of a variational problem without making any use of the associated Euler equation. That is a curious feat. But it is natural to look for ways to use the Euler equation as well, hoping to get a better result. Information of this type has been used in a linear setting by Nesi [59, 60], and in a nonlinear setting by Talbot and Willis [80, 81]. A different but related approach has been pursued by Michel and Suquet [53]. Exploring such ideas led us to an alternative proof of the quartic lower bound for the two-variant material. Our use of the PDE is far less subtle than those of the papers just referenced. But we think it is interesting anyway, as a reminder that the Euler equation may well be of use for proving bounds.

We formulate the “information from the Euler equation” as a lemma.

Lemma 4.12 *For any polycrystal made from the two-variant material, let $\eta(x)$ achieve the minimum in the definition (4.2) of $\bar{\varphi}(f)$. Then we have the estimate*

$$\int_{\Omega} |\nabla \eta - f|^2 dx \leq 1 . \quad (4.62)$$

Proof. The existence of a function $\eta(x)$ minimizing (4.2) is standard, using the convexity of the integrand $\hat{\varphi}$. (We do not assert uniqueness, since $\hat{\varphi}$ is not strictly convex.) Any

minimizer must be a weak solution of the Euler–Lagrange equation, so

$$\nabla \cdot \left[R^T(x) \frac{d\hat{\varphi}}{df}(R(x)\nabla\eta) \right] = 0 . \quad (4.63)$$

Now, for the two-variant material we have

$$\frac{d\hat{\varphi}}{df} = f - \Pi(f) \quad (4.64)$$

where $\Pi : \mathbb{R}^2 \rightarrow \mathbb{R}^2$ is defined by

$$\Pi(f) = \begin{cases} (1, 0) & \text{if } f_1 \geq 1 \\ (f_1, 0) & \text{if } |f_1| \leq 1 \\ (-1, 0) & \text{if } f_1 \leq -1 . \end{cases}$$

The important point is that $\Pi(f)$ is uniformly bounded, specifically $|\Pi(f)| \leq 1$. Substitution of (4.64) into (4.63) gives

$$\Delta\eta = \nabla \cdot [R^T \Pi(R\nabla\eta)] .$$

Thus the function $\tilde{\eta}(x) = \eta(x) - f \cdot x$ satisfies an equation of the form

$$\Delta\tilde{\eta} = \nabla \cdot F \text{ in } \Omega , \quad \tilde{\eta} = 0 \text{ at } \partial\Omega$$

with $|F(x)| \leq 1$. Multiplying the equation by $\tilde{\eta}$ and integrating by parts gives

$$\int_{\Omega} |\nabla\tilde{\eta}|^2 dx \leq \int_{\Omega} |F|^2 dx \leq 1 ,$$

as desired. $\square$

The quartic lower bound is a remarkably simple consequence of this lemma. Indeed, let $\eta(x)$ and $\zeta(x)$ solve the variational problems defining $\bar{\varphi}(f)$ and $\bar{\varphi}(f^\perp)$ respectively. Since the determinant is a null-Lagrangian, we have

$$|f|^2 = \int_{\Omega} \det(\nabla\eta, \nabla\zeta) dx = \int_{\Omega} \det(R(x)\nabla\eta, R(x)\nabla\zeta) dx .$$

Let $h(x) = R(x)\nabla\eta$, $k(x) = R(x)\nabla\zeta$. Then the preceding expression is

$$\int_{\Omega} (h_1 k_2 - h_2 k_1) dx \leq \left(\int_{\Omega} h_1^2 dx \right)^{1/2} \left(\int_{\Omega} k_2^2 dx \right)^{1/2} + \left(\int_{\Omega} h_2^2 dx \right)^{1/2} \left(\int_{\Omega} k_1^2 dx \right)^{1/2} .$$

Now, we have

$$\int_{\Omega} h_2^2 dx \leq 2\bar{\varphi}(f) \quad \text{and} \quad \int_{\Omega} k_2^2 dx \leq 2\bar{\varphi}(f^\perp) ,$$

using the fact that $\hat{\varphi}(f) \geq \frac{1}{2}f_2^2$. And we have

$$\int_{\Omega} h_1^2 dx \leq (|f| + 1)^2 , \quad \int_{\Omega} k_1^2 dx \leq (|f| + 1)^2 ,$$

from Lemma 4.12 and the triangle inequality. Combining these results gives

$$\begin{aligned} |f|^2 &\leq \sqrt{2}(|f| + 1) \left[\bar{\varphi}(f)^{1/2} + \bar{\varphi}(f^\perp)^{1/2} \right] \\ &\leq 2(|f| + 1) \left[\bar{\varphi}(f) + \bar{\varphi}(f^\perp) \right]^{1/2}, \end{aligned}$$

which implies the quartic lower bound

$$\bar{\varphi}(f) + \bar{\varphi}(f^\perp) \geq \frac{1}{4(1 + |f|)^2} |f|^4.$$

Though not exactly the same as (4.23), this estimate has the same (optimal) asymptotic behavior $\frac{1}{4}|f|^4$ near $f = 0$.

5 Elastic problems

We return now to the elastic setting. This section starts with a pair of model problems, the *2D diagonal elastic material* and the *2D diagonal, trace-free elastic material*. For polycrystals made from the first we show that the dimension of $\mathcal{P}$ can be larger than that of $\mathcal{T}$. This demonstrates that the accuracy of the Taylor estimate is a problem-specific matter rather than a universal one. For polycrystals made from second material we prove that $\mathcal{P}$ has the same dimension as $\mathcal{T}$. This model serves as a bridge between our 2D scalar methods and the 3D elastic context.

Then we turn to a class of physically relevant 3D problems, involving a material which undergoes a cubic-tetragonal phase transition. We show that for polycrystals with $\langle 001 \rangle$ texture, the Taylor estimate correctly predicts the dimension of $\mathcal{P}$. We also comment briefly on other 3D problems.

Our main tools are lamination (Section 5.2) and translation (Sections 5.3 and 5.4). The translations used in Sections 5.3 and 5.4 are inspired by recent work on bounds for the effective moduli of 2D elastic polycrystals [4, 50].

5.1 Formulation of the models and summary of results

We shall specify our materials in a different way than in Section 4, describing each material by giving the “mesoscopic energy” of its single crystal.

The alternative would have been to start with the stress-free strains of the martensite variants $\{e^{(i)}\}_{i=1}^k$. They would determine the microscopic elastic energy by

$$\varphi(e) = \min_{i=1, \dots, k} \left\{ \frac{1}{2} |e - e^{(i)}|^2 \right\}. \quad (5.1)$$

The mesoscopic energy $\hat{\varphi}$ would then be determined by relaxation. Recall from Proposition 2.1 that if the stress-free strains are elastically compatible then $\mathcal{S} = \{\hat{\varphi} = 0\}$ is precisely their convex hull.

But our goal is not the direct evaluation of the macroscopic energy. Rather, we care about $\mathcal{P}$, and how it compares with the Taylor estimate $\mathcal{T}$. To answer this question we need not make use of the exact relaxed energy $\hat{\varphi}$. Instead, we may homogenize any nonnegative,

convex function ψ which vanishes on the same set $\mathcal{S}$. Indeed, as explained in Section 2, the central issue is the existence of nonconstant strains satisfying the pointwise relation $e(u) \in R(x)\mathcal{S}R^T(x)$; this clearly depends only on $\mathcal{S}$, not on the details of $\hat{\varphi}$. It is convenient to let ψ be a convex lower bound for $\hat{\varphi}$; then a lower bound for $\bar{\psi}$ implies one for $\bar{\varphi}$, controlling the growth of $\bar{\varphi}$ near $\mathcal{P}$.

We shall henceforth neglect the distinction between the exact relaxation $\hat{\varphi}$ and the convex lower bound ψ . Rather than insist that $\hat{\varphi}$ be the exact relaxation of φ , we permit it to be a convex lower bound instead.

We now specify the three “materials” to be considered, and our results on each.

The 2D diagonal elastic material. In this case the mesoscopic energy is

$$\hat{\varphi}(e) = \frac{1}{2} [(|e_{11}| - 1)_+^2 + (|e_{22}| - 1)_+^2 + 2e_{12}^2] . \quad (5.2)$$

This is the convexification of (5.1) with $k = 4$ and

$$e^{(1)} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad e^{(2)} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad e^{(3)} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \quad e^{(4)} = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} .$$

The set of recoverable strains for the single crystal is the convex hull of $\{e^{(i)}\}$, a two-dimensional square in the three-dimensional space of symmetric matrices:

$$\mathcal{S} = \{e : |e_{11}| \leq 1, |e_{22}| \leq 1, e_{12} = 0\} .$$

This is a consequence of Proposition 2.1, applied separately to $\{e^{(1)}, e^{(2)}, e^{(3)}\}$ and to $\{e^{(2)}, e^{(3)}, e^{(4)}\}$.

The Taylor estimate contains only multiples of the identity:

$$\mathcal{T} = \bigcap_{R \in SO(2)} R\mathcal{S}R^T = \{aI : |a| \leq 1\} ;$$

in particular, it is one-dimensional.

We shall show that the Taylor estimate is not reliable in this case, not even for polycrystals which are macroscopically isotropic. In fact, a polycrystal made from this material can have $\bar{\varphi} \equiv 0$ in a neighborhood of 0. Thus $\mathcal{P}$ can be three-dimensional even though $\mathcal{T}$ is one-dimensional.

Though presented in 2D for the sake of simplicity, this phenomenon is not a consequence of two-dimensionality: the same thing happens for the analogous “3D diagonal elastic material.”

The 2D diagonal, trace-free elastic material. In this case the mesoscopic energy is

$$\hat{\varphi} \begin{pmatrix} a+b & c \\ c & a-b \end{pmatrix} = [a^2 + (|b| - 1)_+^2 + c^2] . \quad (5.3)$$

This is the convexification of (5.1) with $k = 2$ and

$$e^{(1)} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad e^{(2)} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} .$$

In this case $\mathcal{S}$ is the line segment from $e^{(1)}$ to $e^{(2)}$,

$$\mathcal{S} = \left\{ \begin{pmatrix} b & 0 \\ 0 & -b \end{pmatrix} : |b| \leq 1 \right\} ,$$

and the Taylor estimate is trivial:

$$\mathcal{T} = \{0\} .$$

We shall confirm the accuracy of the Taylor estimate, by showing the existence of constants $c_1, c_2 > 0$ such that

$$\bar{\varphi}(e) + \bar{\varphi}(R_{\pi/4}^T e R_{\pi/4}) \geq c_1(\operatorname{tr} e)^2 + c_2|e^D|^4 \quad (5.4)$$

for every polycrystal made from this material (Theorem 5.1). Here $e^D = e - \frac{1}{2}(\operatorname{tr} e)I$ is the deviatoric part of a 2×2 matrix e , and the estimate is only asserted when $|e^D|$ is sufficiently small. It follows, of course, that $\mathcal{P} = \{0\}$ for any polycrystal with sufficient symmetry.

This example is a lot like our scalar two-variant model, and the proof of (5.4) resembles that of Theorem 4.3. We also have a “classification theorem” (Theorem 5.3) analogous to Theorem 4.4, and an upper bound (Theorem 5.5) analogous to Theorem 4.9. The latter says that for any polycrystal with sufficient symmetry,

$$\bar{\varphi}(e) \leq (\operatorname{tr} e/2)^2 + o(|e|^2) .$$

Finally, we have a special lower bound for degenerate polycrystals (Theorem 5.4) analogous to Theorem 4.6.

