THE OVERALL ELASTIC ENERGY OF
POLYCRYSTALLINE MARTENSITIC SOLIDS

By

Oscar P. Bruno
Fernando Reitich
and
Perry H. Leo

IMA Preprint Series # 1387
March 1996

INSTITUTE FOR MATHEMATICS AND ITS APPLICATIONS
UNIVERSITY OF MINNESOTA
514 Vincent Hall
206 Church Street S.E.
Minneapolis, Minnesota 55455
The overall elastic energy of polycrystalline martensitic solids

Oscar P. Bruno*  Fernando Reitich†  Perry H. Leo‡

Abstract

We are concerned with the overall elastic energy in martensitic polycrystals. These are polycrystals whose constituent crystallites can undergo shape-deforming phase transitions as a result of changes in their stress or temperature. We approach the problem of calculation of the nonlinear overall energy via a statistical optimization method which involves solution of a sequence of linear elasticity problems. As a case study we consider simulations on a two-dimensional model in which circular randomly-oriented crystallites are arranged in a square pattern within an elastic matrix. The performance of our present code suggests that this approach can be used to compute the overall energies in realistic three-dimensional polycrystals containing grains of arbitrary shape.

In addition to numerical results we present upper bounds on the overall energy. Some of these bounds apply to the square array mentioned above. Others apply to polycrystals containing circular, randomly oriented crystallites with sizes ranging to infinitesimal, and no intergrain matrix. The square-array bounds are consistent with our numerical results. In some regimes they approximate them closely, thus providing an insight on the convergence of the numerical method. On the other hand, in the case of the random array the bounds carry substantial practical significance, since in this case the energy contains no artificial contributions from an elastic matrix. In all the cases we have considered our bounds compare favorably with those obtained under the well known Taylor hypothesis; they show that, as far as polycrystalline martensite is concerned, calculations of the elastic energy based on the Taylor assumption may lead to substantial overestimates of this quantity.

*Applied Mathematics, California Institute of Technology, Pasadena, CA 91125
†Department of Mathematics and Center for Research in Scientific Computation, North Carolina State University, Raleigh, NC 27695-8205
‡Department of Aerospace Engineering and Mechanics, University of Minnesota, Minneapolis, MN 55455
1 Introduction

Unlike the theory of martensitic transformations in single crystals, which has been advanced considerably in the last forty years (Wechsler, Lieberman and Read, 1953; Bowles and Mackenzie, 1954; Eshelby, 1957; Khachatryan, 1967; Roitburd, 1973; Ericksen, 1975; James, 1986; Otsuka and Shimizu, 1986; Ball and James, 1987; Kohn, 1991), the study of these transitions in polycrystalline structures has only been considered recently (Ono and Sato, 1988; Tanaka, Kobayashi and Sato, 1986; Patoor, Eberhardt and Berveiller, 1987; Boyd and Lagoudas, 1994; Bhattacharya and Kohn, 1995). While the fundamental phase change associated with Martensite can certainly be observed and modeled more easily in single crystals, the study of these materials is sufficiently mature at this time as to justify attempts at understanding the complicated additional effects that take place in the polycrystalline case. Such understanding is of obvious importance in most technological applications, in which single crystals can seldom be used due to the substantial expense involved in their production.

In this paper we study the overall (or effective, or homogenized) strain energy in polycrystals. In particular we present both numerical calculations and closed form bounds for the energy. Our numerical method for this non-linear problem is based on linear elasticity and minimization via simulated annealing. In fact, one of our goals here is to determine whether a combination of simulated annealing, Eshelby integrals and linear elasticity can be used, as proposed in Bruno (1995), to solve the challenging and important problem of computation of nonlinear homogenized energies. As a case study we thus consider simulations for an elastically isotropic two-dimensional model, in which circular randomly-oriented crystallites are arranged in a square pattern within an elastic matrix. The performance of the present code suggests that this approach can be used to compute overall energies in realistic three-dimensional polycrystals containing anisotropic grains of arbitrary shape.

In addition to numerical results we present upper bounds on the effective energy. Some of these bounds apply to the square array mentioned above. Others apply to polycrystals containing circular, randomly oriented crystallites with sizes ranging to infinitesimal, and no intergrain matrix. The square-array bounds are consistent with our numerical results. In some regimes they approximate them closely, thus providing an insight on the convergence of the numerical method, see §§4.2, 5. On the other hand, in the case of the random array the bounds carry substantial practical significance, since in this case the energy contains no artificial contributions from an elastic matrix. In all the cases we have considered our bounds compare favorably with those obtained under the well known Taylor hypothesis; they show that, as far as polycrystalline martensite is concerned, calculations of the elastic energy based on the Taylor assumption may lead to substantial overestimates of this quantity, see §5.

Martensitic transformations are shape-deforming phase transitions which can be induced in certain alloys as a result of changes in the imposed strains, stresses or temperatures. These transitions, which lead to the shape memory effect (that is the recovery of shape as a response to temperature change) occur when a crystalline solid transforms between its parent phase
(Austenite) and any of a number of variants of the product phase (Martensite). Typically, the crystalline structure of each of the Martensite variants has less symmetry than that of the Austenite. Further, the lattices associated with any two of the Martensite variants are identical, and can be superimposed by means of a rotation in the symmetry group of the parent phase. These observations lie at the core of the Crystallographic Theory of Martensite, which has provided an understanding on a number of geometric observables associated with these phase transitions—including the well known occurrence in single crystals of a planar interface separating Austenite on one hand, and fine alternating layers or twins of two different variants of Martensite on the other, see (Wechsler, Lieberman and Read, 1953; Bowles and Mackenzie, 1954; Wayman, 1964).

Since all the phases occurring in this Austenite/twinned-Martensite observation are essentially unstressed, the fineness in the twinned structure mentioned above is interpreted within this geometric theory as the response needed to avoid slips or cracks and thus maintain a coherent interface. A more precise description of this interface and other observed microstructures can be obtained by consideration of the elastic energy within the material. Indeed, in materials which can be modeled in the ideal non-dissipative framework considered here, the observed equilibrium patterns must be associated with states of (local or global) minimum energy, since otherwise non-equilibrated forces must necessarily occur and lead to motions. This simple but fundamental insight is inherent in both the nonlinear but geometrically-linear theory of (Khachaturyan, 1967; Roitburd, 1973) as well as in the more general geometrically nonlinear theory of (James, 1986; Ball and James, 1987). The main difference between these approaches relates to an assumption of smallness of the stress–free strains in the geometrically linear setup; see (Kohn, 1991; Ball and James, 1992; Bhattacharya, 1993) for a complete comparative discussion of these theories.

Here we are concerned with the macroscopic behavior of martensitic polycrystalline aggregates, and we are thus led to a study of their homogenized energy. The homogenized energy associated with a given strain tensor in a polycrystal equals the energy stored in a sample of the material whose boundaries are deformed homogeneously according to that tensor, in the limit of a large sample (for which the grains are infinitely smaller than the sample itself). Of course, one could consider homogenized energies associated with general boundary conditions. But, clearly, calculations associated with homogeneous boundary conditions in a body with a simple shape are much simpler than those associated with general boundary conditions imposed on a body of complicated shape. Fortunately, it is often possible to organize a calculation on a complicated configuration by dividing it into a large number of parts—which are both sufficiently small with respect to macroscopic length-scales and sufficiently large with respect to grain sizes—so as to genuinely allow for the assumptions that the displacements on the boundaries of the parts are given by a linear function, and that the associated energies are given by the homogenization result. This is the basis for a method of optimal design based on homogenization, see (Tartar, 1984; Lurie, Cherkaev and Fedorov, 1982), which uses the homogenized energy to study physical fields within an arbitrary structure under arbitrary boundary conditions.
For instance, one could apply these methods and use the homogenized energy for NiTi polycrystals to study the occurrence of two (macroscopic) interfaces during the elongation of polycrystalline NiTi wires, as reported in Leo, Shield and Bruno (1993). Applications to the study of the onset of plasticity, dissipation and hysteresis in shape memory polycrystals can also be envisioned, see (Ono and Sato, 1988; Bruno, 1995; Bruno, Leo and Reitich, 1995). Another example of interest concerns the energetics in single crystals. Indeed, single crystals can be treated rigorously with our methods, by assuming the random field of crystalline orientations is a given constant. The reduction by means of homogenization and methods of optimal design mentioned above would then permit one to study singly–crystalline microstructure in a mathematical framework in which well known computational problems associated with microstructure (Collins, Kinderlehrer and Luskin, 1991; Collins and Luskin, 1988) have been eliminated. Topics on optimal design cannot be pursued here at any length, however, and their consideration will be left for future work.

Theories of polycrystalline martensite have been advanced in which the nucleation and progress of the phase transition are governed by phenomenological criteria relating elastic and thermodynamic variables (Patoor, Eberhardt and Berveiller, 1987; Tanaka, Kobayashi and Sato, 1986; Boyd and Lagoudas, 1994). Closer in spirit to our work, approaches have been presented which focus on consideration of the energetics of pseudoelasticity, see (Ono and Sato, 1988; Bhattacharya and Kohn, 1995). It is useful here to recall some elements from these contributions. The work in Ono and Sato (1988), for example, is based on a hypothesis (first proposed by Taylor (1938) in the context of plasticity) that the strain is constant throughout the polycrystal. As pointed out in Ono (1991), calculations based on this principle necessarily yield upper bounds for the energy. (The actual results of (Ono and Sato, 1988; Ono, 1991) were obtained under the single assumption that the deviatoric part of the strain is constant, and they include an additional approximation relating to the hydrostatic contribution.) The presentation in Bhattacharya and Kohn (1995), on a related context, contains exact calculations for the (often non-trivial) set $T$ of strains that can be expressed as arbitrary rotations of the possible transformation strains of a single crystal. These calculations have a bearing on our discussion. Indeed $T$ is contained in the set $Z$ of homogeneous overall strains for which the effective energy vanishes. That is, for $\epsilon \in T$, Taylor’s hypothesis is guaranteed to yield the polycrystalline elastic energy (which equals zero) correctly.

While it is quite clear that the Taylor hypothesis is not exactly satisfied in a martensitic polycrystal under general strains, it has been argued that only small departures from its predictions could occur. At the basis of such arguments is the rationale that the large transformation strains found in shape memory alloys would lead to cracks at intergrain boundaries, unless the pseudoelastic deformation is the same in any pair of neighboring grains and thus everywhere in the polycrystal. In this connection, comparison of our numerical calculations and bounds with bounds obtained under the Taylor hypothesis lead us to the following remarks. Our bounds are tighter than the Taylor bounds in all the examples we have considered, and they necessarily vanish whenever the latter do. The Taylor assumption leads to curves which follow qualitative trends correctly, which yield perfectly accurate results
in some regimes but which lead to important departures in others. In some cases these
departures amount to energy overestimates of over 50%, see §5.

The comparison of exact calculations of the Taylor set $T$ with experimental data reported
in Bhattacharya and Kohn (1995) shows that $T$ describes well the trends of recoverability
in shape memory alloys, although it generally underestimates the extent of the recoverable
strains. Energy calculations, both at the microscopic and macroscopic level are relevant
in this connection. On the one hand, they may reveal zero energy configurations in $Z \setminus T$.
Further, combined with experimental results, they may help explain the occurrence of
macroscopically stress-free strains recoverable by shape memory polycrystals beyond the
zero energy sets $T$ and $Z$. (The occurrence of such strains can probably be linked to
microscopic dissipative mechanisms, related to the pseudoelastic hysteresis, which stabilize
positive energy configurations. See Bruno (1995).)

In what follows we will consider model polycrystals whose crystallites enjoy fairly general
modes of transformation, including, possibly, homogeneous strains such as those associated
with singly-crystalline microstructure within the grains. (Completely arbitrary modes of
transformation could be incorporated in our algorithms, and, indeed, while we consider a
non-linear but geometrically linear theory of martensite (Khachaturyan, 1967; Roitburd,
1973), our approach based on iterated solution of linear problems can be applied to the
geometrically nonlinear theory (James, 1986; Ball and James, 1987) as well.) To gain insight
in our numerical method, however, we consider first a case in which each one of the randomly
oriented grains in the polycrystal can either transform fully into a single variant of Martensite
or not transform at all. This may be a reasonable approximation in cases in which the
crystallites are too small to sustain microstructure. Thus, in the case the parent phase has
square symmetry, this simplest scenario assumes each crystallite can support three possible
states: either not transformed, or transformed (with transformation strain in accordance
with the orientation of the crystallite) into one of two possible variants of martensite.

The energy minimization in this case could then proceed by examining each one of the $3^{n^2}$
combinations which are possible in a two-dimensional polycrystal containing $n^2$ grains, and
obtaining, by inspection, the minimum value of the energy. Of course, such a simple-minded
approach would lead to an enormous computational expense, even in this simplest discrete
framework, and even for small values of $n$. Thus, we resort to numerical minimization by
means of simulated annealing (Metropolis, Rosenbluth, Rosenbluth and Teller, 1953; Kirk-
patrick, Gelatt and Vecchi, 1983). This optimization algorithm, which is well adapted to
the treatment of Ising-type optimization problems like ours, allows us to compute homogene-
nized energies efficiently and accurately. (See also Wen, Khachaturyan and Morris (1981)
where a related optimization method was used to obtain minimum energy states in a system
consisting of a prescribed number of precipitate particles within an elastic matrix.)

As we mentioned, it is easy to allow for larger classes of transformation modes, and
thus grain transformations spanning possibly a continuum can be accounted for within this
framework (see §§2, 4, 5). Interestingly, the convergence rate of our algorithm remains
virtually unaffected by the higher complexity associated with this increase in generality.