The cubic–tetragonal material. This material was discussed in Section 3.3. Its set $\mathcal{S}$ of recoverable strains for the single crystal is given by (3.1). There is no loss of generality in restricting our attention to the volume–preserving case $\beta = -2\alpha$. We may also suppose $\alpha > 0$. Then $\mathcal{S}$ is an equilateral triangle centered at the origin in the two–dimensional subspace V of diagonal, trace–free strains,

$$V = \left\{ \begin{pmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{pmatrix} : a + b + c = 0 \right\} . \quad (5.5)$$

The vertices of $\mathcal{S}$ are $\operatorname{diag}[\alpha, \alpha, -2\alpha]$, $\operatorname{diag}[\alpha, -2\alpha, \alpha]$, and $\operatorname{diag}[-2\alpha, \alpha, \alpha]$.

It is not convenient to work with the convexification of φ this time. Instead we shall use the more symmetric function

$$\hat{\varphi}(e) = \frac{1}{2} [(|e'| - \rho)_+^2 + |e''|^2] \quad (5.6)$$

where e' and e'' are the orthogonal projections of e onto V and $V^\perp$:

$$e = \pi_V e + (I - \pi_V)e = e' + e'' ,$$

and $\rho = \sqrt{6}\alpha$ is the radius of the smallest ball in V containing $\mathcal{S}$. This $\hat{\varphi}$ is a convex lower bound for the relaxation of (5.1).

The sets $\mathcal{S}$, $\mathcal{T}$, and $\mathcal{P}$ associated with the real cubic–tetragonal energy are different from those associated with (5.6). To avoid confusion we shall write $\mathcal{S}_{symm}$, $\mathcal{T}_{symm}$, $\mathcal{P}_{symm}$ for the sets defined using the more symmetric energy (5.6). Since this is a lower bound for the true cubic–tetragonal energy we have

$$\mathcal{S} \subset \mathcal{S}_{symm} , \quad \mathcal{T} \subset \mathcal{T}_{symm} , \quad \mathcal{P} \subset \mathcal{P}_{symm} .$$

We shall consider polycrystals with $\langle 001 \rangle$ texture, in other words those in which all the rotations leave the x_3 axis unchanged. No restriction is placed on the geometry of the grains. We evaluated the Taylor estimate in Section 3.3. When specialized to the incompressible case that calculation gives

$$\mathcal{T} = \left\{ \begin{pmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & -2a \end{pmatrix} : -\alpha/2 \leq a \leq \alpha \right\} , \quad (5.7)$$

and a similar calculation gives

$$\mathcal{T}_{symm} = \left\{ \begin{pmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & -2a \end{pmatrix} : |a| \leq \alpha \right\} . \quad (5.8)$$

Our conjecture is that $\mathcal{P}$ should have the same dimension as $\mathcal{T}$, though not necessarily the same size, for polycrystals with sufficient symmetry. We shall prove this assertion for polycrystals with $\langle 001 \rangle$ texture made from a cubic-tetragonal material, by showing that

$$\mathcal{T} \subset \mathcal{P} \subset \mathcal{T}_{symm}$$

for polycrystals with square symmetry about the x_3 axis (Theorem 5.6). We also give a “classification theorem” which requires no further symmetry; it says, roughly speaking, that $\mathcal{P}$ must resemble either $\mathcal{T}$ or a rotation of $\mathcal{S}$ (Theorem 5.8). The crux of our analysis is a lower bound analogous to (5.4): for any polycrystal with $\langle 001 \rangle$ texture

$$\bar{\varphi}(e) + \bar{\varphi}(R_{\pi/4}^T e R_{\pi/4}) \geq c_1 [(\text{tr } e)^2 + e_{13}^2 + e_{23}^2] + c_2 \rho^{-2} [(e_{11} - e_{22})^2 + 4e_{12}^2]^2 , \quad (5.9)$$

where $R_{\pi/4}$ denotes rotation by $\pi/4$ about the x_3 axis, and the estimate is only asserted when $(e_{11} - e_{22})^2 + 4e_{12}^2$ is sufficiently small.

5.2 The 2D diagonal elastic material

Our goal is to show that polycrystals made from this material can have $\bar{\varphi} \equiv 0$ in a neighborhood of 0. Our argument does not really depend on the the specific form (5.2) of the mesoscopic energy. All we use is that

$$\hat{\varphi} \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix} = 0 \quad \text{for } a, b \text{ sufficiently close to 0.}$$

Consider the polycrystal obtained by layering the basic crystal with its rotation by $\pi/4$, using layers normal to $(1, 1)$ and equal volume fractions. A layered composite is spatially

periodic, so it is natural to use the periodic definition of $\bar{\varphi}$. We shall show that for any $\bar{e}$ near 0 there is a locally varying strain field, sharing the periodicity of the microstructure, such that $\hat{\varphi}(R^T(x)e(u)R(x)) \equiv 0$ and $\int e(u) dx = \bar{e}$.

We need only consider strains which are constant in each layer. Then the condition $\hat{\varphi}(R^T(x)e(u)R(x)) \equiv 0$ becomes

$$e(u) = \begin{pmatrix} \alpha & 0 \\ 0 & \beta \end{pmatrix} \text{ where } R = I, \quad e(u) = \begin{pmatrix} \gamma & \delta \\ \delta & \gamma \end{pmatrix} \text{ where } R = R_{\pi/4}, \quad (5.10)$$

with $|\alpha| \leq 1$, $|\beta| \leq 1$, $|\gamma + \delta| \leq 1$, and $|\gamma - \delta| \leq 1$. The constraint of elastic compatibility requires that

$$\begin{pmatrix} \alpha & 0 \\ 0 & \beta \end{pmatrix} - \begin{pmatrix} \gamma & \delta \\ \delta & \gamma \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \odot \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} x & \frac{x+y}{2} \\ \frac{x+y}{2} & y \end{pmatrix} \quad (5.11)$$

for some x and y . This ensures the existence of a continuous deformation u satisfying (5.10). In the present setting, (5.11) amounts to the single linear equation $2(\gamma - \delta) = \alpha + \beta$. Achieving specified mean strain $\bar{e}$ gives three more linear equations, for a total of four equations in the four unknowns α, β, γ and δ . One readily verifies this system is consistent, so it has a unique solution for every $\bar{e}$, and $\alpha, \beta, \gamma, \delta$ are close to zero when $\bar{e}$ is small. Hence $\bar{\varphi} \equiv 0$ in a neighborhood of the origin, as asserted.

The preceding microstructure is far from unique. Virtually *any* rank-one laminate made from the 2D diagonal elastic material has $\bar{\varphi} = 0$ near the origin. This is clear from our argument, which depends mainly on counting equations. We hasten to add, however, that such degeneracy is not a universal feature of every microstructure. For example, the checkerboard microstructure with rotations I and $R_{\pi/4}$ has $\bar{\varphi} = 0$ only at multiples of the identity. (The proof is not trivial, but we leave it as an exercise for the reader's amusement.)

Our rank-one layered example is highly anisotropic. But one can get other, more symmetric examples by mixing this laminated polycrystal with itself in different orientations. One can even get macroscopically isotropic examples, by filling space with a random arrangement of discs then filling each one with our layered example in a randomly chosen orientation. Thus, $\bar{\varphi}$ can vanish in a neighborhood of 0 for a (statistically) isotropic polycrystal made from the 2D diagonal elastic material.

This phenomenon is not special to two space dimensions. A “3D diagonal elastic material” with

$$\hat{\varphi} \begin{pmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{pmatrix} = 0 \quad \text{for } a, b, c \text{ sufficiently close to } 0$$

behaves similarly. The main difference is that one must use rank-two rather than rank-one lamination (choosing the rotations and layering directions with some care) to achieve $\bar{\varphi}(e) \equiv 0$ near $e = 0$.

We have conjectured that $\mathcal{T}$ is usually a good predictor for the dimension of $\mathcal{P}$. The diagonal elastic material provides an important counterexample. It shows this statement can fail, at least for some microstructures, and symmetry alone is not enough to rescue it. It is natural to ask whether the microstructures for which $\bar{\varphi} \equiv 0$ near $e = 0$ are “generic” or “exceptional.” This question remains open.

We are not certain what lesson to draw concerning the behavior of other materials. Perhaps our conjecture fails when the codimension of $\mathcal{S}$ is sufficiently small. We shall return to this point in Section 5.5.

5.3 The 2D diagonal, trace-free elastic material

This material is obtained, roughly speaking, by eliminating the dilational degeneracy of the first example. Its mesoscopic energy (5.3) vanishes on

$$\mathcal{S} = \left\{ \begin{pmatrix} b & 0 \\ 0 & -b \end{pmatrix} : |b| \leq 1 \right\} ,$$

a set of *trace-free* diagonal tensors. Note that this material is not incompressible: dilation is not prohibited, it just costs energy.

Our main goal is to prove the lower bound (5.4). It suffices to work in a basis where e is diagonal, so our task is to show that

$$\bar{\varphi} \begin{pmatrix} a+b & 0 \\ 0 & a-b \end{pmatrix} + \bar{\varphi} \begin{pmatrix} a & b \\ b & a \end{pmatrix} \geq c'_1 a^2 + c'_2 b^4 \quad (5.12)$$

when $|b|$ is sufficiently close to 0.

We shall use the translation method, following more or less the outline of our scalar two-variant example. We begin by identifying the useful translations. Since the goal is to bound a sum of two energies, we must consider a pair of displacement fields $u = (u_1, u_2)$ and $v = (v_1, v_2)$. We denote the associated displacement gradients by

$$M = Du = \begin{pmatrix} u_{1,1} & u_{1,2} \\ u_{2,1} & u_{2,2} \end{pmatrix} , \quad N = Dv = \begin{pmatrix} v_{1,1} & v_{1,2} \\ v_{2,1} & v_{2,2} \end{pmatrix} .$$

The convenient translations are the rotationally invariant null-Lagrangians

$$\begin{aligned} T_1(M, N) &= (M_{11}M_{22} - M_{12}M_{21}) + (N_{11}N_{22} - N_{12}N_{21}) = \det[Du] + \det[Dv] \\ T_2(M, N) &= (M_{11}N_{12} - M_{12}N_{11}) + (M_{21}N_{22} - M_{22}N_{21}) = \det[\nabla u_1, \nabla v_1] + \det[\nabla u_2, \nabla v_2] . \end{aligned}$$

Notice that T_1 and T_2 depend on the full displacement gradients, not just the linear strains $e(u)$ and $e(v)$. These same translations are used in [4] to bound the shear modulus of a 2D elastic polycrystal.

It is clear from the definition that T_1 and T_2 are null-Lagrangians. We claim they are rotationally invariant in the sense that

$$T_i(R^T M R, R^T N R) = T_i(M, N)$$

for any $R \in SO(2)$. This is obvious for T_1 . To see it for T_2 , consider the variables

$$M = \begin{pmatrix} p+q & r+s \\ r-s & p-q \end{pmatrix} \quad N = \begin{pmatrix} w+x & y+z \\ y-z & w-x \end{pmatrix} . \quad (5.13)$$

Under the action of the rotation group, (q, r) and (x, y) transform as vectors while p, s, w, z transform as scalars. So $T_2 = 2(qy - rx) + 2pz - 2sw$ is rotationally invariant.

We need two further observations about T_2 :

(a) If a pair of 2×2 matrices M and N satisfy $\frac{1}{2}(M + M^T) \in \mathcal{S}$ and $\frac{1}{2}(N + N^T) \in \mathcal{S}$ then $T_2(M, N) = 0$.

(b) If $M = \begin{pmatrix} a+b & 0 \\ 0 & a-b \end{pmatrix}$ and $N = \begin{pmatrix} a & b \\ b & a \end{pmatrix}$ then $T_2(M, N) = 2b^2$.

Both properties are easy to verify by direct calculation.

To explain the relevance of T_2 , we now give a simple argument that

$$\bar{\varphi} \begin{pmatrix} a+b & 0 \\ 0 & a-b \end{pmatrix} + \bar{\varphi} \begin{pmatrix} a & b \\ b & a \end{pmatrix} = 0 \implies a = b = 0. \quad (5.14)$$

This statement is analogous to (4.16), and the argument that follows is parallel to (4.17)–(4.21). The hypothesis of (5.14) implies the existence of displacement fields u and v satisfying

$$\begin{aligned} u &= ([a+b]x_1, [a-b]x_2) \text{ at } \partial\Omega, & R^T(x)e(u)R(x) &\in \mathcal{S} \text{ in } \Omega; \\ v &= (ax_1 + bx_2, bx_1 + ax_2) \text{ at } \partial\Omega, & R^T(x)e(v)R(x) &\in \mathcal{S} \text{ in } \Omega. \end{aligned}$$

Applying the rotational invariance of T_2 and observation (a) we see that

$$T_2(Du(x), Dv(x)) = T_2(R^T(x)Du(x)R(x), R^T(x)Dv(x)R(x)) = 0 \text{ pointwise.}$$

But using the fact that T_2 is a null-Lagrangian and observation (b) we have

$$\int T_2(Du, Dv) = T_2(\int Du, \int Dv) = 2b^2.$$

Taken together, these two results imply $b = 0$. The proof that $a = 0$ is different, and easier. The mesoscopic energy satisfies

$$\hat{\varphi}(R^T e R) \geq \frac{1}{4}(\text{tr } e)^2 \quad \text{for any } R \in SO(2).$$

So an application of Jensen's inequality gives

$$0 = \int \hat{\varphi}(R^T e(u)R) \geq \frac{1}{4} \int (\text{tr } e(u))^2 \geq \frac{1}{4} \left(\int \text{tr } e(u) \right)^2 = a^2.$$

The preceding argument uses only the translation T_2 . Moreover, the role of T_2 is parallel to that of the determinant in our scalar calculation. One might therefore anticipate proving the lower bound (5.12) by using the translation method with translation λT_2 . That doesn't work, however, because for any $\lambda \neq 0$ the translated energy

$$\hat{\varphi} \left(\frac{M + M^T}{2} \right) + \hat{\varphi} \left(\frac{N + N^T}{2} \right) - \lambda T_2(M, N)$$

is nonconvex at infinity. This difficulty arises because $\hat{\varphi}$ depends only on the strains while T_2 depends also on the infinitesimal rotations. The resolution is simple: we must augment the translation by a small multiple of T_1 . This works because T_1 is positive definite on the subspace of infinitesimal rotations.

Theorem 5.1 *For any polycrystal made from the 2D diagonal, trace-free material, the macroscopic energy satisfies*

$$\bar{\varphi}(e) + \bar{\varphi}(R_{\pi/4}^T e R_{\pi/4}) \geq c_1(\text{tr } e)^2 + c_2|e^D|^4. \quad (5.15)$$

Here c_1 and c_2 are texture-independent constants, and the estimate is only asserted when $e^D = e - \frac{1}{2}(\text{tr } e)I$ is sufficiently small.

Proof. We treat $\hat{\varphi}$ as a function of 2×2 matrices which only depends on the symmetric part of its argument. Arguing as for (4.25), we see that for any 2×2 matrices M_0, N_0 , $\bar{\varphi}(M_0) + \bar{\varphi}(N_0) - \lambda_1 T_1(M_0, N_0) - \lambda_2 T_2(M_0, N_0)$ is equal to

$$\min_{\substack{u=M_0 \cdot x \text{ at } \partial\Omega \\ v=N_0 \cdot x \text{ at } \partial\Omega}} \int_{\Omega} [\hat{\varphi}(R^T Du R) + \hat{\varphi}(R^T Dv R) - \lambda_1 T_1(Du, Dv) - \lambda_2 T_2(Du, Dv)] dx.$$

Since the translations are rotationally invariant, the integrand is equal to

$$\hat{\varphi}(R^T Du R) + \hat{\varphi}(R^T Dv R) - \lambda_1 T_1(R^T Du R, R^T Dv R) - \lambda_2 T_2(R^T Du R, R^T Dv R). \quad (5.16)$$

The following lemma provides a pointwise lower bound for (5.16).

Lemma 5.2 *Suppose λ_1 and λ_2 satisfy*

$$-1 < \lambda_1 < 0, \quad -\lambda_1(1 - \lambda_1) - \lambda_2^2 > 0, \quad (1 + \lambda_1)^2 - \lambda_2^2 > 0. \quad (5.17)$$

Then we have

$$\min_{M, N \in \mathbb{R}^{2 \times 2}} \{\hat{\varphi}(M) + \hat{\varphi}(N) - \lambda_1 T_1(M, N) - \lambda_2 T_2(M, N)\} = 2 \frac{\lambda_1^2 + \lambda_1 - \lambda_2^2}{(1 + \lambda_1)^2 - \lambda_2^2}. \quad (5.18)$$

Postponing the proof of the lemma, we apply it with $\lambda_1 = -\lambda_2^2$. Conditions (5.17) are satisfied if λ_2 is sufficiently close to 0, and the right hand side of (5.18) becomes

$$2 \frac{\lambda_2^4 - 2\lambda_2^2}{(1 - \lambda_2^2)^2 - \lambda_2^2} = -4\lambda_2^2 + O(\lambda_2^4).$$

It follows that

$$\bar{\varphi}(M_0) + \bar{\varphi}(N_0) \geq -\lambda_2^2 T_1(M_0, N_0) + \lambda_2 T_2(M_0, N_0) - 4\lambda_2^2 + O(\lambda_2^4) \quad (5.19)$$

for any M_0, N_0 , and any sufficiently small λ_2 .

Our goal is to prove (5.15). It suffices to work in a basis where e is diagonal, and to prove (5.12). We apply (5.19) with

$$M_0 = \begin{pmatrix} a+b & 0 \\ 0 & a-b \end{pmatrix}, \quad N_0 = R_{\pi/4}^T e R_{\pi/4} = \begin{pmatrix} a & b \\ b & a \end{pmatrix}.$$

Since $T_1(M_0, N_0) = 2(a^2 - b^2)$ and $T_2(M_0, N_0) = 2b^2$, relation (5.19) gives

$$\bar{\varphi}(M_0) + \bar{\varphi}(N_0) \geq -2\lambda_2^2(a^2 - b^2) + 2\lambda_2 b^2 - 4\lambda_2^2 + O(\lambda_2^4).$$

Remembering that $\hat{\varphi}(e) \geq (\text{tr } e/2)^2$, we also have

$$\bar{\varphi}(N_0) + \bar{\varphi}(M_0) \geq 2a^2$$

by an application of Jensen's inequality. Averaging these two relations gives

$$\bar{\varphi}(N_0) + \bar{\varphi}(M_0) \geq (1 - \lambda_2^2)a^2 + \lambda_2^2 b^2 + \lambda_2 b^2 - 2\lambda_2^2 + O(\lambda_2^4) ,$$

and the choice $\lambda_2 = b^2/4$ yields

$$\bar{\varphi}(M_0) + \bar{\varphi}(N_0) \geq \frac{1}{2}a^2 + \frac{1}{8}b^4$$

when b is sufficiently small. This estimate has the desired form (5.12). $\square$

Proof of Lemma 5.2. Using the variables (5.13) we have

$$\begin{aligned} T_1(M, N) &= p^2 - q^2 - r^2 + s^2 + w^2 - x^2 - y^2 + z^2 , \\ T_2(M, N) &= 2pz + 2qy - 2rx - 2sw , \\ \hat{\varphi}(M) + \hat{\varphi}(N) &= p^2 + (|q| - 1)_+^2 + r^2 + w^2 + (|x| - 1)_+^2 + y^2 . \end{aligned}$$

Therefore $\hat{\varphi}(M) + \hat{\varphi}(N) - \lambda_1 T_1(M, N) - \lambda_2 T_2(M, N)$ can be written as the sum of four decoupled expressions:

$$\begin{aligned} &[(1 - \lambda_1)p^2 - 2\lambda_2 pz - \lambda_1 z^2] + [(|q| - 1)_+^2 + \lambda_1 q^2 - 2\lambda_2 qy + (1 + \lambda_1)y^2] + \\ &[(1 - \lambda_1)w^2 + 2\lambda_2 sw - \lambda_1 s^2] + [(|x| - 1)_+^2 + \lambda_1 x^2 + 2\lambda_2 rx + (1 + \lambda_1)r^2] . \end{aligned} \quad (5.20)$$

Conditions (5.17) ensure that the terms in p, z and w, s are convex, and those in q, y and x, r are convex at infinity.

Our goal is to minimize (5.20). The terms in p, z and s, w are quadratic forms, so their minimum value is 0. Since $-1 < \lambda_1 < 0$, the value of $(1 + \lambda_1) - \lambda_2^2$ is negative, so the optimal values of $|x|$ and $|q|$ are larger than 1. Each of the corresponding terms in (5.20) has minimum value $[\lambda_1^2 + \lambda_1 - \lambda_2^2]/[(1 + \lambda_1)^2 - \lambda_2^2]$. There are two such terms, so this gives (5.18). $\square$

Theorem 5.1 is analogous to our scalar Theorem 4.3. We also have the following analogue of Theorem 4.4.

Theorem 5.3 *For any polycrystal made from the 2D diagonal, trace-free material, the macroscopic energy satisfies*

$$\bar{\varphi}(e) + \bar{\varphi}(R_\theta^T e R_\theta) \geq c_1(\text{tr } e)^2 + c_2(\sin 2\theta)^2 |e^D|^4 \quad (5.21)$$

when $|e^D|$ is sufficiently small. We also have

$$\bar{\varphi}(e) \geq \frac{1}{4}(\text{tr } e)^2 + \frac{1}{2}(|e^D| - \sqrt{2})_+^2 . \quad (5.22)$$

It follows that $\mathcal{P}$ is either $\{0\}$ or else a line segment centered at 0 of length at most $2\sqrt{2}$, contained in the subspace $\text{tr } e = 0$.

Proof. The proof of (5.21) generalizes that of (5.15). It uses (5.19) with $M_0 = e$ and $N_0 = R_\theta^T e R_\theta$, and it gives (5.21) with the same constants c_1, c_2 as in (5.15). The proof of (5.22) is an application of Jensen's inequality, starting from the relation

$$\hat{\varphi}(e) \geq \frac{1}{4}(\operatorname{tr} e)^2 + \frac{1}{2}(|e^D| - \sqrt{2})_+^2 ,$$

which boils down to the fact that

$$a^2 + (|b| - 1)_+^2 + c^2 \geq a^2 + ((b^2 + c^2)^{1/2} - 1)_+^2$$

for any $a, b, c \in \mathbb{R}$. The final assertion about $\mathcal{P}$ follows easily from (5.21) and (5.22). $\square$

We say a polycrystal made from the 2D diagonal, trace-free material is “degenerate” if $\mathcal{P}$ is a line segment. Theorem 5.1 shows that for such polycrystals $\bar{\varphi}$ grows at least quartically in directions transverse to $\mathcal{P}$. We shall improve on this, showing that $\bar{\varphi}$ actually grows quadratically in directions normal to $\mathcal{P}$. This is the analogue of Theorem 4.6. The proof is similar in spirit, but there is a new twist because the rotation of a strain is not a divergence-free “stress” in the 2D in the elastic setting. We focus for convenience on the case of spatially periodic microstructure.