Besides the assumption of a two-dimensional geometry, the most important simplification implied by the setting considered here (circular inclusions and isotropic elasticity) is that the associated linear elasticity problems for single inclusions can be solved in closed form. In particular, our calculations do not incorporate effects such as those arising from anisotropy or grain corners. Both numerical calculations and bounds can be extended to general polycrystals—using, for example, perturbation expansions in the anisotropy and numerical solutions for single inclusions. Whereas a substantial increase in the complexity is to be expected when considering general three dimensional polycrystals with anisotropic inclusions of various shapes, the performance of the present numerics and bounds suggest that our approach should extend successfully to the general case.

2 Elasticity and nonlinear effective energy

Eshelby (1957) considered an inclusion surrounded by an elastic matrix and calculated the strain-energy in the system after the inclusion "transforms"—that is, after the inclusion undergoes a shape deforming phase transition which, in absence of the elastic constraints imposed by the matrix, would lead to a homogeneous strain $\epsilon T$ in the inclusion. In what follows we study the energy in a system consisting of a large number of small transforming inclusions in a matrix under a homogeneous applied deformation. Here we will assume a distribution of grains in two-dimensional space, and transformation strains which are constant within each grain. The transformation strains $\epsilon T$ in the various grains will be allowed to vary in an arbitrary manner from grain to grain as long as the complete configuration remains statistically homogeneous, as explained below.

2.1 Geometry, statistics, elastic constants

We consider an array of grains of arbitrary shape distributed throughout the two-dimensional space. We will assume a numbering $G^{(1)}$, $G^{(2)} \cdots$ on the grains, and we will use functions $\chi^{(n)}$ which are equal to 1 in the region occupied by $G^{(n)}$, and which vanish identically elsewhere:

$$G^{(n)} = \{ x : \chi^{(n)}(x) = 1 \}.$$ 

The array $(G^{(n)})$ will be seen as a random object. The corresponding probability space is defined by a set $G$ of arrays $(G^{(n)})$ together with a probability distribution $P_g$ defined on $G$. As we have said, in our examples we will consider microgeometries in which non-overlapping circular crystallites $G^{(n)}$, possibly of various sizes, are arranged within a domain $B$, and which may or may not cover this domain completely.

An important element in polycrystals is their texture; that is, the statistics in the crystalline orientations of the grains. For the sake of simplicity we assume throughout this paper
that the Austenite has square symmetry. In view of this assumption the orientation of a grain can be described by an angle between 0 and $\frac{\pi}{2}$, and we therefore consider the set $\Theta$ of functions $\theta = \theta^{(n)} = \theta^{(n)}(\omega)$ with

$$0 \leq \theta^{(n)} < \frac{\pi}{2}.$$ 

The number $\theta^{(n)}(\omega)$ gives the orientation, with respect to the horizontal, of the crystalline lattice of the $n$-th grain of the realization $\omega$; the texture is then prescribed by a probability distribution $P_{\theta}$ on the set $\Theta$. In all of the examples considered in this paper $P_{\theta}$ is the product of statistically independent copies of a fixed probability distribution of angles. In fact, the two cases we will consider are those arising from uniform distribution in the interval $[0, \frac{\pi}{2})$ and from the distribution with all of its mass concentrated at $\theta = 0$, see §5.

A realization $\omega$ of our polycrystal is thus a pair $\omega = \{(G^{(n)}), (\theta^{(n)})\}$; the probability distribution on the set $\Omega = \mathcal{G} \times \Theta$ of such realizations will then be taken, naturally, as the product of the probability measures $P_{g}$ and $P_{\theta}$. The “$n$-th grain” and the orientation of its crystalline lattice now become random variables, but the corresponding dependence on $\omega$ will be suppressed when clear from the context. We will thus write, for example, $G^{(n)} = G^{n}(\omega) =$ first coordinate of $\omega$, and $\chi^{(n)} = \chi^{(n)}(x) = \chi^{(n)}(x, \omega)$.

In order for our polycrystals to be macroscopically spatially homogeneous the probability measure $P$ on $\Omega$ must be invariant under translations, that is, for any vector $x$ in the plane we must have

$$P\left(\{\tau_x(\omega) : \omega \in A\}\right) = P(A)$$

where

$$\tau_x(\omega) = \{(G^{(n)}(\omega) + x), \theta^{(n)}(\omega)\}.$$ 

Clearly $P$ is translation invariant if and only if $P_{g}$ is, which we assume in what follows.

In this paper we will consider two main geometrical arrangements: 1) A closely packed square array of circular grains, and 2) A random array of circular grains with sizes ranging to infinitesimal and no intergrain matrix. (A construction of a random array of circles covering all space with a translation invariant probability distribution can be given as in Miller (1969). As for the square array, the issue of translation invariance is resolved, simply, by incorporating all translations of the basic lattice as possible realizations.)

The elastic properties of our polycrystal are characterized by a set of elastic constants, one corresponding to each one of the phases: the Austenite and the various variants of Martensite. Here we consider two-dimensional elasticity under plane strain, and we make the simplest assumption that all the phases are isotropic with identical elastic constants; these will be denoted by

$$\nu = \text{Poisson Ratio and } \mu = \text{Shear Modulus}. \quad (1)$$
We will often represent a strain tensor \( \epsilon \) in terms of its hydrostatic and deviatoric components \( h, d_1 \) and \( d_2 \):

\[
    h = \frac{1}{2} (\epsilon_{11} + \epsilon_{22}),
\]

\[
    d_1 = \frac{1}{2} (\epsilon_{11} - \epsilon_{22})
\]

and

\[
    d_2 = \epsilon_{12} = \epsilon_{21};
\]

and we will write

\[
    \epsilon = [h, d_1, d_2].
\]

The magnitude of the deviator will be denoted by \( d \):

\[
    d = \sqrt{d_1^2 + d_2^2}.
\]

Notice that if \( \epsilon \) is given by (5), and if

\[
    Q(\theta) = \begin{bmatrix}
        \cos(\theta) & \sin(\theta) \\
        -\sin(\theta) & \cos(\theta)
    \end{bmatrix}
\]

then

\[
    Q^t \epsilon Q \equiv [h, \cos(2\theta)d_1 - \sin(2\theta)d_2, \sin(2\theta)d_1 + \cos(2\theta)d_2].
\]

With these notations and calling \( C_{ijkl} \) the isotropic tensor determined by the constants (1) and

\[
    g = 2(1 - 2\nu),
\]

we have

\[
    C_{11kl}\epsilon_{kl} = \frac{2\mu}{g} (2h + gd_1)
\]

\[
    C_{12kl}\epsilon_{kl} = 2\mu d_2
\]

\[
    C_{22kl}\epsilon_{kl} = \frac{2\mu}{g} (2h - gd_1).
\]
2.2 Eigenstrains

To complete the description of our polycrystal we need to characterize its \textit{possible} modes of transformation. To do this it suffices to prescribe the set $\mathcal{S}$ of all strains that may arise as a result of transformation of a fixed single crystal whose axes are, say, parallel to the $(x_1, x_2)$ axes. This set can be prescribed in accordance with any experimental configuration under study; in this paper we assume $\mathcal{S}$ is a set of constant tensors. Note that since the parent phase is assumed to have square symmetry, and thus to be invariant under rotations of $\frac{\pi}{2}$, the set $\mathcal{S}$ must be invariant under conjugation by the matrices of rotation by this angle. Further, $0 \in \mathcal{S}$ since it should be possible for a grain not to transform at all. Once $\mathcal{S}$ is known, the possible modes of transformation $\mathcal{S}^{(n)}$ of a grain $G^{(n)}$ are simply obtained by conjugation of the set $\mathcal{S}$ by a planar rotation of angle $\theta^{(n)}$:

$$\mathcal{S}^{(n)} = \mathcal{S}^{(n)}(\omega) = \left(Q^{(n)}\right)^T \mathcal{S} Q^{(n)},$$

where

$$Q^{(n)} = Q^{(n)}(\omega) = \begin{bmatrix} \cos(\theta^{(n)}(\omega)) & \sin(\theta^{(n)}(\omega)) \\ -\sin(\theta^{(n)}(\omega)) & \cos(\theta^{(n)}(\omega)) \end{bmatrix};$$

see §2.1.

The set $\mathcal{S}$ may be prescribed in such a way as to account for transformation strains resulting from twinning or other microstructure in the grains. In fact, in this paper we will consider two types of sets of transformation strains at the level of grains. We will say an aggregate is a Type I polycrystal if the set $\mathcal{S}$ contains only strain matrices arising from full transformation of a crystal into a single variant of Martensite. A polycrystal of Type II, on the other hand, is one for which the set $\mathcal{S}$ contains all the (constant) matrices that may arise as a result of twinning of the Austenite and/or various variants of Martensite. We might call a polycrystal of Type III if it is not of Types I or II, so that the set $\mathcal{S}$ contains, perhaps, general non-homogeneous strains. Polycrystals of Type III, which could be handled by appropriate versions of our approach, will not be discussed in this paper. Polycrystals whose strains are smaller than the typical length-scales at which singly-crystalline microstructure occurs are probably unable to support such microstructure within the grains, and thus, could be classed under Type I. Polycrystals with larger grains, on the other hand, could behave as polycrystals of Type II or Type III depending on values of their elementary transformation strains and/or applied strains.

In our simple setting in two dimensions and with square-symmetric crystallites the set $\mathcal{S}$ associated with a Type I polycrystal is given by

$$\mathcal{S}_1 = \{[H, D, 0], [H, -D, 0], [0, 0, 0]\}.$$
The corresponding set $S_2$ associated with a polycrystal of Type II, on the other hand, is the set of all strain tensors which can be obtained by combination of the tensors $[H, D, 0], [H, -D, 0]$ and $[0, 0, 0]$ through twinning. It is not hard to check that

$$S_2 = \{ \lambda[H, D, 0] + (1 - \lambda)[H, -D, 0] : 0 \leq \lambda \leq 1 \} \cup \{[0, 0, 0]\}.$$  

or

$$S_2 = \{ [H, (2\lambda - 1)D, 0] : 0 \leq \lambda \leq 1 \} \cup \{[0, 0, 0]\}$$

see (Kohn, 1991; Bhattacharya, 1993). In case $H = 0$ all the strains in these sets are purely deviatoric, and we thus call

$$S_1^{dev} = \{ [0, D, 0], [0, -D, 0], [0, 0, 0] \}. \quad (10)$$

and

$$S_2^{dev} = \{ [0, (2\lambda - 1)D, 0] : 0 \leq \lambda \leq 1 \}. \quad (11)$$

If $D = 0$, on the other hand, $S_1$ and $S_2$ coincide, and while we define

$$S_1^{hydr} = \{ [H, 0, 0], [0,0,0] \}, \quad (12)$$

our definition of the set $S_2^{hydr}$ departs from these conventions, and it will result from a different rationale.

Indeed, the Taylor set $T$ of applied strains which can be obtained as an arbitrary rotation of some element in $S$ is important in the study of martensitic polycrystals, as it yields a family of applied deformations leading to zero elastic energy. In our two dimensional context, unfortunately, we necessarily have $T = \{ [H, 0, 0] \}$ —as it can be seen directly from (8)— and the only deformation which could possibly be accommodated with zero energy is a hydrostatic strain of strength $H$. In order to simulate within our two-dimensional context the occurrence of a non-trivial Taylor set for Type II polycrystals (which is not uncommon in three-dimensional space, see Bhattacharya and Kohn (1995)), we utilize a set of transformation strains

$$S_2^{hydr} = \{ [\lambda H, 0, 0] : 0 \leq \lambda \leq 1 \}. \quad (13)$$

This set cannot be obtained as a result of formation of two-dimensional martensitic twins. Thus, the unphysical postulate of the set $S_2^{hydr}$ as a possible set of transformation strains is justified here as providing a test of the capabilities of our computational methods within the somewhat limited two-dimensional context we consider.

### 2.3 The homogenization limit

In order to account for the smallness of the grains when compared to macroscopic dimensions of the polycrystalline body $B$, we will compute the elastic properties of polycrystals in the
homogenization limit—in which the constituent grains are vanishingly small. To do this we consider the functions

$$\chi^{(n),\delta}(x) = \chi^{(n),\delta}(x, \omega) = \chi^{(n)}\left(\frac{x}{\delta}, \omega\right)$$ (14)

and the corresponding rescaled grains, which occupy the regions

$$G^{(n),\delta} = \{\chi^{(n),\delta} = 1\}.$$

It is easy to convince oneself that the energy averages considered below do not depend on the shape of $B$ in the limit of homogenization, and we therefore assume, without loss of generality

$$B \text{ is a circle of radius one.}$$ (15)

This assumption will prove advantageous in some calculations, see §2.6.

We are concerned with the minimum value the strain energy in our polycrystals may take, by taking advantage of the various modes of transformation available to its grains, when its body is made to accommodate a given homogeneous boundary displacement. To obtain this quantity we begin by computing the strain energy associated with the given boundary conditions and with a given assignment of transformation strains. If a distribution $\epsilon^{T(n)}$ with $\epsilon^{T(n)}(\omega) \in S^{(n)}(\omega)$ is given, we call

$$\epsilon^{T}(x, \delta) = \epsilon^{T}(x, \delta, \omega) = \begin{cases} 
\epsilon^{T(n)} & \text{if } x \in G^{(n),\delta} \\
0 & \text{if } x \notin \cup_n G^{(n),\delta}.
\end{cases}$$ (16)

(As we have mentioned, we allow for cases in which the crystallites $G^{(n),\delta}$ may not cover the whole body of the polycrystal, and in which, unlike in real polycrystals, there is a matrix phase that cannot transform). Once a procedure for the calculation of this strain energy is available, the problem of computation of the minimum energy reduces to one of minimization of a function of many variables. In accordance with our prescription of homogeneous boundary displacements, on the other hand, we assume the assignment $\epsilon^{T(n)}$ of transformation strains is such that tensor field $\epsilon^{T}(x, \delta, \omega)$ is spatially stationary, see equation (17) below.