Theorem 5.4 *Consider a degenerate, spatially periodic polycrystal made from the 2D diagonal, trace-free material, and suppose without loss of generality that*

$$\mathcal{P} = \left\{ \begin{pmatrix} t & 0 \\ 0 & -t \end{pmatrix} : |t| \leq \mu \right\} .$$

Then the macroscopic energy satisfies

$$\bar{\varphi}(e) \geq \frac{1}{4}(\operatorname{tr} e)^2 + c\mu^2(e_{12})^2 , \quad (5.23)$$

with a constant c which is independent of the texture.

Proof. Our essential hypothesis is that

$$\bar{\varphi} \left(\begin{pmatrix} \mu & 0 \\ 0 & -\mu \end{pmatrix} \right) = 0 ,$$

or equivalently that there exists a displacement u with $e(u)$ periodic, such that

$$\int_{\Omega} \hat{\varphi}(R^T(x)e(u)R(x)) dx = 0 \quad \text{and} \quad \int_{\Omega} e(u) dx = \begin{pmatrix} \mu & 0 \\ 0 & -\mu \end{pmatrix} .$$

The first condition can be restated as

$$e(u) = R(x) \begin{pmatrix} \alpha(x) & 0 \\ 0 & -\alpha(x) \end{pmatrix} R^T(x) \quad \text{a.e. in } \Omega, \quad \text{with } |\alpha(x)| \leq 1 . \quad (5.24)$$

Our plan is to bound $\bar{\varphi}$ from below by using the dual variational principle analogous to (4.9), with a test field obtained by “rotating” $e(u)$.

We start with the compatibility relation $e_{11,22} + e_{22,11} = 2e_{12,12}$, which expresses the fact that $e_{ij}(x)$ is the strain of a deformation. Writing this as $(e_{11,2} - e_{12,1})_{,2} = (e_{12,2} - e_{22,1})_{,1}$, we deduce the existence of a unique periodic function p such that

$$p_{,1} = e_{11,2} - e_{12,1} , \quad p_{,2} = e_{12,2} - e_{22,1} , \quad \oint p = 0 . \quad (5.25)$$

Setting

$$\tilde{e} = \begin{pmatrix} e_{12} & -e_{11} \\ e_{22} & -e_{12} \end{pmatrix}$$

we see that

$$\sigma = \tilde{e} + pI \quad (5.26)$$

is divergence-free. Starting from an arbitrary strain σ is not in general symmetric. However our $e(u)$ is trace-free as a consequence of (5.24). Therefore our σ is symmetric, and we also have

$$\tilde{e} = R_{\pi/4}^T e R_{\pi/4} . \quad (5.27)$$

We need an estimate for the “pressure” p . Differentiation of (5.25) gives the equation

$$\Delta p = e_{11,21} - e_{12,11} + e_{12,22} - e_{22,12} ,$$

from which it follows by an easy Fourier calculation that

$$\oint p^2 \leq C \oint |e|^2 \leq 2C . \quad (5.28)$$

Now we apply the dual variational principle analogous to (4.9):

$$\bar{\varphi}(f) \geq \max_{\nabla \cdot \eta = 0} \oint \{ f \cdot \eta(x) - \hat{\varphi}^*(R^T(x)\eta(x)R(x)) \} dx . \quad (5.29)$$

One verifies that for the 2D diagonal, trace-free material (5.3),

$$\hat{\varphi}^* \begin{pmatrix} a+b & c \\ c & a-b \end{pmatrix} = a^2 + b^2 + c^2 + 2|b| .$$

We consider test fields of the form

$$\eta = -\tau\sigma + \bar{p}I$$

where σ is given by (5.26) and $\tau, \bar{p}$ are real numbers. One verifies that

$$\hat{\varphi}^*(R^T(x)\eta R(x)) = \frac{1}{2}|\eta|^2$$

as a consequence of (5.24) and (5.27). Therefore (5.29) becomes

$$\begin{aligned} \bar{\varphi}(f) &\geq 2\tau\mu f_{12} + \bar{p} \operatorname{tr} f - \frac{1}{2} \oint (\tau^2 |\tilde{e}|^2 + 2\tau^2 p^2 + 2\bar{p}^2) \\ &\geq (2\tau\mu f_{12} - C'\tau^2) + (\bar{p} \operatorname{tr} f - \bar{p}^2) . \end{aligned}$$

Optimization in τ and $\bar{p}$ gives the desired estimate (5.23). $\square$

We chose to focus on periodic polycrystals because the estimate (5.28) is elementary in that case. The result is also true when $\bar{\varphi}$ is defined using affine boundary conditions; the justification of (5.28) then uses the boundedness of the Riesz transform.

We turn now to the matter of upper bounds. Here, too, the situation is very similar to that of the scalar two-variant model. The natural choice for a linear comparison material is

$$\hat{\varphi}_\varepsilon \left(\begin{array}{cc} a+b & c \\ c & a-b \end{array} \right) = a^2 + \varepsilon b^2 + c^2$$

with $\varepsilon > 0$ small. The following result extends Theorem 4.7, Lemma 4.8, and Theorem 4.9 to this 2D elastic setting.

Theorem 5.5 *Consider a polycrystal made from the 2D diagonal, trace-free material, with texture $R(x)$ and macroscopic energy $\bar{\varphi}(e)$. For $\varepsilon > 0$ let $\bar{\varphi}_\varepsilon(e)$ be the effective energy of the linear polycrystal made from the comparison material $\hat{\varphi}_\varepsilon$ using the same texture $R(x)$. Then we have an estimate of the form*

$$\bar{\varphi}(e) \leq \bar{\varphi}_\varepsilon(e) + C_\varepsilon |e|^{2+\delta(\varepsilon)}. \quad (5.30)$$

If the linear comparison material is macroscopically isotropic (for example on account of symmetry) then its effective behavior is completely determined, and $\bar{\varphi}_\varepsilon(e) \leq (\text{tr } e/2)^2 + C'\sqrt{\varepsilon}|e^D|^2$. It follows that

$$\bar{\varphi}(e) \leq (\text{tr } e/2)^2 + o(|e|^2). \quad (5.31)$$

Thus the macroscopic energy of an isotropic polycrystal is flatter than quadratic, when restricted to the deviatoric subspace $\text{tr } e = 0$.

Proof. The proof of (5.30) is similar to that of (4.37). There is one technical difference: to justify the analogue of (4.40) we must use a version of Meyers' theorem adapted to the system of elasticity — see for example [3, 34].

Lurie and Cherkaev have shown that the shear modulus of an isotropic 2D polycrystal made from an elastic material with square symmetry is completely determined [50]. A more general result is proved in [4]. Specializing the formula of Lurie and Cherkaev to the case at hand, we see that if $\bar{\varphi}_\varepsilon$ is isotropic then

$$\bar{\varphi}_\varepsilon \left(\begin{array}{cc} a+b & c \\ c & a-b \end{array} \right) = a^2 + \bar{\mu}(b^2 + c^2) \quad \text{with } \bar{\mu} = \frac{\varepsilon}{-\varepsilon + \sqrt{2\varepsilon(1+\varepsilon)}}. \quad (5.32)$$

Since $\bar{\mu} \sim \sqrt{\varepsilon/2}$ as $\varepsilon \rightarrow 0$, (5.31) follows easily from (5.30) and (5.32). $\square$

5.4 Cubic–tetragonal polycrystals with $\langle 001 \rangle$ texture

This is our main three-dimensional example. We shall concentrate on the “symmetric” mesoscopic energy (5.6) and its associated sets $\mathcal{S}_{\text{symm}}$, $\mathcal{T}_{\text{symm}}$, $\mathcal{P}_{\text{symm}}$. The desired conclusions about $\mathcal{P}$ will be obtained as corollaries.

Throughout this section our attention is restricted to polycrystals with $\langle 001 \rangle$ texture: the grain shapes are arbitrary, but all the rotations $R(x)$ leave the x_3 axis unchanged. Our main goal is to prove that $\bar{\varphi}(e) + \bar{\varphi}(R_{\pi/4}^T e R_{\pi/4})$ satisfies the lower bound (5.9). Here $R_{\pi/4}$ is rotation by angle $\pi/4$ about the x_3 axis.

The argument is roughly parallel to that of the preceding section. Since the goal involves a sum of two energies, we must consider two displacement fields $u = (u_1, u_2, u_3)$ and $v = (v_1, v_2, v_3)$. We denote the associated displacement gradients by $M = Du$ and $N = Dv$. With the indexing convention $M_{ij} = u_{i,j}$, the useful translations are now

$$S_1(M, N) = \frac{1}{2} \sum_{i,j=1}^3 (M_{ii}M_{jj} - M_{ij}M_{ji}) + \frac{1}{2} \sum_{i,j=1}^3 (N_{ii}N_{jj} - N_{ij}N_{ji})$$

and

$$\begin{aligned} S_2(M, N) = & (M_{11}N_{12} - M_{12}N_{11}) + (M_{21}N_{22} - M_{22}N_{21}) + (M_{31}N_{32} - M_{32}N_{31}) + \\ & \frac{1}{2}(M_{33}N_{12} - M_{32}N_{13}) - \frac{1}{2}(M_{33}N_{21} - M_{31}N_{23}) - \frac{1}{2}(M_{12}N_{33} - M_{13}N_{32}) + \\ & \frac{1}{2}(M_{21}N_{33} - M_{23}N_{31}) . \end{aligned}$$

It is obvious from the definitions that S_1 and S_2 are null-Lagrangians, since each is a sum of 2×2 determinants. They are also rotationally invariant in the sense that

$$S_i(R^T M R, R^T N R) = S_i(M, N)$$

for any rotation fixing the x_3 axis. This is clear for S_1 . To see it for S_2 , we observe that if $M = (M_{ij})$, then under the action of $R =$ rotation by angle θ about the x_3 axis

$$\begin{aligned} (M_{11} - M_{22}, M_{12} + M_{21}) & \quad \text{transforms as a vector, rotated by angle } 2\theta; \\ (M_{13}, M_{23}) \text{ and } (M_{31}, M_{32}) & \quad \text{transform as vectors, rotated by angle } \theta; \\ M_{11} + M_{22}, M_{12} - M_{21} \text{ and } M_{33} & \quad \text{transform as scalars.} \end{aligned}$$

Therefore the first two terms of S_2 are rotationally invariant by the argument used for T_2 in Section 5.2; the third term is immediately seen to be invariant; and the last four terms are invariant because they may be regrouped as

$$\frac{1}{2}M_{33}(N_{12} - N_{21}) - \frac{1}{2}(M_{12} - M_{21})N_{33} + \frac{1}{2}(M_{31}N_{23} - M_{32}N_{13}) - \frac{1}{2}(M_{23}N_{31} - M_{13}N_{32}) .$$

We need two further observations about S_2 . Preparing to state them, we define for any $a, b, c, d, e \in \mathbb{R}$ the pair of matrices

$$\begin{aligned} M_0 &= \begin{pmatrix} a+b+c & 0 & d \\ 0 & a-b+c & e \\ d & e & -2a+c \end{pmatrix} \\ N_0 &= \begin{pmatrix} a+c & b & (d-e)/\sqrt{2} \\ b & a+c & (d+e)/\sqrt{2} \\ (d-e)/\sqrt{2} & (d+e)/\sqrt{2} & -2a+c \end{pmatrix} . \end{aligned} \tag{5.33}$$

Notice that M_0 is an arbitrary 3×3 matrix with diagonal upper left 2×2 block, and $N_0 = R_{\pi/4}^T M_0 R_{\pi/4}$. We also recall that V is the two-dimensional subspace (5.5) of diagonal, trace-free strains. Our two observations are as follows:

- (a) If a pair of 3×3 matrices M and N satisfy $\frac{1}{2}(M + M^T) \in V$ and $\frac{1}{2}(N + N^T) \in V$, then $S_2(M, N) = 0$.
- (b) The matrices M_0 and N_0 defined by (5.33) satisfy $S_2(M_0, N_0) = 2b^2 + O(d^2 + e^2)$.