The homogenized energy will be defined as the minimum value of the energy over all admissible distributions of transformation strains in the limit as $\delta \to 0$, see (22), (23). The existence of this limit, its independence from the realization $\omega$ and the commutativity of the operations of limit and infimum—which are clear from our numerics—are assumed in what follows; mathematical proofs of these homogenization theorems will be left for future considerations; compare (Koslov, 1979; Zhikov, Koslov and Ngoan, 1979; Müller, 1987). In a closely related connection it is useful to recall that under a hypothesis of ergodicity (which is satisfied by all the probability distributions we use (Dunford and Schwartz, 1958; Halmos,
1956), we can substitute volume averages calculated for any realization

\[ <q>_B = \frac{1}{|B|} \lim_{\delta \to 0} \int_B q\left(\frac{y}{\delta}, \omega\right) dy \]

by ensemble averages calculated at any point \( x \)

\[ <q>_\Omega = \int_\Omega q(x, \omega) P(d\omega). \]

as long as the quantity \( q \) is stationary, that is

\[ q(x, \tau^{-y}(\omega)) = q(x + y, \omega); \quad (17) \]

for all \( y \), see Dunford and Schwartz (1958). That is, for a stationary \( q \) we have

\[ <q>_B = <q>_\Omega, \]

and thus the volume average is independent from the realization \( \omega \).

### 2.4 Homogenized energy

Assume a homogeneous displacement

\[ \epsilon_{ij}^0 x_j \]

is applied on the boundary of our body \( B \). Further, let \( \epsilon^T(x) = \epsilon^T(x, \delta, \omega) \) be a given assignment of transformation strains, and call \( u = u(x) = u(x, \delta, \omega) \) the displacement which results from both the boundary displacement and the prescribed set of transformation strains. In other words, calling

\[ \epsilon_{ij}(x) = \frac{1}{2} (u_{i,j}(x) + u_{j,i}(x)) \]

the strain at the point \( x \in B \) and \( \sigma \) the associated stress,

\[ \sigma_{ij}(x) = C_{ijkl}(u_{k,l}(x) - \epsilon^T_{kl}(x)), \quad (18) \]

\( u \) satisfies the equations

\[ \partial_j \sigma_{ij} = 0 \quad (19) \]
and

\[ u_i|_{\partial B} = \epsilon_i^0 x_j. \] (20)

(Of course, equation (19) is meant to imply continuity of tractions

\[ \sigma_{ij} n_j = C_{ijkl} (u_{k,l} - \epsilon_{kl}) n_j \] (21)

across the boundary of the grains, see (16).)

The elastic energy produced by a given distribution \( \epsilon^T \) of transformation strains under the boundary conditions (20) is given by

\[ W = W_{\epsilon^T} \equiv \lim_{\delta \to 0} W_{\epsilon^T}^\delta = \frac{1}{2} < \sigma_{ij} (u_{i,j} - \epsilon_{ij}^T) + \gamma(\epsilon^T) >_B = \frac{1}{2} < \sigma_{ij} (u_{i,j} - \epsilon_{ij}^T) + \gamma(\epsilon^T) >_\Omega. \] (22)

Here \( \gamma(\epsilon^T) \) is the free energy of the phase associated with the transformation strain \( \epsilon^T \). Our discussion will be restricted to the homogenization problem at the critical temperature, at which the free energies of Austenite and Martensite coincide, and we will thus take

\[ \gamma(\epsilon^T) = 0 \]

for all phases \( \epsilon^T \). The general case admits, of course, an analogous treatment.

The overall (or homogenized) energy \( E \) is defined by the minimum value of \( W \) over all admissible stationary distributions of transformation strains, that is

\[ E = \inf_{\epsilon^T \in \Lambda} W \] (23)

where

\[ \Lambda = \{ \epsilon^T : \epsilon^T \text{ is stationary and } \epsilon_{T(n)}(\omega) \in \mathcal{S}^{(n)}(\omega) \text{ for all } n \text{ and all } \omega \}, \] (24)

see §§2.2, 2.3.

For future reference we note some useful relations. The volume–average of the strain is given by

\[ < \epsilon_{ij} >_B = \frac{1}{2|B|} \lim_{\delta \to 0} \int_B (u_{i,j} + u_{j,i}) dx = \epsilon_{ij}^0, \]

whereas for the volume–average of the stress we have

\[ < \sigma_{ij} >_B = \frac{1}{|B|} \lim_{\delta \to 0} \int_B C_{ijkl} (u_{k,l} - \epsilon_{kl}^0(x)) dx \]

12
\[ \sigma_{ij}^0 = C_{ijkl} \epsilon_{kl}^0 \]
\[ = \sigma_{ij}^0 - tv C_{ijkl} \epsilon_{kl}^T. \]

Here we have put \( \sigma_{ij}^0 = C_{ijkl} \epsilon_{kl}^0 \), and we have denoted by \( t = f(\epsilon^T) \), \( v \) and \( \bar{\epsilon} \) the number fraction of transformed inclusions, the volume fraction occupied by all the inclusions and the number average of the strain, respectively, in the limit of small \( \delta \). Thus, calling \( N^T = N^T_{\epsilon^T}(\delta, \omega) \) the number of transformed inclusions (the number of inclusions within \( B \) for which \( \epsilon^T(n) \neq 0 \)) we have

\[
\epsilon_{kl}^T = \lim_{\delta \to 0} \frac{1}{N^T} \sum_{n \in I} \epsilon_{kl}^{T(n)},
\]

where \( I \) denotes the set

\[
I = I^\delta = \{ n : G^{(n),\delta} \subseteq B \}.
\]

(25)

The values of \( v \) for the square and random arrays we consider (see §2.1) are \( v = \pi/4 \) and \( v = 1 \) respectively. Note that if \( N = N(\delta, \omega) \) denotes the total number of inclusions within \( B \) then the number fraction \( f(\epsilon^T) \) of transformed inclusions is given by

\[
f(\epsilon^T) = \lim_{\delta \to 0} \frac{N^T_{\epsilon^T}(\delta)}{N(\delta)}
\]

(27)

(a limit which exists and is independent of the realization by ergodicity). We will call \( \epsilon^{T(\text{av})} \) the ensemble average of \( \epsilon^T \); clearly we have

\[
\epsilon_{kl}^{T(\text{av})} = < \epsilon_{kl}^T >_\Omega = < \epsilon_{kl}^T >_B = tv \epsilon_{kl}^T.
\]

(28)

The hydrostatic and deviatoric components of \( \epsilon^{T(n)} \) and \( \epsilon^{T(\text{av})} \) will be denoted by

\[
\epsilon^{T(n)} = [h^{T(n)}, d_1^{T(n)}, d_2^{T(n)}] \in S^{(n)}
\]

(29)

and

\[
\epsilon^{T(\text{av})} = [h^{T(\text{av})}, d_1^{T(\text{av})}, d_2^{T(\text{av})}]
\]

respectively, see §2.1.

### 2.5 Boundary conditions

The displacements, strains and stresses mentioned above are compounds of the corresponding quantities produced by the boundary displacements on one hand, and by the transformation
of the inclusions on the other. It is convenient here to discriminate between these contributions. Call $u_0$ the displacement field resulting from the imposed boundary displacements alone, in the absence of transformation of the inclusions. Thus, $u^0$ satisfies

$$\partial_j C_{ijkl} u^0_{k,l} = 0$$

and

$$u^0_i|_{\partial B} = \epsilon^0_{ij} x_j;$$

clearly we have

$$u^0_i = \epsilon^0_{ij} x_j$$

in $B$. Call $\bar{u}$, on the other hand, the displacement that would be produced solely by transformation of the inclusions, under the assumption of zero boundary displacements. Thus, $\bar{u}$ is continuous everywhere, and it satisfies

$$\partial_j C_{ijkl}(\bar{u}_{k,l}(x) - \epsilon^T(x)) = 0,$$

and

$$\bar{u}|_{\partial B} = 0.$$

(Equation (31) is meant to imply continuity of tractions across the grain boundaries; see (21).)

The solution to our full elasticity problem, resulting from both boundary conditions and grain transformations, is thus equal to $u^0 + \bar{u}$. The associated average strain energy contained in the polycrystal is given by

$$W = \frac{1}{2|B|} \lim_{\delta \to 0} \int_B (\sigma^0_{ij} + \bar{\sigma}_{ij})(u^0_{i,j} + \bar{u}_{i,j} - \epsilon^T_{ij}(x))dx$$

where we have put

$$\bar{\sigma}_{ij} = C_{ijkl}(\bar{u}_{k,l}(x) - \epsilon^T(x)).$$

To simplify our expression (33) for the strain energy, note first that, in view of equations (30), (31) and (32) and since $\sigma^0_{ij}$ and $u^0_{i,j}$ are constant, the divergence theorem gives

$$W = \frac{1}{2|B|} \lim_{\delta \to 0} \left[ |B| \sigma^0_{ij} u^0_{i,j} - \sigma^0_{ij} \int_B \epsilon^T_{ij} dx + \int_B \bar{\sigma}_{ij} u^0_{i,j} dx - \int_B \bar{\sigma}_{ij} \epsilon^T_{ij} dx \right].$$

Further, we have

$$\lim_{\delta \to 0} \int_B \epsilon^T_{ij} dx = |B| \epsilon_{ij}^{T(\text{av})}.$$
from equation (28), whereas, by the divergence theorem,

$$\lim_{\delta \to 0} \int_B \tilde{\sigma}_{ij} u^0_{i,j} dx = -|B| C_{ijkl} T^{(av)}_{kl} u^0_{i,j}.$$ 

It follows that

$$W = \frac{1}{2} \tilde{\sigma}_{ij} u^0_{i,j} - \frac{1}{2} \tilde{\sigma}_{ij} T^{(av)}_{ij} - \frac{1}{2} u^0_{i,j} C_{ijkl} \epsilon_{kl} T^{(av)}_{ij} - \lim_{\delta \to 0} \frac{1}{2|B|} \int_B \tilde{\sigma}_{ij} \epsilon_{ij} T^{(av)}_{ij}$$

$$= \frac{1}{2} \tilde{\sigma}_{ij} u^0_{i,j} - \frac{1}{2} \tilde{\sigma}_{ij} T^{(av)}_{ij} - \lim_{\delta \to 0} \frac{1}{2|B|} \int_B \tilde{\sigma}_{ij} \epsilon_{ij} T^{(av)}_{ij} dx.$$ 

This leaves only the limit of the quantity

$$\mathcal{L}^{(\delta)} = -\frac{1}{2|B|} \int_B \tilde{\sigma}_{ij} \epsilon_{ij} T^{(av)}_{ij} dx$$ (35)

to be evaluated.

### 2.6 Eshelby integrals

It is now convenient to decompose the fields $\tilde{u}$ and $\tilde{\sigma}$ in the forms

$$\tilde{u} = u^1 + u^2$$

$$\tilde{\sigma} = \sigma^1 + \sigma^2$$

where $u^1$ and $\sigma^1$ are the displacement and stress caused by the transformation of our inclusions (which are contained in $B$) when they are thought of as embedded in an elastic matrix occupying all the plane, and $u^2$ and $\sigma^2$ are the corresponding corrections. Consideration of these fields in the plane will permit us to reduce the calculation of the strain energy to the evaluation of a quadratic function given by a certain “interaction matrix” $M$ which, under our assumptions of circular grains and homogeneous elastic moduli, can be computed in closed form.

Explicitly, call $w^{(n)} = w^{(n),\delta}$ the solution to the equations

$$\begin{cases} 
\partial_j \sigma^{(n)}_{ij} = 0 & \text{in the plane} \\
 w^{(n)}(x) \to 0 & \text{as } |x| \to \infty 
\end{cases}$$ (36)
(with continuity of displacements and tractions across the boundary of $G^{(n),\delta}$), where

\[
\begin{cases}
\sigma_{ij}^{(n)} = C_{ijkl} (w_{k,l}^{(n)}(x) - \epsilon_{kl}^{(n)}) & \text{inside } G^{(n),\delta} \text{ and} \\
\sigma_{ij}^{(n)} = C_{ijkl} w_{k,l}^{(n)}(x) & \text{in the plane minus } G^{(n),\delta}.
\end{cases}
\] (37)

Taking into account (26) we obtain the representations

\[
u^1 = \sum_{n \in I} u^{(n)}_{i,k,l},
\]

\[
\sigma_{ij}^1(x) = C_{ijkl} \left( u_{k,l}^1(x) - \epsilon_{kl}^1(x) \right) = \sum_{n \in I} \sigma_{ij}^{(n)},
\] (38)

and

\[
\sigma_{ij}^2(x) = C_{ijkl} u_{k,l}^2(x);
\]

note that equation (34) is satisfied. Of course, $u^1$ and $u^2$ are continuous and we have

\[
\partial_j \sigma_{ij}^1 = 0
\] (39)

and

\[
\partial_j \sigma_{ij}^2 = 0.
\] (40)

Since $\tilde{u}$ vanishes on the boundary of $B$ we see that

\[
\frac{\partial}{\partial B} u^2 = -\frac{\partial}{\partial B} u^1.
\] (41)

Interestingly — in view of (15) — the boundary values of $u^1$, and therefore those of $u^2$, can be calculated exactly in the limit as the grain size $\delta$ tends to zero. To calculate these boundary values we appeal to Eshelby's representation for the displacement caused by a transforming inclusion within an elastic matrix. This representation uses the free space Green's function, which, in the two dimensional isotropic plane-strain case we consider is given by

\[
\Gamma_{ij}(x_1, x_2) = \frac{1}{8\pi(1-\nu)\mu} \left( \frac{x_i x_j}{r^2} - (3 - 4\nu) \delta_{ij} \log(r) \right),
\] (42)

with $r = \sqrt{x_1^2 + x_2^2}$. (Simple substitutions for these elastic constants give the Green's function for the related plane stress problems, see Mura (1993)).
Since \( \Gamma_{ij}(x - x') \) is the \( i \)-th component of the displacement produced by a unit point force at \( x \) in the \( j \)-th Cartesian direction, we see, with Eshelby (1957), that the displacement \( V \) produced by an eigenstrain \( \epsilon^T \) within an inclusion \( C \) of arbitrary shape is given by

\[
V_i(x) = \int_{\partial C} C_{jkrst} \epsilon^T_{rs} n_k \Gamma_{ij}(x - x') dS'.
\]