Observation (a) follows easily from the calculation that if

$$\begin{aligned} \operatorname{div} u &= 0, & u_{1,3} + u_{3,1} &= 0, & u_{2,3} + u_{3,2} &= 0, \\ \operatorname{div} v &= 0, & v_{1,3} + v_{3,1} &= 0, & v_{2,3} + v_{3,2} &= 0 \end{aligned} \quad (5.34)$$

then

$$S_2(Du, Dv) = [e_{11}(u) - e_{22}(u)]e_{12}(v) - [e_{11}(v) - e_{22}(v)]e_{12}(u).$$

Observation (b) is a straightforward calculation. (The exact result is $S_2(M_0, N_0) = 2b^2 + \sqrt{2}(d^2 + e^2)$.)

Clearly S_2 is analogous to the translation T_2 of Section 5.3. To highlight the similarities we give the simple proof that

$$\bar{\varphi}(e) + \bar{\varphi}(R_{\pi/4}^T e R_{\pi/4}) = 0 \implies e = \begin{pmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & -2a \end{pmatrix} \text{ for some } a. \quad (5.35)$$

The hypothesis of (5.35) implies the existence of displacements u and v satisfying

$$\begin{aligned} u &= e \cdot x \text{ at } \partial\Omega, & \hat{\varphi}(R^T(x)e(u)R(x)) &= 0 \text{ in } \Omega; \\ v &= R_{\pi/4}^T e R_{\pi/4} \cdot x \text{ at } \partial\Omega, & \hat{\varphi}(R^T(x)e(v)R(x)) &= 0 \text{ in } \Omega. \end{aligned}$$

Using the relation

$$\hat{\varphi}(R^T e R) \geq \frac{1}{6}(\operatorname{tr} e)^2 + e_{13}^2 + e_{23}^2 \quad \text{when } R \text{ is a rotation about the } x_3 \text{ axis} \quad (5.36)$$

we deduce that u and v satisfy (5.34), whence

$$\operatorname{tr} e = e_{13} = e_{23} = 0.$$

Now comes the interesting part: showing that the upper left 2×2 block of e is a multiple of the identity. It suffices to work in a basis which makes this block diagonal, i.e. to consider $e = M_0$ and $R_{\pi/4}^T e R_{\pi/4} = N_0$ defined by (5.33) with $c = d = e = 0$. Using the rotational invariance of S_2 and observation (a) we get

$$S_2(Du(x), Dv(x)) = 0 \quad \text{pointwise.}$$

Using the fact that S_2 is a null-Lagrangian and observation (b) we get

$$\oint S_2(Du(x), Dv(x)) dx = 2b^2.$$

This validates the conclusion of (5.35).

We are ready to address the quantitative lower bound.

Theorem 5.6 *For the symmetrized cubic-tetragonal energy (5.6), any polycrystal with $\langle 001 \rangle$ texture satisfies*

$$\bar{\varphi}(e) + \bar{\varphi}(R_{\pi/4}^T e R_{\pi/4}) \geq c_1[(\text{tr } e)^2 + e_{13}^2 + e_{23}^2] + c_2 \rho^{-2}[(e_{11} - e_{22})^2 + 4e_{12}^2]^2. \quad (5.37)$$

Here c_1 and c_2 are absolute constants, independent of texture and the value of ρ . The estimate is asserted only when $(e_{11} - e_{22})^2 + 4e_{12}^2$ is sufficiently small.

Proof. We argue as in the proof of Theorem 5.1. It suffices to work in a basis where the upper left 2×2 block of e is diagonal, so our task is to show that if M_0 and N_0 are defined by (5.33) with $|b|$ sufficiently small then

$$\bar{\varphi}(M_0) + \bar{\varphi}(N_0) \geq c'_1[c^2 + d^2 + e^2] + c'_2 \rho^{-2} b^4. \quad (5.38)$$

Our starting point is the fact that $\bar{\varphi}(M) + \bar{\varphi}(N) - \lambda_1 S_1(M, N) - \lambda_2 S_2(M, N)$ equals

$$\min_{\substack{u=M \cdot x \text{ at } \partial\Omega \\ v=N \cdot x \text{ at } \partial\Omega}} \int_{\Omega} [\hat{\varphi}(R^T Du R) + \hat{\varphi}(R^T Dv R) - \lambda_1 S_1(Du, Dv) - \lambda_2 S_2(Du, Dv)] dx. \quad (5.39)$$

Since the translations are rotationally invariant, the integrand is equal to

$$\hat{\varphi}(R^T Du R) + \hat{\varphi}(R^T Dv R) - \lambda_1 S_1(R^T Du R, R^T Dv R) - \lambda_2 S_2(R^T Du R, R^T Dv R). \quad (5.40)$$

The following lemma provides a pointwise bound for (5.40).

Lemma 5.7 *There are positive constants A , C , and δ with the following property: for any $|\lambda_2| \leq \delta$ the choice $\lambda_1 = -A\lambda_2^2$ satisfies*

$$\min_{M, N \in \mathbb{R}^{3 \times 3}} \{\hat{\varphi}(M) + \hat{\varphi}(N) - \lambda_1 S_1(M, N) - \lambda_2 S_2(M, N)\} \geq -C\rho^2 \lambda_2^2. \quad (5.41)$$

The constants A , C , and δ are independent of ρ .

Given the Lemma, the proof of (5.38) is easy. One verifies that $S_1(M_0, N_0) = 6c^2 - 6a^2 - 2b^2 - 2d^2 - 2e^2 \leq 6c^2$ and $S_2(M_0, N_0) = 2b^2 + O(d^2 + e^2)$, so (5.39) gives

$$\begin{aligned} \bar{\varphi}(M_0) + \bar{\varphi}(N_0) &\geq -A\lambda_2^2 S_1(M_0, N_0) + \lambda_2 S_2(M_0, N_0) - C\rho^2 \lambda_2^2 \\ &\geq 2\lambda_2 b^2 - C\rho^2 \lambda_2^2 - O(\lambda_2^2 c^2 + |\lambda_2| d^2 + |\lambda_2| e^2) \end{aligned}$$

when $|\lambda_2| \leq \delta$. We also have

$$\bar{\varphi}(M_0) + \bar{\varphi}(N_0) \geq 3c^2 + 2d^2 + 2e^2$$

from (5.36). Averaging these inequalities gives

$$\bar{\varphi}(M_0) + \bar{\varphi}(N_0) \geq c'_1[c^2 + d^2 + e^2] + \lambda_2 b^2 - C\rho^2 \lambda_2^2 / 2$$

when $|\lambda_2|$ is sufficiently small. The value of λ_2 optimizing the last two terms is $b^2 / C\rho^2$, which is admissible when $|b|$ is sufficiently small. The resulting bound has the desired form (5.38). $\square$

Proof of Lemma 5.7. The first and main step is a bound for

$$\hat{\varphi}(M) + \hat{\varphi}(N) - \lambda_1 S_1(M, N) - \lambda_2 S_2(M, N) \quad (5.42)$$

analogous to (5.20). It will be derived by estimating S_1 and S_2 appropriately.

We can decompose a 3×3 matrix M into its symmetric and anti-symmetric parts,

$$e(M) = \frac{1}{2}(M + M^T) \text{ and } \omega(M) = \frac{1}{2}(M - M^T), \quad (5.43)$$

and the symmetric part can be further decomposed as

$$e(M) = \pi_V e(M) + (I - \pi_V) e(M) = e'(M) + e''(M) \quad (5.44)$$

with V defined by (5.5). Since S_2 is quadratic, writing $M = e'(M) + e''(M) + \omega(M)$ and $N = e'(N) + e''(N) + \omega(N)$ yields an expression for $S_2(M, N)$ as a sum of 9 terms. However *four of these terms vanish as a result of the special structure of S_2* . Indeed, our observation (a) can be stated as

$$e''(M) = 0 \text{ and } e''(N) = 0 \implies S_2(M, N) = 0.$$

Therefore S_2 has no terms coupling $(e'(M), e'(N))$, $(e'(M), \omega(N))$, $(\omega(M), e'(N))$, or $(\omega(M), \omega(N))$. We can therefore estimate it by

$$|S_2(M, N)| \leq c \{ |e''(M)| |e'(N)| + |e''(M)| |\omega(N)| + |e'(M)| |e''(N)| + |\omega(M)| |e''(N)| + |e''(M)| |e''(N)| \}$$

for a suitable choice of the constant c .

The estimate for S_1 is easier. Since $(\text{tr } M)^2$ and $(\text{tr } N)^2$ are positive we have

$$\begin{aligned} S_1(M, N) &= \frac{1}{2}[(\text{tr } M)^2 - \text{tr}(M^2)] + \frac{1}{2}[(\text{tr } N)^2 - \text{tr}(N^2)] \\ &\geq -\frac{1}{2}[\text{tr}(M^2) + \text{tr}(N^2)] \\ &= -\frac{1}{2}[|e(M)|^2 + |e(N)|^2] + \frac{1}{2}[|\omega(M)|^2 + |\omega(N)|^2]. \end{aligned}$$

Combining these results and using the formula (5.6) for $\hat{\varphi}$, we deduce after some manipulation that for any $\lambda_1 \leq 0$, (5.42) is bounded below by the sum

$$\begin{aligned} &[\frac{1}{4}(1 - 2|\lambda_1|)|e''(M)|^2 - c|\lambda_2||e''(M)||\omega(N)| + \frac{1}{2}|\lambda_1||\omega(N)|^2] + \\ &[\frac{1}{2}(|e'(M)| - \rho)_+^2 - \frac{1}{2}|\lambda_1||e'(M)|^2 - c|\lambda_2||e'(M)||e''(N)| + \frac{1}{8}|e''(N)|^2] + \\ &[\frac{1}{4}(1 - 2|\lambda_1|)|e''(N)|^2 - c|\lambda_2||e''(N)||\omega(M)| + \frac{1}{2}|\lambda_1||\omega(M)|^2] + \\ &[\frac{1}{2}(|e'(N)| - \rho)_+^2 - \frac{1}{2}|\lambda_1||e'(N)|^2 - c|\lambda_2||e'(N)||e''(M)| + \frac{1}{8}|e''(M)|^2] + \\ &[\frac{1}{8}|e''(M)|^2 - c|\lambda_2||e''(M)||e''(N)| + \frac{1}{8}|e''(N)|^2]. \end{aligned}$$

This is the anticipated analogue of (5.20).