The divergence theorem allows us to write, equivalently,

\[
V_i(x) = \int_C C_{jkrst} \epsilon^T_{rs} \Gamma_{ij,k}(x - x') dx'.
\] (43)

It follows that \( u^1 \) is given by

\[
u^1_i(x, \delta) = \int_{\cup \{G^{(n)}, \delta; n \in I\}} C_{jkrst} \epsilon^T_{rs}(x', \delta) \Gamma_{ij,k}(x - x') dx',
\]

see (26). In the limit as \( \delta \) tends to zero this expression becomes

\[
u^1_i(x, 0) = \int_B C_{jkrst} \epsilon^{T(\text{av})}_{rs} \Gamma_{ij,k}(x - x') dx',
\] (44)

since, clearly, \( \epsilon^T \) converges weakly to

\[
< \epsilon^T >_B = < \epsilon^T >_\Omega = \epsilon^{T(\text{av})}.
\]

Now, in view of equation (43) we may reinterpret (44) as giving the displacement caused by the "inclusion" \( B \) in an infinite matrix, as \( B \) transforms with transformation strain \( \epsilon^{T(\text{av})} \). It follows from our assumption (15) that \( u^1(x, 0) \) and in particular its boundary values (41)

are homogeneous (and they are given by (106), with \([h, d, d] = \epsilon^{T(\text{av})}\)). In view of the \( H^{1/2} \) convergence of the boundary values of \( u^1 \) (established in Appendix A.1), and thus of those of \( u^2 \), it follows from the weak formulation of equations (40) and Korn's inequality that \( u^2(x, \delta) \) converges in the Sobolev space \( H^{1}(B) \) to \(-u^1(x, 0)\) as \( \delta \to 0 \). (Note that the gradient of \( u^1(x, \delta) \) does not itself converge in square mean, in general.) Thus, \( \sigma_{ij}^2(x, \delta) \) converges within
$B$ to the constant value $-C_{ijkl}u^{1}_{k,l}(x,0)$ in the square mean, and, since $\epsilon^{T}$ converges weakly to $\epsilon^{T(\text{av})}$ we can write

$$
\lim_{\delta \to 0} \int_{B} \sigma^{2}_{ij}(x,\delta)\epsilon^{T}_{ij}(x,\delta) = - \int_{B} C_{ijkl}u^{1}_{k,l}(x,0)\epsilon^{T(\text{av})}_{ij}
$$

(45)

As we said, the symmetrized gradient of $u^{1}(x,0)$ gives the strain in an inclusion within a matrix which transforms with transformation strain $\epsilon^{T(\text{av})}$. Thus, the quantity (45) can be evaluated easily from the results in Appendix D.1; we obtain

$$
\frac{1}{|B|} \lim_{\delta \to 0} \int_{B} \sigma^{2}_{ij}\epsilon^{T}_{ij} = - \frac{4\mu}{g(2+g)} \left[ 4(h^{T(\text{av})})^{2} + g(1+g) \left( (d^{T(\text{av})}_{1})^{2} + (d^{T(\text{av})}_{2})^{2} \right) \right].
$$

(46)

2.7 Interaction matrix

Returning to the integral (35) and calling

$$
W^{\delta}_{1} = - \frac{1}{2|B|} \int_{B} \sigma^{1}_{ij}\epsilon^{T}_{ij} dx
$$

and

$$
W^{\delta}_{2} = - \frac{1}{2|B|} \int_{B} \sigma^{2}_{ij}\epsilon^{T}_{ij} dx
$$

we have

$$
L^{\delta} = W^{\delta}_{1} + W^{\delta}_{2}.
$$

From (46) we obtain

$$
W^{\delta}_{2} = \lim_{\delta \to 0} W^{\delta}_{2} = \frac{2\mu}{g(2+g)} \left[ 4(h^{T(\text{av})})^{2} + g(1+g) \left( (d^{T(\text{av})}_{1})^{2} + (d^{T(\text{av})}_{2})^{2} \right) \right].
$$

(47)

The quantity $W^{\delta}_{1}$, on the other hand, can be expressed, for any finite value of $\delta$, by a closed formula which lends itself easily for numerical computations; the limit of $W^{\delta}_{1}$ as $\delta \to 0$ will
thus be approximated, simply, by the values of $W_1^\delta$ for sufficiently small positive values for this parameter. Indeed, in view of (38) we have

$$W_1^\delta = \frac{1}{2|B|} \sum_{k,p \in I} \int_{G(k),\delta} \sigma_{ij}^{(p)} e_{ij}^c T^{(k)}.$$  \hspace{1cm} (48)

Let us write

$$W_1^\delta = W_{\text{self}}^\delta + W_{\text{int}}^\delta$$ \hspace{1cm} (49)

where

$$W_{\text{self}}^\delta = -\frac{1}{2|B|} \sum_{k \in I} \int_{G(k),\delta} \sigma_{ij}^{(k)} e_{ij}^c T^{(k)} \, dx$$  \hspace{1cm} (50)

gives the self energy of the grains, and

$$W_{\text{int}}^\delta = -\frac{1}{2|B|} \sum_{k \neq p, k,p \in I} \int_{G(k),\delta} \sigma_{ij}^{(p)} e_{ij}^c T^{(k)} \, dx$$  \hspace{1cm} (51)

the interaction energy among the grains. The quantity $W_{\text{int}}^\delta$, which should not be confused with the energy of interaction of a inhomogeneity with an imposed field, see Eshelby (1957), accounts for strain energies arising from mismatch of the various transformation strains in the polycrystal. The integrals in (50) and (51) can be calculated in terms of elementary functions, as shown in Appendix D.2; there we derive an expression

$$W_{\text{self}}^\delta + W_{\text{int}}^\delta = e M^\delta e^t$$ \hspace{1cm} (52)

where $M^\delta$ is an explicit $(3N) \times (3N)$ matrix, and where $e$ is a $(3N)$ vector formed by the transformation strains of all the grains, see (122).

Summing up the results of §2.2 to §2.6, we see that the strain energy (22) is given by

$$W = \frac{1}{2} \sigma_{ij}^0 u_{ij}^0 - \sigma_{ij}^0 e_{ij}^c T^{(av)} + \lim_{\delta \to 0} \mathcal{L}^\delta$$

$$= \frac{1}{2} \sigma_{ij}^0 u_{ij}^0 - \sigma_{ij}^0 e_{ij}^c T^{(av)} + \lim_{\delta \to 0} W_2^\delta + \lim_{\delta \to 0} W_1^\delta.$$
In view of (47) and (49) we obtain, finally

\[ W = \frac{1}{2} \sigma_{ij}^{0} u_{ij}^{0} - \sigma_{ij}^{0} T^{(av)} + \]

\[ \frac{2 \mu}{g(2+g)} \left[ 4 (\kappa T^{(av)})^2 + g (1+g) \left( (d_1 T^{(av)})^2 + (d_2 T^{(av)})^2 \right) \right] + \lim_{\delta \to 0} [W_{self}^{\delta} + W_{int}^{\delta}] \]  \hspace{1cm} (53)

see (52). As we said, the homogenized energy \( E \) results from \( W \) by minimization, see (23). The theoretical considerations, bounds and numerical calculations of §§3–5 are based on equations (52) and (53).

3 Bounds

The patterns of transformation in polycrystals result as a compromise between two factors. On one hand they recognize a tendency which, in order to avoid conflicts with the imposed boundary conditions, would have the grains transform with an average transformation strain as close as possible to the applied strain. A second tendency, on the other hand, would have the grains not transform at all in order to avoid increases in energy resulting from mismatch between the transformation strains of neighboring grains. In particular, the transformation strains of different grains in a minimum energy configuration are likely to exhibit statistical correlations. Thus, a calculation of the homogenized energy based on a hypothesis of independence in the transformation strains of different grains must lead to an upper bound for this quantity.

In §3.1 we explore the implications of this remark, and we obtain explicit bounds in closed form for the energy in the square and random arrays. Additional bounds, based on the Taylor hypothesis, are derived in §3.2. (Previous studies of energies in shape memory polycrystals based on the Taylor hypothesis include (Ono and Sato, 1988; Ono, 1991; Otsuka and Shimizu, 1986); our simple exact calculations in this connection are somewhat different from the approximate ones given earlier). The comparisons of the various numerical results and bounds given in §5 show that our new bound based on the assumption of uncorrelated grains (UG) can be substantially tighter than the Taylor bound. Unlike the Taylor bound, which is not restricted to particular geometries, the UG bounds depend on the grain shapes, and they would require (simple) numerical calculations for treatment of shapes other than circular, elliptical or ellipsoidal. Our bounds do show rigorously, however, that estimates of the energy based on the Taylor hypothesis may differ substantially from actual values, and that the Taylor assumption may therefore lead to inaccuracies in structural calculations.

In addition to its implications on the physics of polycrystals, consideration of bounds provide a valuable test for our numerics. Our numerical results for the square array always
lie below our corresponding bound, as they should. In most regimes, further, the bound
does approximate the numerical results very closely—a clear indication of an excellent
convergence in our numerics; see §4.2.

3.1 Uncorrelated grains and upper bounds

The derivation of our bounds proceeds roughly as follows: under the assumption of independ-
ence of the eigenstrains in any two of the constituent grains, and, further, of transformation
strains which may either vanish or result only from rotations of a single tensor $\xi \in \mathcal{S}$, an
expression for the energy is obtained which depends only on $\xi$ and the average value $\epsilon^{T(\text{av})}$
of the eigenstrains. An explicit finite dimensional minimization with respect to $\xi$ and $\epsilon^{T(\text{av})}$
then concludes the calculation. The value obtained for the energy by this procedure is an
upper bound for the actual homogenized energy, since it equals the actual minimum value
taken by the energy expression (22) in a subclass of the set of all admissible stationary
distributions of eigenstrains (24).

Explicitly, given a tensor $\xi \in \mathcal{S}$, a number $t \in [0, 1]$ and a set $C \subseteq [0, \frac{\pi}{2}]$ let us call

$$\phi_C = \phi_C(x, \delta, \omega) = \begin{cases} 
\phi^{(n)}_C & \text{if } x \in \mathcal{G}^{(n)} \delta \\
0 & \text{if } x \not\in \cup_n \mathcal{G}^{(n)} \delta 
\end{cases}$$

with

$$\phi^{(n)}_C = \begin{cases} 
\theta^{(n)} & \text{if } \theta^{(n)} \in C \\
\theta^{(n)} + \frac{\pi}{2} & \text{if } \theta^{(n)} \not\in C.
\end{cases}$$

We then define

$$\Lambda_{\xi, t, C} = \{ \epsilon^T \in \Lambda : f(\epsilon^T) = t \text{ and for each } x \text{ either } \epsilon^T = 0, \text{ or } \epsilon^T = Q^T(\phi_C) \xi Q(\phi_C) \},$$

see (7), (27). Our upper bound is given by

$$U = \inf_{\xi \in \mathcal{S}} \inf_{0 \leq t \leq 1} \inf_{\epsilon^T \in \Lambda_{\xi, t, C}} W.$$  \hspace{1cm} (54)

Note that the transformation strains assigned by an element of $\Lambda_{\xi, t, C}$ to any two grains are
mutually statistically independent, since so are the angles assigned by the distribution $\theta^{(n)}$
for two different values of $n$. The energy $W$ is constant in the set $\Lambda_{\xi, t, C}$, as we shall show.
This constant will be computed explicitly in terms of $\xi$, $t$ and two additional real parameters
\( y \text{ and } z \text{ associated with the set } C. \text{ An explicit minimization on this parameters (the details of which are given in Appendix C) yields an expression in closed form for } U. \)

The value that \( W \) takes on \( \Lambda_{\xi, t, C} \) can be calculated by ensemble averaging of (53); an explicit expression follows immediately once a formula for the quantity

\[
Z^\delta = < W^\delta_{\text{int}} >_\Omega = -\frac{1}{2|B|} \sum_{k, p \neq p} \int_{G^{(k), \delta}} < \sigma_{ij}^{(p)} \epsilon_{ij}^{T(k)} >_\Omega \, dx
\]

is known, see (51). (The self energy can be calculated easily, since the transformation strains associated with an element of \( \Lambda_{\xi, t, C} \) are rotations of the fixed tensor \( \xi \).) Now, \( \sigma^{(p)} \) is proportional to \( \epsilon^{T(p)} \), see e.g. (109), and thus we obtain, by independence

\[
< \sigma_{ij}^{(p)} \epsilon_{ij}^{T(k)} >_\Omega = < \sigma_{ij}^{(p)} >_\Omega \cdot < \epsilon_{ij}^{T(k)} >_\Omega
\]

for \( k \neq p \), so that for an element of \( \Lambda_{\xi, t, C} \)

\[
Z^\delta = -\frac{1}{2|B|} \sum_{k, p \neq p} \int_{G^{(k), \delta}} < \sigma_{ij}^{(p)} >_\Omega < \epsilon_{ij}^{T(k)} >_\Omega \, dx = \sum_{k \neq p} \left[ \frac{h^{T(\text{av})}}{d_1^{T(\text{av})}} \begin{array}{c} d_1^{T(\text{av})} \\ d_2^{T(\text{av})} \end{array} \right] M_{kp} \left[ \frac{d_1^{T(\text{av})}}{d_2^{T(\text{av})}} \right],
\]

see (121), and the problem can be treated by consideration of averages of eigenstrains.