The second step is to restrict the values of λ_1 and λ_2 appropriately, then minimize over M and N . We want the quadratic forms

$$\frac{1}{4}(1 - 2|\lambda_1|)x^2 - c|\lambda_2|xy + \frac{1}{2}|\lambda_1|y^2, \quad \frac{1}{2}|\lambda_1|x^2 - c|\lambda_2|xy + \frac{1}{8}y^2, \quad \frac{1}{8}x^2 - c|\lambda_2|xy + \frac{1}{8}y^2$$

to be positive definite, so we need

$$|\lambda_1| > 4c^2\lambda_2^2, \quad |\lambda_1|(1 - 2|\lambda_1|) > 2c^2\lambda_2^2, \quad 1 > 16c^2\lambda_2^2.$$

All three requirements are met by the choice $\lambda_1 = -A\lambda_2^2$, provided that A is sufficiently large and $|\lambda_2|$ is sufficiently small. For such λ_1 and λ_2 , (5.42) is bounded below by

$$\frac{1}{2}(|e'(M)| - \rho)_+^2 - |\lambda_1||e'(M)|^2 + \frac{1}{2}(|e'(N)| - \rho)_+^2 - |\lambda_1||e'(N)|^2. \quad (5.45)$$

Minimization over $|e'(M)|$ and $|e'(N)|$ gives

$$\min_{M, N \in \mathbb{R}^{3 \times 3}} (5.45) = \frac{-2A\rho^2\lambda_2^2}{1 - 2A\lambda_2^2}.$$

The right hand side is of order $-C\rho^2\lambda_2^2$ when λ_2 is sufficiently small, so this gives the desired result (5.41). $\square$

If a polycrystal has sufficient symmetry — for example, if $\bar{\varphi}(e) = \bar{\varphi}(R_{\pi/4}^T e R_{\pi/4})$ — then Theorem 5.6 restricts $\mathcal{P}_{\text{symm}}$ to the line through $\mathcal{T}_{\text{symm}}$. But it does not determine the extent of $\mathcal{P}_{\text{symm}}$ within this line.

We can do better. The following “classification theorem” shows that for all polycrystals, with no symmetry hypothesis aside from $\langle 001 \rangle$ texture, either (i) $\mathcal{P}_{\text{symm}} = \mathcal{T}_{\text{symm}}$, or else (ii) $\mathcal{P}_{\text{symm}}$ resembles a rotation of $\mathcal{S}_{\text{symm}}$. Polycrystals with sufficient symmetry must naturally be of type (i). Thus, for the symmetrized cubic–tetragonal energy (5.6) the Taylor estimate predicts more than just the dimension of $\mathcal{P}_{\text{symm}}$ — it even predicts its size.

Theorem 5.8 *For the energy (5.6), every polycrystal with $\langle 001 \rangle$ texture satisfies*

$$\bar{\varphi}(e) + \bar{\varphi}(R_\theta^T e R_\theta) \geq c_1 [(tr e)^2 + e_{13}^2 + e_{23}^2] + c_2 \rho^{-2} (\sin 2\theta)^2 [(e_{11} - e_{22})^2 + 4e_{12}^2]^2, \quad (5.46)$$

where R_θ denotes rotation by angle θ about the x_3 axis and the constants c_1, c_2 are independent of θ . We also have

$$\bar{\varphi}(e) \geq \frac{1}{2} [(|\pi_W e| - \rho)_+^2 + |\pi_{W^\perp} e|^2] \quad (5.47)$$

where W is smallest subspace containing V which is invariant under rotation about the x_3 axis:

$$W = \{e : tr e = 0, e_{13} = 0, e_{23} = 0\}.$$

As a consequence, one of the following alternatives must hold: either the Taylor estimate is exact,

$$\mathcal{P}_{\text{symm}} = \mathcal{T}_{\text{symm}}, \quad (5.48)$$

or else the polycrystal resembles a single crystal in the sense that

$$\mathcal{P}_{\text{symm}} \subset R_\theta \mathcal{S}_{\text{symm}} R_\theta^T \quad (5.49)$$

for some θ .

Proof. We argue as for Theorems 4.4 and 5.3. The proof of (5.46) is similar to that of (5.37), using $R_\theta^T M_0 R_\theta$ in place of N_0 . Inequality (5.47) follows from the analogous statement for $\hat{\varphi}$ via Jensen's inequality.

We turn to the classification of $\mathcal{P}_{symm}$. It is obvious from (5.46)–(5.47) that

$$\mathcal{P}_{symm} \subset \{e : \operatorname{tr} e = 0, e_{13} = 0, e_{23} = 0, |e| \leq \rho\}.$$

Suppose $\mathcal{P}_{symm}$ contains some strain e_0 whose upper left block is not a multiple of the identity. Then every element of $\mathcal{P}$ must be simultaneously diagonal with e_0 , by (5.46), and this implies (5.49). If, on the other hand, $\mathcal{P}$ contains only strains whose upper left block is a multiple of the identity, then we easily deduce (5.48). $\square$

All these results concern the “symmetrized” cubic–tetragonal energy (5.6) rather than the “real” cubic–tetragonal energy defined via (5.1). But we have the following easy corollary concerning the real set of recoverable strains $\mathcal{P}$:

Corollary 5.9 *For any polycrystal with $\langle 001 \rangle$ texture made from the cubic–tetragonal material, one of the following alternatives must hold: either*

- (i) $\mathcal{T} \subset \mathcal{P} \subset \mathcal{T}_{symm}$, in which case the Taylor estimate correctly predicts the dimension of $\mathcal{P}$; or
- (ii) $\mathcal{T} \subset \mathcal{P} \subset R_\theta \mathcal{S}_{symm} R_\theta^T$ for some θ , in which case the polycrystal resembles a single crystal.

Polycrystals with sufficient symmetry about the x_3 axis must naturally be of type (i).

Proof. This follows easily from Theorem 5.8, using the fact that $\mathcal{T} \subset \mathcal{P} \subset \mathcal{P}_{symm}$.

5.5 Some comments about 3D polycrystals

Most of our rigorous results are for scalar or 2D elastic model problems. Even the last example, concerning 3D cubic–tetragonal polycrystals, is somewhat two–dimensional due to the hypothesis of $\langle 001 \rangle$ texture. This section explains briefly the difficulties involved in extending our results to other classes of 3D polycrystals.

Cubic–tetragonal polycrystals with general texture. For polycrystals made from a cubic–tetragonal material with no restriction on the texture, the Taylor estimate $\mathcal{T}$ is trivial. We believe that $\mathcal{P}$ is also trivial, assuming sufficient symmetry.

The natural extension of our argument would consider a sum of six energies. It is convenient to label the associated displacement fields as $u^{ij} = (u_1^{ij}, u_2^{ij}, u_3^{ij})$, with the symmetry convention $u^{ij} = u^{ji}$. We shall use the notation

$$u_{k,l}^{ij} = \frac{\partial u_k^{ij}}{\partial x_l}, \quad M = (M_{kl}^{ij}) = (u_{k,l}^{ij}). \quad (5.50)$$

Notice that M_{kl}^{ij} is symmetric only in the upper indices, not the lower ones. The distinction between upper and lower indices has nothing to do with contravariance or covariance; rather, it serves to distinguish the different properties of the two pairs of indices.

The analogue of T_1 and S_1 is clearly

$$Q_1 = \sum_{i,j,k,l=1}^3 \left(M_{kk}^{ij} M_{ll}^{ij} - M_{kl}^{ij} M_{lk}^{ij} \right) .$$

This is obviously a null-Lagrangian. Since each quadratic term is obtained from an expression of the form $M_{kl}^{ij} M_{rs}^{pq}$ by contracting pairs of indices, it is rotationally invariant in the following sense: for any $R \in SO(3)$, if

$$\tilde{M}_{kl}^{ij} = R_{i'i} R_{j'j} R_{k'k} R_{l'l} M_{k'l'}^{i'j'} \quad (5.51)$$

then

$$Q_1(\tilde{M}) = Q_1(M) .$$

This is different from the notion of rotational invariance used in Sections 5.3 and 5.4: here the rotation acts on *all* the indices, whereas before it acted only on the “lower indices.”

The analogue of T_2 and S_2 is less clear, however. To make our usual argument work, we would need a Q_2 which is quasiconvex, rotationally invariant in the sense of (5.51), and which has the following two additional properties:

- (a) For any M , if $\frac{1}{2}[M^{ij} + (M^{ij})^T] \in V$ for every i, j then $Q_2(M) \leq 0$.
- (b) For any symmetric matrix e there exist rotations $\{R^{ij}\}_{i,j=1}^3$ such that $Q_2(M) \geq |e^D|^2$ when $M^{ij} = (R^{ij})^T e R^{ij}$ for every i, j .

Given such Q_1 and Q_2 , an argument similar to those of the previous sections would show that

$$\sum_{i,j} \bar{\varphi}(R^{ijT} e R^{ij}) \geq c_1(\text{tr } e)^2 + c_2 \rho^{-2} |e^D|^4 .$$

for any polycrystal made from the symmetrized cubic-tetragonal energy (5.6). It would follow that $\mathcal{P} = \{0\}$ for polycrystals with sufficient symmetry.

Unfortunately, we have not been able to identify a translation Q_2 satisfying the conditions listed above.

Polycrystals with special textures: elastic comparison bounds. For the 2D diagonal, trace-free material we used $\hat{\varphi}_\varepsilon$, the perturbed linearization of $\hat{\varphi}$, as a linear comparison material. For polycrystals with sufficient symmetry the linear effective behavior was completely determined, leading to the flatter-than-quadratic upper bound in Theorem 5.5.

For 3D polycrystals the linear effective behavior is not determined by symmetry alone. Therefore the elastic comparison bounds may be richer, i.e. they may carry some texture-dependent information. However, we know rather little about the range of possible values of $\bar{\varphi}_\varepsilon$. A natural question is this: do there exist 3D cubic-tetragonal polycrystals with special textures such that $\bar{\varphi}_\varepsilon(e)$ remains uniformly convex as the perturbation parameter ε tends to 0? For such polycrystals we would expect $\bar{\varphi}$ to behave quadratically near 0.

Cubic-trigonal polycrystals. For the 2D diagonal material we showed that our conjecture fails: $\mathcal{T}$ is one-dimensional but $\mathcal{P}$ can be a set with interior. The source of this behavior was unclear, but it seemed linked to the lower codimension of $\mathcal{S}$.

For a cubic–trigonal material there are 4 variants of martensite, so $\mathcal{S}$ is a 3 dimensional simplex in the 5 dimensional space of deviatoric strains. It is natural to ask whether our conjecture might fail in such a case, since the codimension of $\mathcal{S}$ is only 2.

To get a counterexample by the method of Section 5.2, we should start by finding a layered composite whose set of recoverable strains $\mathcal{P}$ has dimension greater than that of $\mathcal{S}$. A generic layered composite does not have this property. Indeed, consider the polycrystal obtained by mixing the material in its standard orientation with the material rotated by rotation R , in volume fractions γ and $1 - \gamma$ respectively, with layer normal n . If $\bar{e} \in \mathcal{P}$ then there must exist a pair of (constant) strains $e_1 \in \mathcal{S}$ and $e_2 \in RSR^T$ such that $\gamma e_1 + (1 - \gamma)e_2 = \bar{e}$ and $e_1 - e_2 = \frac{1}{2}(a \otimes n + n \otimes a)$. This can be viewed as a system of 18 linear equations for the 21 degrees of freedom $\bar{e}, e_1, e_2$ and a . So the set of possible $\bar{e}$ should be 3 dimensional – the same size as $\mathcal{S}$.

The situation might be different, however, for special choices of the parameters defining the polycrystal (the rotation R , the layering direction n , and the volume fraction γ). If for some choices the linear system cited above were degenerate then the resulting polycrystal would have a set $\mathcal{P}$ of dimension at least 4. It is quite plausible that this might occur; it is exactly what happens for the “3D diagonal elastic material.” If rank–one layering gives polycrystals with $\mathcal{P}$ of dimension 4, then we might expect rank–two layering to give polycrystals with $\mathcal{P}$ of dimension 5.

This argument suggests (but does not prove) that there should be cubic–trigonal polycrystals with special textures for which $\mathcal{P}$ is a set with interior in the space of deviatoric strains. But it also suggests that such behavior should be non–generic.

6 Discussion

This section summarizes our accomplishments, highlighting the strengths and shortcomings of our method.

6.1 Mechanical issues

We have identified the recoverable strains of a shape–memory polycrystal with the strains achievable by stress–free mixtures of martensite variants. When the basic crystal has many variants of martensite the Taylor estimate gives a nontrivial lower bound; we have argued that the actual set of recoverable strains should generally be larger. When the basic crystal has few variants of martensite the Taylor estimate is trivial; we have argued that the set of recoverable strains should also be trivial. Special textures can lead to nontrivial but lower–dimensional Taylor estimates; we have argued that for these polycrystals the set of recoverable strains should be similarly lower–dimensional.

Our model captures many of the trends observed experimentally. It explains why materials such as NiAl and FeNiC, which undergo cubic–tetragonal transformations, make poor shape–memory polycrystals. It explains why CuAlNi and TiNi, which undergo cubic–orthorhombic and cubic–monoclinic transformations, make better shape–memory polycrystals. And it explains why specially textured CuAlNi polycrystals have much larger recoverable strains than untextured ones.

However our analysis does not fully explain the excellent shape-memory behavior of TiNi. In this material, the recoverable strain of a single martensite variant ranges from 3 to 10%, depending on direction. Polycrystalline wires and strips are observed to recover 6 to 8% strain. Because the martensite has monoclinic-I symmetry, we do not know the exact form of its Taylor estimate. But we doubt that the excellent shape-memory behavior of this material can be explained by the Taylor estimate alone. The recoverable strain of TiNi wires varies considerably with processing and manufacturer; perhaps the best shape-memory wires have special textures, and correspondingly larger Taylor estimates. Our principles predict that for polycrystals made from a cubic-monoclinic material, $\mathcal{P}$ should be larger than $\mathcal{T}$; perhaps in the case of TiNi it is much larger.

Our model predicts that deformation beyond the set of recoverable strains will result in damage to the crystalline lattice. But it does not predict the consequences of such damage. The material might undergo plastic deformation or brittle failure. For copper based alloys such as CuAlNi and CuZnSn, where the martensite has orthorhombic or monoclinic-II symmetry, our analysis predicts that polycrystals should be able to recover some strain. That is indeed observed, however these materials are subject to brittle failure at larger strains, making them difficult to use in practice.

Our identification of “recoverable strain” with “stress-free microstructure” serves to reduce the problem to one of nonlinear homogenization. Of course this identification is just an approximation to the truth. It ignores issues of dissipation, dynamics and accessibility, and it disregards the effects of limited fineness. Yet our conclusions are in general agreement with experimental data for most cases. Thus our approach seems to be adequate, for the limited goal of understanding the dependence of recoverable strain on crystallography and texture. Explaining this adequacy — for example, explaining why the constraints of dynamics and accessibility are of lesser importance — remains a task for future research.

We have chosen to use the language of energy minimization, estimating the “macroscopic energy” $\bar{\varphi}$. The mechanical interpretation of our results raises an interesting question. Which is a better approximation of the true set of recoverable strains: the set where $\bar{\varphi} = 0$, or the set where $\bar{\varphi} < \delta$ for some $\delta > 0$? The many approximations implicit in our model might seem to favor the latter. But when $\bar{\varphi} > 0$ the system is, on average, stressed. Even a small average stress may be amplified greatly at multigrain junctions by the effect of elastic anisotropy (which makes junctions behave like corners). So strains for which $\bar{\varphi} > 0$ might easily lead to damage at grain junctions.

A related comment is in order concerning the local fields. We have routinely used the same Hooke’s law for each variant, since we are mainly interested in bounding the macroscopic energy $\bar{\varphi}$. In real materials the variants have different (symmetry-related) Hooke’s laws. Keeping this elastic inhomogeneity would have little influence on our bounds (except in materials “soft moduli”). But it would greatly change the local characteristics of the energy minimizers.

6.2 Mathematical issues

Our modelling hypotheses led us to a class of nonlinear homogenization problems. The (mesoscopic) energy of the “basic crystal” is degenerate in some directions, and we wish to know whether the energy of a polycrystal is similarly degenerate.

Our main accomplishment has been to discern certain principles which are in some sense “universal.” In particular, for polycrystals with sufficient symmetry:

- if the Taylor estimate $\mathcal{T}$ is trivial then the set of recoverable strains $\mathcal{P}$ should also be trivial;
- if the Taylor estimate $\mathcal{T}$ has maximal dimension then the set of recoverable strains $\mathcal{P}$ should generally be larger;
- if the Taylor estimate $\mathcal{T}$ has intermediate dimension, the set of recoverable strains $\mathcal{P}$ should be restricted to the same subspace.

We have given proofs (and some counterexamples) in various settings, using a combination of translation bounds, elastic comparison bounds, periodic homogenization and lamination.

The idea of considering *sums of energies* has been crucial. Our lower bounds, proved by translation, are texture-independent. They apply to *all* polycrystals — even single crystals, which are trivial examples of polycrystals. But the bounds involve sums of energies at *symmetry-related* strains. Therefore they look different and more powerful when applied to polycrystals with sufficient symmetry.

There is some danger in focussing on texture-independent bounds. This approach identifies the most extreme behavior, but not necessarily the typical behavior. We have dealt with this issue primarily through examples, which give some sense of what the typical behavior should be. Where possible we have given upper as well as lower bounds, bracketing the typical behavior in between.

We have conjectured that $\mathcal{P}$ has the same dimension as $\mathcal{T}$, for polycrystals with sufficient symmetry. But this conjecture should not be taken too literally. It is true in some settings (e.g. for cubic-tetragonal polycrystals with $\langle 001 \rangle$ texture) but false in others (e.g. the 2D diagonal material). We wonder what further conditions on $\mathcal{S}$ are needed to make the conjecture true. Perhaps it would suffice to know that for every simply-laminated polycrystal, the dimension of $\mathcal{P}$ is no greater than that of $\mathcal{S}$.

We find the success of the translation method rather mysterious. It seems natural enough for the two-variant scalar model, where the topology of the plane appears relevant and the determinant is the only null-Lagrangian in sight. But our elastic examples follow the same pattern. We wonder whether there may be some underlying structural reason. Is the existence of a translation like T_2 or S_2 necessary as well as sufficient for $\mathcal{T} = \{0\}$ to imply $\mathcal{P} = \{0\}$? Can our analysis be somehow extended to cover 3D cubic-tetragonal polycrystals with general textures?

For all its power, the translation method has one major failing: it does not easily incorporate textural information such as grain shapes, the orientation distribution or higher-order statistics. Perhaps such features might be captured by an appropriate use of the elastic comparison bound. Recent developments such as the work of Nesi [59, 60] may also be relevant.

Our entire discussion has been based on geometrically linear elasticity. Now that the linear case is partly understood, we hope some extension to the geometrically nonlinear setting might be possible.

Acknowledgements. Some of this research was conducted while KB held a postdoctoral position at the Courant Institute. This work was partially supported by grants from ARO (KB and RVK), NSF (KB and RVK), ONR (KB) and the Powell Foundation (KB).

References

- [1] Acerbi, E. and Fusco, N., “Semicontinuity problems in the calculus of variations”, *Arch. Rat. Mech. Anal.* 86 (1984) 125-145.
- [2] Attouch, H., *Variational Convergence of Functions and Operators*, Pitman, 1984.
- [3] Avellaneda, M., “Iterated homogenization, differential effective medium theory, and applications”, *Comm. Pure Appl. Math.* 40 (1987) 803-847.
- [4] Avellaneda, M., Cherkaev, A.V., Gibiansky, L.V., Milton, G.W., and Rudelson, M., “A complete characterization of the possible bulk and shear moduli of planar polycrystals”, *J. Mech. Phys. Solids*, submitted.
- [5] Avellaneda, M., Cherkaev, A.V., Lurie, K.A., and Milton, G.W., “On the effective conductivity of polycrystals and a three-dimensional phase-interchange inequality”, *J. Appl. Phys.* 63 (1988) 4989-5003.
- [6] Ball, J.M. and James, R.D., “Fine phase mixtures as minimizers of energy”, *Arch. Rat. Mech. Anal.* 100 (1987) 13-52.
- [7] Ball, J.M. and James, R.D., “Proposed experimental tests of a theory of fine microstructure and the two well problem”, *Phil. Trans. Roy. Soc. London* 338A (1992) 389-450.
- [8] Bhattacharya, K., “Self-accommodation in martensite”, *Arch. Rat. Mech. Anal.* 120 (1992) 201-244.
- [9] Bhattacharya, K. “Comparison of the geometrically nonlinear and linear theories of martensitic transformation”, *Cont. Mech. Thermodyn.* 5 (1993) 205-242.
- [10] Bhattacharya, K., Firoozye, N.B., James, R.D. and Kohn, R.V., “Restrictions on microstructure”, *Proc. Roy. Soc. Edinburgh* 124A (1994) 843-878.
- [11] Bhattacharya, K. and Kohn, R.V., “Symmetry, texture, and the recoverable strain of shape-memory polycrystals”, *Acta Metall. Mater.*, in press.
- [12] Bhattacharya, K., Kohn, R.V. and Kozlov, S., “Some examples of nonlinear homogenization involving nearly degenerate energies”, in preparation.
- [13] Bishop, J.F.W. and Hill, R., “A theory of the plastic distortion of a polycrystalline aggregate under combined stresses”, *Phil. Mag.* 42 (1951) 414-427.
- [14] deBotton, G. and Ponte Castañeda, P., “Variational estimates for the creep behavior of polycrystals”, *Proc. R. Soc. Lond. A* 448 (1995) 121-142.

- [15] Boyd, J. and Lagoudas, D., “A thermodynamical constitutive model for shape memory materials. Part I: The monolithic shape memory alloy and Part II: The SMA composite material”, submitted to *Int. J. Plasticity*.
- [16] Brinson, L.C. and Moran, B. eds., *Mechanics of phase transformations and shape memory alloys*, AMD-Volume 189, ASME, 1994.
- [17] Bruno, O., Reitich, F. and Leo, P., “The overall elastic energy of polycrystalline martensitic solids,” submitted to *J. Mech. Phys. Solids*.
- [18] Chipot, M. and Kinderlehrer, D., “Equilibrium configurations of crystals”, *Arch. Rat. Mech. Anal.* 103 (1988) 237-277.
- [19] Dacorogna, B., *Direct Methods in the Calculus of Variations*, Springer-Verlag, 1989.
- [20] Dal Maso, G., *An Introduction to Γ -Convergence*, Birkhauser, 1993.
- [21] De Simone, A. and Friesecke, G., “On the problem of two linearized wells”, submitted to *Calc. of Variations and PDE*.
- [22] Dykhne, A.M., “Conductivity of a two-dimensional two-phase system”, *Soviet Physics JETP* 32 (1971) 63-65.
- [23] Enami, K., Martynov, V.V., Tomie, T., Khandros, L.G. and Nenno, S., “Deformation behavior of Ni-Al L1₀ (3R) martensite”, *Trans. Jap. Inst. Metals* 22 (1981) 357-366.
- [24] Eucken, S. and Hirsch, J., “The effect of textures on shape memory behaviour”, *Mat. Sci. Forum* 56-58 (1990) 487-492.
- [25] Falk, F., “Pseudoelastic stress-strain curves of polycrystalline shape memory alloys calculated from single crystal data”, *Int. J. Engng. Sci.* 27 (1989) 277-284.
- [26] Fannjiang, A. and Papanicolaou, G., “Convection enhanced diffusion for periodic flows”, *SIAM J. Appl. Math.* 54 (1994) 333-408.
- [27] Firoozye, N.B., “Optimal use of the translation method and relaxation of variational problems”, *Comm. Pure Appl. Math.* 44 (1991) 643-678.
- [28] Fonseca, I., “The lower quasiconvex envelope of the stored energy function for an elastic crystal”, *J. Math. Pures Appl.* 67 (1988) 175-195.
- [29] Francfort, G. and Müller, S., “Combined effects of homogenization and singular perturbation in elasticity”, *J. Reine Angew. Math.* 454 (1994) 1-35.
- [30] Francfort, G. and Murat, F., “Optimal bounds for conduction in two-dimensional, two-phase, anisotropic media”, in R.J. Knops and A.A. Lacey, eds., *Non-Classical Continuum Mechanics*, London Math. Society Lecture Notes Vol. 122, Cambridge University Press, 1987, 197-212.
- [31] Francfort, G. and Murat, F., “Homogenization and optimal bounds in linear elasticity”, *Arch. Rat. Mech. Anal.* 94 (1986) 307-334.