In order to find the possible values of such averages, call

\[
\xi = [h^\xi, d_1^\xi, d_2^\xi]
\]

the hydrostatic and deviatoric components of \( \xi \), and take

\[
\epsilon^T \in \Lambda_{\xi, t, C}.
\]

The hydrostatic component of \( \epsilon^{T(n)} \) equals \( h^\xi \) for all transforming grains, and thus

\[
h^{T(\text{av})} = tvh^\xi,
\]

see (28). Since a rotation of the tensor \( \xi \) by angle \( \phi_C \) can be represented as

\[
[h^\xi, \cos(2\phi_C)d_1^\xi - \sin(2\phi_C)d_2^\xi, \sin(2\phi_C)d_1^\xi + \cos(2\phi_C)d_2^\xi],
\]

22
see (8), an average \([h^{av}, d_1^{av}, d_2^{av}]\) of such rotated tensors over a distribution \(\phi_C(x, \delta, \omega)\) is given by
\[
d_1^{av} = d_1^\delta < \cos(2\phi_C) >_\Omega - d_2^\delta < \sin(2\phi_C) >_\Omega
\]
and
\[
d_2^{av} = d_1^\delta < \sin(2\phi_C) >_\Omega + d_2^\delta < \cos(2\phi_C) >_\Omega.
\]
These averages can in turn be related to number averages of the values of trigonometric functions in the \(N^T\) transforming grains. Indeed, for \(\epsilon^T \in \Lambda_{\xi,t,C}\) we have, by ergodicity
\[
\frac{d_1^{av}}{\pi} = \frac{2tv}{\pi} (d_1^\delta y - d_2^\delta z) \tag{58}
\]
and
\[
\frac{d_2^{av}}{\pi} = \frac{2tv}{\pi} (d_1^\delta z + d_2^\delta y), \tag{59}
\]
where
\[
y = \frac{\pi}{2} \lim_{\delta \to 0} \frac{1}{N^T} \sum_{\{k \in E; \epsilon^T(k) \neq 0\}} \cos(2\phi_C^{(k)}) \tag{60}
\]
and
\[
z = \frac{\pi}{2} \lim_{\delta \to 0} \frac{1}{N^T} \sum_{\{k \in E; \epsilon^T(k) \neq 0\}} \sin(2\phi_C^{(k)}) \tag{61}
\]
Now, the quantity \(W = W_{\epsilon^T}\) in (53) does not depend on the realization \(\omega\) by ergodicity; see comments in §2.3. In view of (55), (56), (57), (58), (59) and (113) and the results of Appendices B.1 and B.2, ensemble averaging of \(W_{\epsilon^T}\) (which is constant with respect to \(\omega\)) leads to an expression
\[
W_{\epsilon^T} = m(y, z, t, \xi, \epsilon^0) = A(ty - a)^2 + A(tz - b)^2 + \alpha(t - c)^2 + \beta + \lim_{\delta \to 0} Z^\delta \tag{62}
\]
which can be calculated explicitly in terms of the arguments of \(m\) and the various parameters, see Appendix C. (Incidentally, this expression shows that \(W\) is constant on \(\Lambda_{\xi,t,C}\); as claimed earlier). All of our statistics is now contained in these number averages of trigonometric
functions, and optimization with respect to $C$ is equivalent to optimization with respect to $y$ and $z$.

To obtain our bounds it is necessary to find the ranges of variation for the various minimization parameters, and to effect the minimization of $m$ in those ranges. (For simplicity we only present results for purely hydrostatic and purely deviatoric polycrystals.) The domain of variation for the parameters $t$, $h^\xi$, $d_1^\xi$, and $d_2^\xi$ is clear from our context: we have

$$0 \leq t \leq 1$$

and

$$[h^\xi, d_1^\xi, d_2^\xi] \in \mathcal{S}.$$  \hspace{1cm} (64)

The range of possible values of the variables $y$ and $z$ as the set $C$ is varied, on the other hand, is the circle

$$y^2 + z^2 \leq 1$$  \hspace{1cm} (65)

as shown in Appendix B.1. The corresponding minimization calculation is shown in detail in Appendix C, leading to the UG bounds (93), (94), (104) and (105).

### 3.2 Taylor bounds

Bounds for the overall elastic energies can also be obtained, as is known, by means of the constant strain hypothesis of Taylor, see also (Ono and Sato, 1988; Ono, 1991; Bhattacharya and Kohn, 1995). Under the Taylor assumption the strain is everywhere constant in the material and equal to the applied strain $\epsilon^0$. Now, if the transformation strain in the grain $G^{(n),\delta}$ equals $\epsilon^{T(n)}$, then the elastic energy arising in that grain as a result of the constant strain $\epsilon^0$ is

$$\frac{1}{2} \epsilon_{ij}^0 C_{ijkl} (\epsilon_{kl} - \epsilon_{kl}^{T(n)}) |G^{(n),\delta}|.$$  \hspace{1cm} (66)

Thus, the best bound to be obtained under the Taylor assumption, which we call the Taylor bound, results by addition of all these grain energies (and the matrix energy, if such an elastic matrix exists) where the transformation strain $\epsilon^{T(n)} \in \mathcal{S}^{(n)}$ is chosen so as to minimize the expression (66) for each $n$.

As illustrations we present Taylor bounds for purely deviatoric and purely hydrostatic Type II polycrystals with random orientations, see (11) and (13). In either case, the admissible transformation strains in the $n$-th grain are given by constant multiples of a tensor $\xi^{(n)}$

$$\xi^{(n)} = \gamma \xi^{(n)},$$  \hspace{1cm} (67)
where $\xi^{(n)}$, in turn, is a rotation of the fixed tensor

$$\xi = [H, D, 0].$$

For purely deviatoric Type II polycrystals $\xi^{(n)}$ and $\gamma$ are given by

$$\xi^{(n)} = Q^t(\theta^{(n)})[0, D, 0]Q(\theta^{(n)}) \quad \text{and} \quad -1 \leq \gamma \leq 1 \quad (68)$$

whereas for hydrostatic Type II polycrystals we have

$$\xi^{(n)} = [H, 0, 0] \quad \text{and} \quad 0 \leq \gamma \leq 1. \quad (69)$$

In either case the vertex $\gamma_{\text{ver}}$ of the (parabolic) function of $\gamma$

$$(\varepsilon^0 - \xi^{(n)}_\gamma)C(\varepsilon^0 - \xi^{(n)}_\gamma) \quad (70)$$

is given by

$$\gamma^{(n)}_{\text{ver}} = \frac{C_{ijkl}\xi^{(n)}_{ij} \xi^{(n)}_{kl}}{C_{ijkl}\xi^{(n)}_{ij} \xi^{(n)}_{kl}}.$$ 

The minimum energy in the $n$-th grain is thus given by (70) with $\gamma = \gamma^{(n)}_{\text{ver}}$ provided $\gamma^{(n)}_{\text{ver}}$ lies between $-1$ and $1$ in the deviatoric case, or between $0$ and $1$ in the hydrostatic case; otherwise the minimum occurs at one of the endpoints of the intervals of admissibility for the parameter $\gamma$.

To obtain the Taylor bound for a given applied strain $\varepsilon^0$ in the cases (68) and (69), we express $\varepsilon^0$, for each $n$, as a multiple of $\xi^{(n)}$ plus a tensor $\xi^{(n)}_\perp$ which is orthogonal to $\xi^{(n)}$ in the sense that

$$C_{ijkl}\xi^{(n)}_{ij} \xi^{(n)}_\perp = 0.$$ 

Thus,

$$\varepsilon^0 = \gamma^{0(n)}(\varepsilon^{(n)} + \xi^{(n)}_\perp),$$

and clearly $\gamma^{(n)}_{\text{ver}} = \gamma^{0(n)}$.

As we said, we consider purely hydrostatic and purely deviatoric Type II polycrystals with random orientations only; as usual we denote

$$\varepsilon^0 = [h^0, d^0_1, d^0_2].$$

In the case of purely hydrostatic polycrystals and provided $0 < h^0 < h^\xi$, we obtain $\xi^{(n)}_\perp = [0, d^0_1, d^0_2]$ and $\xi^{(n)}_\gamma = [h^0, 0, 0]$. The Taylor bound for $0 < h^0 < h^\xi$ is then given by

$$V = 2v\mu(d^0)^2 + (1 - v)\left(\frac{4\mu}{g}(h^0)^2 + 2\mu(d^0)^2\right),$$

25
see (6). In the complementary case the bound is obtained, analogously, by substitution of $\gamma = 1$ in (70) and averaging.

Let us now consider a deviatoric Type II polycrystal with random orientations. Since the orientations of our polycrystal are uniformly distributed, it is easy to see that the Taylor bound is invariant under rotations of the applied strain. We may thus assume, without loss of generality, that $d^0_2 = 0$ and $d^0_1 = d^0$. Provided $|d^0| < |d^\xi|$ we then obtain

$$
\xi^{(n)\perp} = Q^t(\theta^n)[h, 0, -d^0 \sin(2\theta^n)]Q(\theta^n), \text{ and the energy in the } n\text{-th grain equals } \frac{2\mu R^2}{g} (g(d^0)^2 \sin^2(2\theta^n) + 2h^2). \text{ In the limit of small } \delta, \text{ the sum of all these energies becomes an integral which results in the Taylor bound}
$$

$$
V = \frac{v\mu}{g} \left( 4(h^0)^2 + g(d^0)^2 \right) + (1 - v) \frac{2\mu}{g} \left( 2(h^0)^2 + g(d^0)^2 \right).
$$

valid for $|d^0| < |d^\xi|$.

## 4 Numerics

In §4.1 we describe the implementation of our numerical method, and, in §4.2 we discuss a number of tests demonstrating its convergence. A variety of numerical results and bounds are then presented in §5.

The elastic constants used in the following two sections are given by the following reasonable but otherwise arbitrary choices: $g = 1$ and $\mu = 100 \text{ GPa}$; see (9), (1). Also, we have used 2% deviatoric and hydrostatic transformation strains. The actual values used for the transformation strains are not of importance in this presentation. The particular choices above resulted from our requirement that the values of the elastic energies be within the ranges of those observed experimentally. To accomplish this in our two dimensional square array case-study which contains an elastic matrix it was necessary to use values for the transformation strains of the grains which are smaller than some of those observed in practice. (Note the small energy values in Figure 10, in a case in which an elastic matrix does not exist; see also comments at the end of §5.) Curves with identical qualitative characteristics are obtained by assignment of transformation strains of the order of, say, 10%. Further, the quality of our numerics does not seem to depend on the values of these parameters.
4.1 Numerical method

Equation (53) gives the value of the elastic energy associated with a prescribed applied deformation, and with a given admissible distribution of transformation strains $\varepsilon^{T(n)}$, see (29). The homogenized energy $E$ is the minimum value of these quantities over all (admissible and translation invariant) distributions of transformation strains, see (23). For a given distribution, all the terms in (53) can be evaluated explicitly — except for the limit of $W_{\text{int}}^{\delta}$. Thus $E$ can be obtained numerically by substitution of this limit by the value of $W_{\text{int}}^{\delta}$ with a sufficiently small value of $\delta$, followed by minimization with respect to the assignments of transformation strains.

In §4.2 we will present numerical results showing that the result of the process of minimization for a fixed $\delta$ does indeed converge to a well defined value as $\delta \to 0$. In what follows we describe our solution of the minimization problem for fixed $\delta$ which, as mentioned in the introduction, is based on optimization via simulated annealing.

Let a fixed imposed deformation be given and consider, for a fixed positive value of $\delta$, an admissible distribution of transformations for all the (finitely many) grains within $B$

$$\varepsilon^{T(n)} \in S^{(n)}.$$ 

Further, call $W_{\text{current}}$ the corresponding value of the elastic energy. To decrease the value of $W$ our application of the method of simulated annealing (Metropolis, Rosenbluth, Rosenbluth and Teller, 1953; Kirkpatrick, Gelatt and Vecchi, 1983) proceeds by choosing one grain at random with probability (number of grains)$^{-1}$ and changing the transformation strain of the chosen grain $G^{(k)}_{\delta}$, again randomly and with a uniform probability distribution, to some other element of $S^{(k)}$. Note that the sets $S^{(n)}$ may be finite or infinite. The choice of a random element in $S^{(k)}$ thus amounts, in the cases we consider, to generation of either a random integer or a real number in a finite interval; see §2.2. The vector of transformation strains will be denoted by $e$ as in Appendix D.2, see (122); the current distribution is denoted by $e_{\text{current}}$, while the one obtained from $e_{\text{current}}$ by changing one element at random will be called $e_{\text{new}}$.

Once a new vector $e_{\text{new}}$ has been obtained, the value $W_{\text{new}}$ of the energy associated with this modified distribution of eigenstrains is computed. (Notice that, since $e_{\text{current}}$ and $e_{\text{new}}$ differ in their $k$-th triple only,

$$e_{\text{new}} = e_{\text{current}} + \Delta e$$

with

$$\Delta e = (0, \cdots, 0, \Delta h^{(k)}, \Delta d^{(k)}_1, \Delta d^{(k)}_2, 0 \cdots, 0),$$

it is not necessary to recompute the complete quadratic $(W_{1}^{\delta})_{\text{new}} = e_{\text{new}}M^{\delta}e_{\text{new}}^{t}$, see (49).

Instead it is advantageous to use the expression

$$\left(W_{1}^{\delta}\right)_{\text{new}} = \left(W_{1}^{\delta}\right)_{\text{current}} + 2(\Delta e)M^{\delta}e_{\text{current}}^{t} + (\Delta e)M^{\delta}(\Delta e)^{t}$$

27
which leads to a substantially reduced operation count. Similar remarks apply to the updates of the other terms in (53). If $W_{\text{new}}$ is smaller than $W_{\text{current}}$ then the new distribution is accepted as current and the energy is updated accordingly: $W_{\text{current}} = W_{\text{new}}$. If $W_{\text{new}}$ is larger than $W_{\text{current}}$, on the other hand, the new distribution $e_{\text{new}}$ could be rejected, but it could also be accepted — in accordance with the basic principle of simulated annealing. This principle, which accepts a new, less favorable distribution with probability

$$
p = \exp \left[ - \frac{(W_{\text{new}} - W_{\text{current}})}{T} \right] \tag{71}
$$

allows the method to exit a region containing a local minimum, to sample the configuration space more fully, and thus, to obtain a good approximation of the global minimum. The quantity $T$ in (71) is the *artificial temperature*. It is through this parameter that the method determines whether an unfavorable distribution ought to be accepted.