- [32] Funakubo, H., *Shape Memory Alloys*, translated from the Japanese by J.B. Kennedy, Gordon and Breach, 1987.
- [33] Geymonat, G., Müller, S., and Triantafyllidis, N., “Homogenization of nonlinearly elastic materials, microscopic bifurcation and macroscopic loss of rank-one convexity”, *Arch. Rat. Mech. Anal.* 122 (1993) 231-290.
- [34] Giaquinta, M., *Multiple Integrals in the Calculus of Variations and Nonlinear Elliptic Systems*, Princeton University Press, 1983.
- [35] Golden, K. and Papanicolaou, G.C., “Bounds for effective parameters of heterogeneous media by analytic continuation”, *Comm. Math. Phys.* 90 (1983) 473-491.
- [36] Gotthard, R. and Van Humbeeck, J., eds., Proceedings of the International Conference on Martensitic Transformations (ICOMAT 95), *J. de Physique Colloque*, to appear.
- [37] Jikov, V.V., Kozlov, S.M., and Oleinik, O.A., *Homogenization of Differential Operators and Integral Functionals*, Springer-Verlag, 1994.
- [38] Kajiwara, S. and Kikuchi, T., “Shape memory effect and related transformation behavior in Fe-Ni-C alloys”, *Acta Metall. Mater.* 38 (1990) 847-855.
- [39] Keller, J.B., “A theorem on the conductivity of a composite medium”, *J. Math. Phys.* 5 (1964) 548-549.
- [40] Khachaturyan, A.G., *Theory of Structural Phase Transformations in Solids*, John Wiley & Sons, 1983.
- [41] Kohler, W. and Papanicolaou, G.C., “Bounds for the effective conductivity of random media”, in R. Burridge et al. eds., *Macroscopic Properties of Disordered Media*, Lecture Notes in Physics Vol. 154, Springer-Verlag, 1982, 111-130.
- [42] Kim, Y.D. and Wayman, C.M., “Shape recovery and phase transformation behavior in Ni-Al alloys”, *Metall. Trans.* 23A (1992) 2981-2986.
- [43] Kinderlehrer, D. and Pedregal, P., “Characterizations of gradient Young measures”, *Arch. Rat. Mech. Anal.* 115 (1991) 329-365.
- [44] Kohn, R.V., “The relaxation of a double-well energy”, *Cont. Mech. Thermodyn.* 3 (1991) 193-236.
- [45] Kohn, R.V. and Little, T., in preparation.
- [46] Kohn, R.V. and Vogelius, M., “Relaxation of a variational problem from impedance computed tomography”, *Comm. Pure Applied Math.* 40 (1987) 745-777.
- [47] L’Excellent, C. ed., “Mechanisms and mechanics of solid-solid phase transformations: MECAMAT 95”, *Journal de Physique IV*, to appear.
- [48] Ling, H.C. and Kaplow, R., “Stress-induced shape changes and shape memory in the R and martensite transformations in equiatomic NiTi”, *Metall. Trans.* 12A (1981) 2101-2111.

- [49] Ling, H.C and Kaplow, R., “Variation in the shape recovery temperature in Ni-Ti alloys”, *Mat. Sci. Engng.* 48 (1981) 241-247.
- [50] Lurie, K.A. and Cherkayev, A.V., “G- closure of some particular sets of admissible material characteristics for the problem of bending of thin plates”, *J. Optim. Th. Appl.* 42 (1984) 305-316.
- [51] Marcellini, P., “Periodic solutions and homogenization of nonlinear variational problems”, *Ann. Mat. Pura Appl.* 117 (1978) 139-152.
- [52] Meyers, N.G., “An L^p estimate for the gradient of solutions of second order elliptic divergence equations”, *Ann. Scuola Norm. Sup. Pisa* 17 (1963) 189-206.
- [53] Michel, J.C. and Suquet, P.M., “On the strength of composite materials: variational bounds and computational aspects”, in M.P. Bendsoe and C.A. Mota Soares, eds., *Topology Design of Structures*, Kluwer, 1993, 355-374.
- [54] Milton, G.W., “On characterizing the set of possible effective tensors of composites: The variational method and the translation method”, *Comm. Pure Appl. Math.* 43 (1990) 63-125.
- [55] Miyazaki, S., Otsuka, K. and Suzuki, Y., “Transformation pseudoelasticity and deformation behavior in Ti-50.6at.%Ni alloy”, *Scripta Metall.* 15 (1981) 287-292.
- [56] Miyazaki, S., Kimura, S., Otsuka, K. and Suzuki, Y., “The habit plane and transformation strains associated with the martensitic transformation in NiTi single crystals”, *Scripta Metall.* 18 (1984) 883-888.
- [57] Miyazaki, S. and Otsuka, K., “Development of shape memory alloys”, *ISIJ Inter.* 29 (1989) 353-377.
- [58] Müller, S. and Šverák, V., “Attainment results for the two-well problem by convex integration”, in preparation.
- [59] Nesi, V., “Quasiconformal mappings as a tool to study certain two dimensional G-closure problems”, *Arch. Rat. Mech. Anal.*, to appear.
- [60] Nesi, V., “Homogenized coefficients, quasiregular mappings, and higher integrability of the gradients in two dimensional linear conductivity: an elementary connection”, preprint.
- [61] Olson, T., “Improvements on Taylor’s upper bound for rigid-plastic composites”, *Mat. Sci. Engng. A* 175 (1994) 15-20.
- [62] Ono, N. and Sato, A., “Plastic deformation governed by the stress induced martensitic transformation in polycrystals”, *Trans. Jap. Inst. Metals* 29 (1988) 267-273.
- [63] Ono, N., Satoh, A., and Ohta, H., “A discussion on the mechanical properties of shape memory alloys based on a polycrystal model”, *Mat. Trans. Jap. Inst. Metals* 30 (1989) 756-764.

- [64] Ono, N., “Pseudoelastic deformation in a polycrystalline Cu-Zn-Al shape memory alloy”, *Mat. Trans. Jap. Inst. Metals* 31 (1990) 381-385.
- [65] Ono, N., “Pseudoelastic behavior in a polycrystalline CuAlNi shape memory alloy in comparison with the modified Taylor model”, *Mat. Trans. Jap. Inst. Metals* 31 (1990) 855-860.
- [66] Patoor, E., Eberhardt, A. and Berveiller, M., “Micromechanical modelling of superelasticity in shape memory alloys”, in M. Chipot, ed., *Progress in Partial Differential Equations: the Metz Surveys 2*, Pitman Research Notes in Mathematics 296, 1993, 38-54.
- [67] Patoor, E., Bensalah, M., Eberhardt, A. and Berveiller, M., “Micromechanical aspects of shape memory behavior”, in C.M. Wayman and J. Perkins, eds., *Proc. ICOMAT-92*, Monterey Inst. Adv. Studies, 1994, 401-406.
- [68] Piao, M., Otsuka, K., Miyazaki, S. and Horikawa, H., “Mechanism of the A_s temperature increase by pre-deformation in the thermoelastic alloys”, *Mater. Trans. Japan Inst. Metals* 34 (1993) 919-929.
- [69] Ponte Castañeda, P., “The effective mechanical properties of nonlinear isotropic composites”, *J. Mech. Phys. Solids* 39 (1991) 45-71.
- [70] Ponte Castañeda, P., “Variational methods for estimating the effective behavior of nonlinear composite materials”, in *Proc. 8th International Symposium on Continuum Models and Discrete Systems (CMDS 8)*, K.Z. Markov, ed., World Scientific, to appear.
- [71] Potapov, P.L., Polyakova, N.A., and Udovenko, V.A., “A shape memory behavior of powder 64.0Ni-Al alloy”, in *Proc. ICOMAT-95*, *J. de Physique — Colloque*, to appear.
- [72] Roytburd, A.L., “Martensitic transformation as a typical phase transformation in solids”, *Solid State Phys.* 33 (1978) 317-390.
- [73] Sab, K., “On the homogenization and the simulation of random materials”, *Euro. J. Mech. A/Solids* 11 (1992) 585-607
- [74] Saburi, T. and Nenno, S., “The shape memory effect and related phenomena”, in H.I. Aaronson et al. eds., *Proc. Int. Conf. on Solid-Solid Phase Transformations*, The Metall. Soc. AIME, New York (1981) 1455-1479.
- [75] Saburi, T., Tatsumi, T. and Nenno, S., “Effects of heat treatment on mechanical behavior of Ti-Ni-alloys”, *J. de Physique* 43 (1982) Colloque C4, 261-266.
- [76] Saburi, T., Yoshida, M. and Nenno, S., “Deformation behaviour of shape-memory Ti-Ni alloy crystals”, *Scripta Metall.* 18 (1984) 363-366.
- [77] Silberschmidt, V.V., “On statistical thermodynamics of deformation twinning”, *Cont. Mech. Thermodyn.* 4 (1992) 269-277.

- [78] Sun, Q.P. and Hwang, K.C., “Micromechanics modelling for the constitutive behavior of polycrystalline shape memory alloys I. Derivation of general relations” and “Micromechanics modelling for the constitutive behavior of polycrystalline shape memory alloys II. Study of the individual phenomena”, *J. Mech. Phys. Solids* 41 (1993) 1-17 and 19-33.
- [79] Tadaki, T., Otsuka, K. and Shimizu, K., “Shape memory alloys”, *Ann. Reviews Mater. Sci.* 18 (1988) 25-45.
- [80] Talbot, D.R.S. and Willis, J.R., “Upper and lower bounds for the overall properties of a nonlinear composite dielectric. I. Random microgeometry”, *Proc. Roy. Soc. Lond.* 447A (1994) 365-384.
- [81] Talbot, D.R.S. and Willis, J.R., “Upper and lower bounds for the overall properties of a nonlinear composite dielectric. II. Periodic microgeometry”, *Proc. Roy. Soc. Lond.* 447A (1994) 385-396.
- [82] Tartar, L., “Estimations fines des coefficients homogénéisés”, in P. Kree, ed., *Ennio de Giorgi Colloquium*, Research Notes in Mathematics Vol. 125, Pitman, 1985, 168-187.
- [83] Taylor, G.I., “Plastic strain in metals”, *J. Inst. Metals* 62 (1938) 307-324.
- [84] Wayman, C.M., “Shape memory and related phenomena”, *Prog. Mater. Sci.* 36 (1992) 203-224.