![Figure 1](image)

**Figure 1:** Convergence of the parameter $\lambda$ for grains centered at positions $(0, 0), (-5, -5), (-5, 5), (5, -5), (5, 5)$ in a hydrostatic Type II square array containing 317 grains (21 grains on the horizontal diameter of $B$) under a hydrostatic applied strain with $h^0 = 0.01$.

The calculation proceeds by choosing a "large" value of the temperature which is then incrementally decreased to produce the annealing effect. At every fixed value of the temperature a number of random steps are performed, each one consisting of a change of one of the
transformation strains, leading to a new energy value $W_{new}$ and to acceptance or rejection of the new configuration as described above.

In a particular implementation of simulated annealing, choices have to be made with regards to parameters mentioned above: initial temperature, number of random steps at each temperature and percentage of decrease of the temperature from one temperature step to the next. According to general recommendations, e.g. Press, Teukolsky, Vetterling and Flannery (1992), these parameters would be selected as follows. An estimate of the order of magnitude for the initial temperature given by the quantity $T = O(W_{new} - W_{current})$ corresponding to two neighboring distributions would be used. (This choice leads to probabilities of order 1 in (71)). At each temperature the algorithms could be made to perform 100-(number of grains) random steps, and the temperature would be decreased to 90\% of its previous value at each temperature step.

In our problem, however, we have observed that use of initial temperatures which are ten orders of magnitude smaller than those generally recommended lead to results for the homogenized energy which are indistinguishable from those obtained from conventional choices. (Of course, once a vanishing value of the initial temperature is chosen, the remaining parameter choices are irrelevant.) Interestingly, the convergence to the minimum value is much faster if such a vanishing value of the initial temperature is used. This phenomenon can be explained in light of our numerical experiments, which suggest that in our problem there are no substantial differences between the energy values associated with local and global minima.

4.2 Convergence

In order to study the convergence properties of our algorithm we have performed a variety of tests which we discuss below. These tests comprise cases in which the modes of transformation of the individual grains are either purely deviatoric or purely hydrostatic, and they contain comparisons of numerical results with our rigorous bounds. Finally, they include an example of an array in which the crystalline lattices of all the crystallites are oriented in a fixed direction, and whose behavior can therefore be anticipated as similar to that of a single crystal. The results of these tests indicate an excellent overall performance of our algorithm. In particular, our code is robust, reliable, and, interestingly, it is also rather fast: it produces the energy value for a given applied strain in a 1 to 5 minutes calculation in a Sparc 20 for any of the configurations we have treated.

In our first convergence test we consider a hydrostatic Type II square array, for which the set of possible eigenstrains is given by (13) with $H = 0.02$. Since this set of tensors is invariant under arbitrary rotations, we expect that a minimizing distribution of transformation should assign a fixed eigenstrain to all grains—at least in the limit of small $\delta$. In Figure 1 we show the evolution of the value of $\lambda$ (which characterizes the eigenstrain, see (13)) for five grains in a square array containing 317 grains. The locations of the test grains were chosen as
follows: one at the origin, and the other four half way from the center to the circumference of $B$. (Note that in this example the horizontal diameter of $B$ contains 21 grains.) A clear convergence to the value $\lambda = 0.6035$ in all cases is observed.

<table>
<thead>
<tr>
<th># of grains</th>
<th>Energy: $\epsilon_{11}^0 = 0.01$</th>
<th>Energy: $d_1^0 = 0.01$</th>
</tr>
</thead>
<tbody>
<tr>
<td>149</td>
<td>11.41</td>
<td>5.70</td>
</tr>
<tr>
<td>317</td>
<td>11.43</td>
<td>5.78</td>
</tr>
<tr>
<td>529</td>
<td>11.44</td>
<td>5.84</td>
</tr>
<tr>
<td>901</td>
<td>11.45</td>
<td>5.86</td>
</tr>
</tbody>
</table>

Table 1: Convergence study of the homogenized energy (in MPa) for a deviatoric Type II square array with randomly oriented grains ($D = 0.02$ in (11)). Left: uniaxial applied strains, $\epsilon_{11}^0 = .01$ (AE=15 MPa). Right: deviatoric applied strain, $d_1^0 = 0.01$ (AE= 20 MPa).

Figure 2: Deviatoric Type I square array ($D = 0.02$ in (10)) with constant orientations under a deviatoric applied strain with $d_1^0 = 0.006$ and $d_2^0 = 0$. Left: Initial configuration (random guess). Right: minimizing configuration. Initial and final number fractions of transformed grains: 0.6877 and 0.3312 respectively. Initial energy: 20.41 MPa; Final energy: 2.24 MPa.

Our next test is a straightforward study of the numerical values of the minimum energy for decreasingly smaller values of $\delta$, see Table 1; again, a clear convergence pattern is observed.
Figure 3: Hydrostatic Type I square array \((H = 0.02 \text{ in (12))}. \) Left: uniaxial applied strain \(\varepsilon_{11}^0\); Right: hydrostatic applied strain \(h^0\). Upper curve: AE; Lower curve: UG upper bound; Diamonds: numerical results.

The figures given in this table correspond to a deviatoric Type II square array with randomly oriented grains and with \(D = 0.02\), see (11). We note that these values are subject to statistical uncertainty associated with the random character of the grain orientations. While large fluctuations could be expected in general, a number of 300 grains or more seems to reduce such large oscillations to a set of realizations of rather small probability. Indeed, at these grain numbers the statistical fluctuations we have found reduce to less than 1% of the value of the Austenite Energy (AE). (We define the AE as the energy \(C_{ijkl} x_{ij}^0 x_{kl}^0\) which would result in the material under the imposed deformations and under the assumption of zero eigenstrains in all the grains.

In the next convergence test we consider a deviatoric Type I square array of circles in which the crystallographic orientations of all the crystallites coincide and are parallel to the coordinate axes. Figure 2 gives representations of this polycrystal. (In this and similar subsequent figures, a pair of points indicates one of the crystallographic axes in an untransformed grain; the other axis lies at right angles with the one shown. Further, an arrow indicates a grain transformed with a deviatoric eigenstrain. The direction of the arrow defines the \(x\)-axis in the right-handed coordinate system in which the transformation strain is given by \([0, D, 0]\).) In the left portion of Figure 2 we show the initial (random) distribution of transformation strains; on the right we show the minimizing distribution. We observe that the minimizing structure matches quite closely the twinned structure which
Figure 4: Deviatoric Type I square array ($D = 0.02$ in (10)). Left: uniaxial applied strain $c_{11}^0$; Right: deviatoric applied strain $d_{1}^0$. Upper curve: AE, Lower curve: UG upper bound; Diamonds: numerical results.

occurs in a single crystal with the same modes of transformations and under identical loads (the purely deviatoric transformation strain used in this example, which corresponds to a shear parallel to the bisector of either the first or third quadrant, allows for a coherent $45^\circ$ Austenite-Martensite interface). Note that the virtually perfect arrangement of lines in the minimizing microstructure is only broken at a few boundary points, where our approximation by a finite sample manifests itself.

Finally we consider the comparison of numerical results and bounds given in Figures 3, 4, 7 and 8. The upper curve in these figures represents the AE, the lower curve is the estimate given by the UG bounds of §3.1, and the intermediate curve in Figures 7 and 8 is the Taylor bound $V$, see §3.2. Not only do the numerical results lie, as they should, below the UG bounds—we have not yet encountered a situation in which our numerical results violate our bounds—but they also approximate them closely in a number of regimes. This consistency constitutes a clear indication of good quality in our numerics and bounds.

5 Results

In this section we discuss some of the most salient characteristics of the energy curves and microstructures we have found in our two-dimensional simulations. We have assumed elastic
constants and transformation strains as those described in the introduction to §4. As we explained there, these particular choices are somewhat arbitrary, and they do not carry particular significance in this presentation.

To begin our discussion of numerical results, we consider the right graph in Figure 3, which shows a non-convex overall energy curve. Non-convexities in the overall energies have been reported, even in single crystals, and they have been linked to geometric incompatibilities among the various variants of martensite (Kohn (1991)). In our case, however, the lack of convexity is closely related to the particular nature of Type I polycrystals. Indeed, increasing hydrostatic deformations imposed on this polycrystal can be accommodated best by transformation of a certain fraction of crystallites. These eigenstrains, however, cause energy increases as they interact through an elastic matrix on which the boundary conditions impose smaller deformations. Thus, such grain transformations are indeed better suited to accommodate even larger applied strains, and thus further increases in the applied strain result in reductions in the elastic energy and non-convexity. (A simplified picture of this phenomenon can be obtained by consideration of a single crystal with possible transformation strains $\sigma_1^{hyd}$ under hydrostatic loads.) Notice that our upper bound follows our numerical curve closely, and it shares its non-convex structure. In Figure 4 right, on the other hand, the non-convexity of the UG bound does not correspond to non-convexity in the actual energy curve.
Figure 6: Deviatoric Type I randomly oriented square array ($D = 0.02$ in (10)). Deviatoric applied strain: $d^0_1 = 0.02$. Left: Initial configuration (random guess); Right: Minimizing configuration. Initial number fraction: 0.6814; Final number fraction: 0.8864. Initial energy: 94.91 MPa; Final energy: 31.05 MPa.

As discussed in §4.2, Figure 2 contains a representation of the initial and minimizing configurations in an array with constant orientations. We observed there that the minimizing structure corresponds quite closely to the one associated found in true single crystals. It is to be noted that the minimizing microstructure is not unique, and, in particular, that twins at plus or minus 45° lead to identical values of the energy. In Figures 5 and 6 we present corresponding results for randomly oriented arrays. Note that the minimizing configuration in Figure 5 contains, roughly, lines at ±45° formed by grains which carry transformation strains in directions as close as possible to the most favorable one: $\theta = 0$, see §2.1. That is, the minimizing configuration is associated with an arrangement in which on one hand the transforming crystallites are some of those oriented in the most favorable angles, while, on the other hand, the transforming crystallites “attempt” to arrange themselves, as much as possible, in “lines” parallel to the most favorable directions. In Figure 6 most of the crystallites have transformed under an increased applied strain and arrangements of crystallites in lines cannot be distinguished; note that each grain in the final configuration, with no exceptions, has transformed in the direction that is closest to “horizontal”, as expected.

In Figures 7 to 10 we present results corresponding to polycrystals of Type II. Let us first consider Figures 7 and 8, where we present calculations corresponding to the square array which we compare with the associated Taylor bounds and UG bounds. Note the remarkably good qualitative and quantitative approximations provided by the UG bounds. In Figures 9
Figure 7: Hydrostatic Type II square array \((H = 0.02 \text{ in } 13)\). Left: uniaxial applied strain \(e_{11}^0\); Right: hydrostatic applied strain \(h^0\). Upper curve: AE; Middle curve: Taylor bound; Lower curve: UG bound; Diamonds: numerical results.

and 10, finally, we compare the Taylor bound and the UG bound for the Type II random array with no intergrain matrix described in §2.1. We note that, as is apparent from Figures 7 to 9 and as stated in the introduction, the Taylor bound can produce overestimates of the energy of over 50%. The UG bound in Figure 9 right, for example, which does not contain contributions to the energy of an elastic matrix, tells us that the elastic energy at \(d_1^0 = 0.02\) is less than 26.42, while the corresponding value given by the Taylor bound is 40.

In the configuration corresponding to Figure 10, the Taylor and UG bounds coincide, since in this case the UG bound is attained by a distribution \(e^T\) satisfying the Taylor hypothesis. For all applied strains in \(T\) the overall energy and the bounds vanish. Thus, in Figure 10 right we depart from our previous practice, and we present results for a purely hydrostatic polycrystal under applied strains which are not purely hydrostatic. We used applied strains of the form \([0.75e_{11}^0, 0.25e_{11}^0, 0] (0 \leq e_{11}^0 \leq 0.02)\) which contain a significant deviatoric component; we see that the overall energy remains extremely small. A comparison of Figures 7 to 10 demonstrates the influence the elastic matrix occurring in the square array may have in the values of the overall energy. In the deviatoric arrays considered in Figures 8 and 9, for which zero energy configurations do not exist, the energetic effect of the elastic matrix is qualitatively negligible; quantitatively it amounts energy increases of about 30%. Comparison of Figures 7 and 10, on the other hand, shows more dramatic matrix effects which arise in a configuration in which a non-trivial Taylor set exists.
Figure 8: Deviatoric Type II square array ($D = 0.02$ in (11)). Left: uniaxial applied strain $\epsilon_{11}^0$; Right: deviatoric applied strain $a_{1}^0$. Upper curve: AE; Middle curve: Taylor bound; Lower curve: UG bound; Diamonds: numerical results.

Acknowledgements: OB gratefully acknowledges support from NSF (through an NYI award and through grants No. DMS-9200002 and DMS-9523292), from the Sloan Foundation (through the fellowships program), from the Powell Research Foundation, and from the AFOSR (contract No. F49620-96-1-0008). FR gratefully acknowledges support from AFOSR through grant No. F49620-95-1-0113. PHL gratefully acknowledges support from NSF through grant CMS-9503393.

A Appendix: Finely-grained Eshelby solutions

A.1 Convergence of boundary values

Let $(G^{(n)})$ be an distribution of grains of arbitrary shape in the plane, and let $F$ be an arbitrary plane domain. Call $u^1$ the solution

$$u^1(x, \delta) = \sum_{G^{(n)}, \delta \subseteq F} u^{(n), \delta}(x),$$
Figure 9: Deviatoric Type II random array with no inter-grain matrix ($D = 0.02$ in (11)). Left: uniaxial applied strain $e_{11}^0$; Right: deviatoric applied strain $d_1^0$. Upper curve: AE; Middle curve: Taylor bound; Lower curve: UG bound.

see (36), (37), and assume the distribution of transformation strains $\varepsilon^T$ converges weakly within $F$ to $\varepsilon^{T(\text{av})} = [h^{T(\text{av})}, d_1^{T(\text{av})}, d_2^{T(\text{av})}]$ as $\delta \to 0$. In what follows we show that under these conditions the following three points hold true:

1. For any bounded set $F'$, $u^1(x, \delta)$ converges to

$$u_i^1(x, 0) = \int_{F'} C_{jkr} \varepsilon_{rs}^{T(\text{av})} \Gamma_{ij,k}(x - x')dx'$$

(72)

in $H^1(F' \setminus F)$ as $\delta \to 0$, and the convergence is uniform outside any domain containing the closure of $F$ in its interior. If $F$ is a circle then $u^1(x, 0)$ equals the displacement in (106), (107) with $[h, d_1, d_2] = [h^{T(\text{av})}, d_1^{T(\text{av})}, d_2^{T(\text{av})}]$.

2. The values of $u^1(x, \delta)$ on the boundary of $F$ converge in $H^{\frac{1}{2}}(\partial F)$.

3. If, in addition, $\varepsilon^T$ converges strongly in the square mean within $F$ then $u^1(x, \delta)$ converges to $u^1(x, 0)$ in $H^1(F')$ for any bounded domain $F'$. 

37
Figure 10: Hydrostatic Type II random array with no inter-grain matrix ($H = 0.02$ in (13)).
Left: uniaxial applied strain $\epsilon_{11}^0$; Right: $\epsilon_{11}^0 = 2\epsilon_{22}^0$, $\epsilon_{12}^0 = 0$. Upper curve: AE; Lower curve: UG and Taylor bounds (the bounds coincide).

To establish point 1) we consider the representation

$$u_i^1(x, \delta) = \int_{\bigcup \{(G^{(n)}_i, \delta, G^{(n)}_l, \delta) \subseteq F\}} \bar{C}_{jkr} \bar{\epsilon}_{rs}^T(x', \delta) \Gamma_{ij,kl}(x - x') dx',$$

see §2.6. It follows from this expression that the limit of $u^1(x, \delta)$ at any point outside $F$ is given by (72), since the kernel $\Gamma_{ij,kl}(x)$ is continuous for $x \neq 0$. Further, since this kernel is locally integrable as well as uniformly continuous in the complement of any small ball around the origin, it is easy to check that the convergence is indeed uniform in the complement of any open set containing the closure of $F$ in its interior.

To establish the convergence $H^1(F' \setminus F)$ for a bounded set $F'$, and thus conclude with our proof of point 1), we first note that for $x$ outside $F$ the partial derivatives of $u^1(x, \delta)$ with respect to $x_l$ are given by the expression

$$u_{i,l}^1(x, \delta) = \int_F C_{jkr} \bar{\epsilon}_{rs}^T \Gamma_{ij,kl}(x' - x') dx'.$$

(73)
To estimate this quantity we use polar coordinates around the point \( x \in F' \setminus F \). Calling \( r = |x - x'| \) and letting \( M_x \) be an upper bound on \( |x - x'| \) for all \( x' \in F' \setminus F \) and \( \text{dist}(x, F) \) the distance from \( x \) to \( F \) we obtain from (42), (73)

\[
|u_{1,1}^1(x, \delta)| < K \int_{\text{dist}(x,F)}^{M_x} \frac{1}{r} dr
\]

and thus

\[
|u_{1,1}^1(x, \delta)| < K \log(\text{dist}(x, F))
\]

for some constant \( K \). It follows that the squares of the derivatives of \( u^1(x, \delta) \) are bounded by an integrable function and the \( H^1 \) convergence in \( F' \setminus F \) follows from the result of uniform convergence away from \( F \). The limiting form (72) of Eshelby’s integral tells us that \( u^1(x, 0) \) equals the displacement caused by the inclusion \( F \) as it transforms in the plane with eigenstrain \( \epsilon^{T(au)} \). Thus, if \( F \) is a circle \( u^1 \) is given by (106), (107) with \([h, d_1, d_2] = [h^{T(au)}, d_1^{T(au)}, d_2^{T(au)}]\) as claimed.

The convergence of the boundary values of point 2) now follows directly from the trace Theorem (e.g. Necas (1967)) applied in the region \( F' \setminus F \) for any bounded domain \( F' \) containing the closure of \( F \) in its interior. To establish point 3), finally, assume the field of transformation strains converges strongly in mean square within \( F \). In order to establish the convergence of \( u^1(x, \delta) \) in \( H^1(F') \) for a bounded domain \( F' \) it suffices, in view of point 1) to establish the corresponding result in the case \( F' = F \). This, in turn, follows easily from the \( H^{1/2} \) convergence of the values of \( u^1 \) on the boundary of \( F \), by considering the weak formulation of the equations (39) and Korn’s inequality.

### A.2 A region bounded by two circles

Let \( D_{c,r} \) be the circle of radius \( r \) centered at \( c \). In this section we consider a distribution of transformations strains \( \epsilon^T(x, \delta) \) supported in \( B \setminus D_{c,r} \), where \( D_{c,r} \subseteq B \), see (15). We show that if \( \epsilon^T \) converges weakly in \( B \setminus D_{c,r} \) to a constant strain \( \xi \) as \( \delta \to 0 \), then the strain \( \epsilon_{c,r} = \epsilon_{c,r}(x, \delta) \) produced by \( \epsilon^T \) in the plane tends to zero within \( D_{c,r} \). Further, given an arbitrary \( r' < r \), we show the convergence is jointly uniform in the region \( \mathcal{R}_{r'} \subseteq \mathbb{R}^4 \) of all pairs \((c, x)\) such that \( D_{c,r} \subseteq B \) and \( x \in D_{c,r'} \).

We establish first the simpler theorem stating that \( \epsilon_{c,r} \) actually vanishes within \( D_{c,r} \) in case \( \epsilon^T = \xi \) in \( B \setminus D_{c,r} \). Indeed, the Eshelby strain \( \epsilon_\xi' \) caused within a transforming circular inclusion (with transformation strain \( \xi \)) is a constant tensor which does not depend on the size of the inclusion, see (108). It follows that for \( x \in D_{c,r} \) we can write

\[
\epsilon_{c,r} + \epsilon_\xi' = \epsilon_\xi'
\]
(since the strain at \( x \) equals the strain produced by transformation of \( D_{c,r} \) plus the strain produced by transformation of \( B \setminus D_{c,r} \)) and thus

\[
\epsilon_{c,r} = 0
\]
in this case, as claimed.

To establish the proof in the general case it now suffices to show that \( \epsilon_{c,r} \) converges uniformly in \( \mathcal{R}_{r^*} \). The fact that the limit is 0 then follows directly from the result for constant eigenstrain and the representation in terms of Eshelby integrals of \( \S \) 2.6, which tells us that within \( D_{c,r} \) the limit equals the strain caused by transformation of \( B \setminus D_{c,r} \) with transformation strain \( \xi = \epsilon_{T(a^0)} \). Now, the uniform convergence within \( D_{c,r} \) for a fixed \( c \) follows directly from the results of the previous Appendix; the joint uniform convergence with respect to \( (c,x) \) can be established, analogously, from consideration of the uniform continuity of the associated kernels away from their singularities.

B Appendix: Uncorrelated grains, ranges of averages, interactions

In \( \S \) B.1 we find the range of values of the variables \( y \) and \( z \), see (62), and in \( \S \) B.2, B.3 we calculate the quantity \( Z^\delta \) for the square and random arrays, see \( \S \) 3.1.

B.1 The range of values of \( y \) and \( z \)

From (60) we clearly have

\[
y = \frac{\pi}{2} \lim_{\delta \to 0} (a(\delta, \omega) - b(\delta, \omega))
\]

where

\[
a = \frac{1}{N_T} \sum_{\substack{k \mid \tau(k) \neq 0 \\theta^{(k)} \in C}} \cos(2\theta^{(k)})
\]

and

\[
b = \frac{1}{N_T} \sum_{\substack{k \mid \tau(k) \neq 0 \\theta^{(k)} \in C}} \cos(2\theta^{(k)}).
\]
In view of our assumption of a uniform distribution of grain orientations, the law of large numbers tells us that

\[ \lim_{\delta \to 0} a = \frac{2}{\pi} \int_C \cos(2\theta) d\theta \]

and

\[ \lim_{\delta \to 0} b = \frac{2}{\pi} \int_{[0, \frac{\pi}{2}] \setminus C} \cos(2\theta) d\theta \]

so that

\[ y = \left( \int_C \cos(2\theta) d\theta - \int_{[0, \frac{\pi}{2}] \setminus C} \cos(2\theta) d\theta \right). \]

Analogously,

\[ z = \left( \int_C \sin(2\theta) d\theta - \int_{[0, \frac{\pi}{2}] \setminus C} \sin(2\theta) d\theta \right) \]

see (61).

Since

\[ \int_0^{\frac{\pi}{2}} \cos(2\theta) d\theta = 0 \]

and

\[ \int_0^{\frac{\pi}{2}} \sin(2\theta) d\theta = 1 \]

we have

\[ y = 2 \int_C \cos(2\theta) d\theta \]

and

\[ z = 2 \int_C \sin(2\theta) d\theta - 1. \]

(74)

(75)
Note from (74) that $y$ lies between $-1$ and $1$. To describe the range of values taken by $(y, z)$ as $C \subseteq [0, \frac{\pi}{2}]$ varies, we compute the maximum and minimum values that $z$ may take for a given $y$. That is, we seek the extrema of the integral expression

$$J_1 = \int_C \sin(2\theta) d\theta$$

over all $C \subseteq [0, \frac{\pi}{2}]$ given that

$$J_2 = \int_C \cos(2\theta) d\theta = \frac{y}{2}. \quad (76)$$

Let us consider first the case

$$0 \leq y \leq 1. \quad (77)$$

To find the maximum values of $J_1$ consistent with (76) we first show that the corresponding maximizing sets must be of the form

$$C = [0, b] \quad (78)$$

for some $b \in [\frac{\pi}{4}, \frac{\pi}{2}]$. To see this notice that the maximizing set $C$ must contain the interval $[0, \frac{\pi}{4}]$, since otherwise the set $[0, \frac{\pi}{2}] \setminus C$ could be added to $C$, together with a corresponding portion within the interval $[\frac{\pi}{4}, \frac{\pi}{2}]$ in such a way that the integral (76) is unchanged but $J_1$ is increased. Further, if the set $C$ contains a portion $\tilde{C}$ of the interval $[\frac{\pi}{4}, \frac{\pi}{2}]$

$$\tilde{C} = C \cap \left[\frac{\pi}{4}, \frac{\pi}{2}\right]$$

then $\tilde{C}$ must be a set of the form $[\frac{\pi}{4}, b]$ for some $b \leq \frac{\pi}{2}$. Indeed, there is a number $b \leq \frac{\pi}{2}$ such that the integral of $\cos(2\theta)$ on $[\frac{\pi}{4}, b]$ equals the integral of this function on $\tilde{C}$. Since $\cos(2\theta)$ decreases from 0 in $[\frac{\pi}{4}, \frac{\pi}{2}]$ we see the measure of $[\frac{\pi}{4}, b]$ is larger than the measure of $\tilde{C}$, and since $\sin(2\theta)$ decreases in the interval $[\frac{\pi}{4}, \frac{\pi}{2}]$ it follows that the integral of this function over $\tilde{C}$ is strictly smaller than its integral over $[\frac{\pi}{4}, b]$ unless $\tilde{C} = [\frac{\pi}{4}, b]$. We conclude that $C$ is given by (78), as claimed.
Now it is an easy matter to compute the maximum of $J_1$ subject to (76), and thus to
describe the set of values of the pair $(y, z)$ which can be obtained from (74)-(75). Indeed,
for the maximizer (78) we obtain from (76)

$$\sin(2b) = y;$$

from which it follows that

$$\cos(2b) = -\sqrt{1 - y^2}$$

since $\frac{\pi}{2} \leq 2b \leq \pi$, and thus that the maximum value of $J_1$ is $\frac{1}{2} \left( \sqrt{1 - y^2} + 1 \right)$. It follows

that the maximum value of $z$ in the case (77) is

$$z_{\max} = \sqrt{1 - y^2}. \tag{79}$$

A similar argument shows that the maximum value of $z$ is indeed given by (79) for all $y,
-1 \leq y \leq 1$, and that the minimum value of $z$ is given by

$$z_{\min} = -\sqrt{1 - y^2}$$

for $-1 \leq y \leq 1$. In other words, the pair $(y, z)$ is restricted to lie within the circle

$$y^2 + z^2 \leq 1.$$ 

It is now easy to check that all $(y, z)$ within this circle can be obtained as values corresponding
to some set $C \subseteq \frac{\pi}{2}$, and the best of the upper bounds (62) can be obtained by minimization
in $y, z, t$ and $\xi$ subject to (63), (64) and (65).

### B.2 Random array: $Z^\delta = 0$

Here we show that the quantity $Z^\delta$ vanishes in case the circular grains cover all of $B$. To do
this let us denote by $W_{\text{self}}^\delta(h, d_1, d_2)$ the self energy per unit volume arising from a constant
eigenstrain $\epsilon^T = [h^T, d_1^T, d_2^T]$ in a circle $F$ of radius $R$ contained in an infinite matrix. That
is, calling $\sigma$ the corresponding stress we have from (112)

$$W_{\text{self}}(h^T, d_1^T, d_2^T) = -\frac{1}{2\pi R^2} \int_F \epsilon^T \sigma = \frac{2\mu}{(2 + g)} \left( 2(h^T)^2 + (d^T)^2 \right);$$
note that $W_{self}$ is independent of the radius $R$. To show that $Z^{\delta} = 0$ we consider the self energy per unit volume $W_{self}(h_{T^{(av)}}, d_{1}^{T^{(av)}}, d_{2}^{T^{(av)}})$ in our body $B$ when considered as a transforming inclusion $F = B$ with transformation strain $[h_{T^{(av)}}, d_{1}^{T^{(av)}}, d_{2}^{T^{(av)}}]$. We note that since the set $B$ is the infinite disjoint union of the grains $G^{(n), \delta}$ we have

$$\epsilon^{T^{(av)}} = \sum_{n \in I} \chi^{(n), \delta} \epsilon^{T^{(av)}},$$

see (14). Since this sum converges in mean square, the $H^{1}$ convergence result given in point 3) of Appendix A.1 applies. It implies, in particular, that if $\epsilon^{T^{(n)}} = \epsilon^{T^{(av)}}$ for all $n$, the infinite sum (38) converges in square mean. From (48), (51), (56) (note that $N = \infty$ here) and the independence of $W_{self}$ on the grain size we thus obtain

$$W_{self}(h_{T^{(av)}}, d_{1}^{T^{(av)}}, d_{2}^{T^{(av)}}) = W_{self}(h_{T^{(av)}}, d_{1}^{T^{(av)}}, d_{2}^{T^{(av)}}) + Z^{\delta},$$

and thus $Z^{\delta} = 0$, as desired.

### B.3 Square array: $Z^{\delta} \neq 0$

In the case of a square array of circles the transforming regions do not cover all space. As a result $Z^{\delta}$ is not zero and it makes a (small) contribution to the total energy. To compute $Z^{\delta}$ in this limit let us first write $a = (h_{T^{(av)}}, d_{1}^{T^{(av)}}, d_{2}^{T^{(av)}})$ and

$$Z^{(k), \delta} = \sum_{p \neq k} a M_{kp}^{\delta} a^{t}$$

so that

$$Z^{\delta} = \sum_{k=1}^{N} Z^{(k), \delta}.$$ 

Now, given a small number $r > 0$, call

$$I_{r}^{\delta} = \{ k \in I^{\delta} : G^{(k), \delta} \subseteq D_{1-r,0} \},$$

44
see (26), where \( D_{1-r,0} = \{ x : |x| \leq 1 - r \} \). From (121), the weak form of equations (18), (19) and the convergence results of Appendix A.1 one can show that

\[
\sum_{k \in I_r^\delta \setminus I_r^\delta} Z^{(k),\delta} \to 0 \text{ as } r \to 0
\]  

(80)

uniformly in \( \delta \). It is therefore sufficient to consider the contributions from \( Z^{(k),\delta} \) with \( k \in I_r^\delta \).

Let \( F^{(k),r} \) be the circle of radius \( r \) concentric with \( G^{(k),\delta} \), and assume \( k \in I_r^\delta \) (which implies \( F^{(k),r} \subseteq B \)). By the results in Appendix A.2, the strain produced in \( G^{(k),\delta} \) by all the grains contained outside \( F^{(k),r} \) tends to zero as \( \delta \to 0 \). (The limiting strain produced by the grains inside \( F^{(k),r} \) does not vanish, and will be considered below.) Further, the convergence to zero is uniform for all such configurations. It follows that the contribution to \( Z^{(k),\delta} \) from all grains that are at a distance larger than \( r \) from the center of \( G^{(k),\delta} \) is bounded by the area of \( G^{(k),\delta} \) times a quantity which tends to zero with \( \delta \). Thus, from the formulae of Appendix D.2 we have, for \( k \in I_r^\delta \) we have

\[
Z^{(k),\delta} = \left( (d_2^{(av)})^2 - (d_1^{(av)})^2 \right) \sum_{\substack{p \neq k \in G^{(p),\delta} \cap F^{(k),r} \neq \emptyset}} \frac{2\mu R^4}{(2 + g)} \cos(4\eta_{kp}) \frac{(6R^2 - 2\ell_{kp}^4)}{\ell_{kp}^4} + \delta^2 O(\delta).
\]

(Indeed, by square symmetry, the contributions of all but the (2, 2) and (3, 3) entries of \( M_{kp}^\delta \) cancel out.) In the present case in which the radii equal \( \delta/2 \) we obtain

\[
\lim_{\delta \to 0} \frac{Z^{(k),\delta}}{\delta^2} = \left( (d_2^{(av)})^2 - (d_1^{(av)})^2 \right) \frac{\mu}{8(2 + g)} S^0
\]

uniformly for \( k \in I_r^\delta \), where \( S^0 \) is given by the limit

\[
S^0 = \lim_{\delta \to 0} \sum_{0 < i^2 + j^2 \leq \delta^{-2}} \cos \left( 4\tan^{-1}(j/i) \right) \frac{3 - 4(i^2 + j^2)}{2(i^2 + j^2)^2}.
\]

A direct numerical evaluation gives

\[
S^0 \approx -0.29.
\]

(81)
In view of (80) and since \( N \delta^2 \to \pi \) we obtain

\[
\lim_{\delta \to 0} Z^\delta = \lim_{\delta \to 0} \sum_{k \in I^\delta} Z^{(k),\delta} = \lim_{\delta \to 0} N \left( (d_2^{T(\text{av})})^2 - (d_1^{T(\text{av})})^2 \right) \frac{\mu \delta^2}{8(2 + g)} S^\delta
\]

\[
= \left( (d_2^{T(\text{av})})^2 - (d_1^{T(\text{av})})^2 \right) \frac{\mu \pi}{8(2 + g)} S^0.
\]

Using (57), (58), (59) (with \( v = \frac{\pi}{4} \)), we may rewrite this expression as

\[
\lim_{\delta \to 0} Z^\delta = -\frac{(d^T)^2 \mu \pi}{32(2 + g)} S^0 t^2 \left( y^2 - z^2 \right) = \eta t^2 (y^2 - z^2).
\]

where

\[
\eta = -\frac{(d^T)^2 S^0 \mu \pi}{32(2 + g)} \approx \frac{0.03(d^T)^2 \mu}{2 + g}.
\]

see (81).

C Appendix: Finite dimensional minimization

In this section we calculate the minimum value of the function in (62) as its various arguments are varied, and we obtain, in a number of cases, expressions in closed form for the UG bound \( U \). In view of (54), (62) and (65) this bound is given by

\[
U = U(e^0) = \min_{\xi \in \delta} m_\xi(e^0)
\]

with

\[
m_\xi(e^0) = \min_{0 \leq z, t, \xi \leq 1} m(y, z, t, \xi, e^0).
\]

Expressions in closed form for \( U \) can indeed be obtained for the random array of circles (in which the particles cover all space and \( Z^\delta = 0 \)) under general boundary conditions. In the
case of the square lattice, on the other hand, explicit calculations can also be given provided that, in a basis parallel to the lattice of grains the applied strain tensor is diagonal.

To begin we write down explicit expressions for the parameters $A$, $a$, $b$, $\alpha$ and $\beta$ characterizing the function $m$ in (62)

$$m(y, z, t, \xi, \epsilon^0) = A(ty - a)^2 + A(tz - b)^2 + \alpha(t - c)^2 + \beta + Z^\delta.$$  

These parameters, which do not depend on $(y, z, t)$, can be calculated easily from (53)–(58); calling $d^\xi = \sqrt{(d_1^\xi)^2 + (d_2^\xi)^2}$ and $d^0 = \sqrt{(d_1^0)^2 + (d_2^0)^2}$ we obtain

$$A = \frac{8\mu v^2 (d^\xi)^2 (1 + g)}{\pi^2 (2 + g)} \quad (84)$$

$$\alpha = \frac{8\mu v^2 (h^\xi)^2}{g (2 + g)}$$

$$\beta = -\frac{\mu}{8 (1 + g) (2 + g) (h^\xi)^2} \left[ 16 (h^\xi)^2 (2 + g) \left( (1 + g) (h^0)^2 + (d^0)^2 \right) 
- 8 h^\xi (2 + g) (1 + g) \left( 2 \left( h^\xi \right)^2 + (d^\xi)^2 \right) h^0 + g \left( 2 \left( h^\xi \right)^2 + (d^\xi)^2 \right)^2 (1 + g) \right]$$

$$a = \frac{\pi (2 + g) d_1^0}{2v (1 + g) d^\xi}$$

$$b = -\frac{\pi (2 + g) d_2^0}{2v (1 + g) d^\xi}$$

$$c = \frac{4h^0 h^\xi (2 + g) - g \left( 2 \left( h^\xi \right)^2 + (d^\xi)^2 \right)}{8v (h^\xi)^2}.$$  

From Appendices B.2, B.3 we know that $Z^\delta$ in (56) satisfies

$$Z^\delta = 0 \quad \text{for the randomly oriented random array of circles covering all of } B \quad (85)$$

and

$$\lim_{\delta \to 0} Z^\delta = \eta \ell^2 (y^2 - z^2) \quad \text{for a square array of circles.} \quad (86)$$
C.1 Minimization in \((y, z, t)\)

We begin by simplifying our minimization problem. In the case of the random array \(Z^\xi = 0\) (see (85)) and \(m\) is given by

\[
m = A(ty - a)^2 + A(tz - b)^2 + \alpha(t - c)^2 + \beta.
\]

For given \(\xi\) and \(e^0\) call \((y_0, z_0, t_0)\) the point at which the minimum (83) is achieved. Hence, if \((a^2 + b^2) \leq t_0^2\) we see that necessarily \(y_0 = \frac{a}{t_0}\) and \(z_0 = \frac{b}{t_0}\), while if \((a^2 + b^2) > t_0^2\) then \((y_0, z_0)\) is the only multiple of \((\frac{a}{t_0}, \frac{b}{t_0})\), with a positive factor, which lies on the boundary of the circle (65). In any case, the minimizer \((t_0, y_0, z_0)\) satisfies \(t \cdot (y_0, z_0) = \gamma \cdot (a, b)\) for some \(\gamma > 0\), and therefore

\[
m_\xi(e^0) = \min_{0 \leq \gamma \leq 1/s} As^2(\gamma - 1)^2 + \alpha(t - c)^2 + \beta \tag{87}
\]

where

\[
s = \sqrt{a^2 + b^2} = \frac{\pi(2 + g)d_0}{2v(1 + g)d_0}. \tag{88}
\]

As for the square array, on the other hand, we have \(b = 0\) provided \(d_0^0 = 0\), see (84), and thus the minimizer must have \(z_0 = 0\). In order to obtain \(m_\xi\) in case \(d_0^0 = 0\), then, we may set \(z = 0\) in our expression for \(m\). In view of (86) we have

\[
m_\xi = \min_{0 \leq \gamma \leq 1} (A + \eta) \left(\frac{ty - a}{1 + \eta/A}\right)^2 + \alpha(t - c)^2 + \beta + \eta \frac{a^2}{1 + \eta/A}.
\]

Thus, calling

\[
A_\eta = A + \eta
\]

\[
s_\eta = \frac{s}{1 + \eta/A}\]

\[
\beta_\eta = \beta + \eta \frac{a^2}{1 + \eta/A}, \tag{89}
\]

48
we obtain
\[ m_\xi(e^0) = \min_{0 \leq t \leq 1, 0 \leq \gamma \leq \gamma_{t/s}} A_\eta^2 \eta^2 (\gamma - 1)^2 + \alpha(t - c)^2 + \beta_\eta. \] (90)

We see that in either of the cases considered here, the calculation of \( m_\xi \) reduces to finding a minimum of the form
\[ m_\xi(e^0) = \min_{0 \leq s' \leq 1, 0 \leq \gamma \leq \gamma_{t/s}} A'(s')^2 (\gamma - 1)^2 + \alpha(t - c)^2 + \beta' \] (91)

for some values of \( A' \), \( s' \) and \( \beta' \).

To compute this minimum we consider separately the cases: \( s' < 1 \) and \( s' \geq 1 \). In case \( s' \geq 1 \) it is easy to see from (91) that the minimizer occurs on the line \( \gamma = t/s' \) in the \( (t, \gamma) \) plane. With this substitution the problem reduces to minimization of a one-dimensional quadratic in \( t \) in the interval \( 0 \leq t \leq 1 \). Thus, denoting by
\[ t_{\text{ver}} = \frac{A's' + \alpha c}{A' + \alpha}. \] (92)

the vertex of this quadratic, we obtain,
\[ \text{for } s' \geq 1, \quad m_\xi = \begin{cases} 
\frac{A'\alpha}{(A' + \alpha)}(s' - c)^2 + \beta' & \text{if } 0 \leq t_{\text{ver}} \leq 1 \\
A'(1 - s')^2 + \alpha(1 - c)^2 + \beta' & \text{if } t_{\text{ver}} > 1 \\
A'(s')^2 + \alpha c^2 + \beta' & \text{if } t_{\text{ver}} < 0.
\end{cases} \] (93)

Let us now consider the case \( s' < 1 \). It is not hard to show that, again, the minimum must satisfy \( \gamma = t/s' \) provided \( c < s' \), and minimization of a one-dimensional quadratic yields the result in this case. If \( s' < c < 1 \) the minimum equals \( \beta' \), as it is checked easily. Finally, if \( c > 1 \) the minimum is achieved at \( t = 1 \) and \( \gamma = 1 \). Summing up,
\[ \text{for } s' < 1, \quad m_\xi = \begin{cases} 
\frac{A'\alpha}{(A' + \alpha)}(s' - c)^2 + \beta' & \text{if } c \leq s' \text{ and } 0 \leq t_{\text{ver}} \\
A'(s')^2 + \alpha c^2 + \beta' & \text{if } c \leq s' \text{ and } t_{\text{ver}} < 0 \\
\beta' & \text{if } s' < c \leq 1 \\
\alpha(1 - c)^2 + \beta' & \text{if } c > 1.
\end{cases} \] (94)

We remark that the values of the function \( m_\xi \) in the cases of purely hydrostatic and purely deviatoric eigenstrains can be obtained as limits of the expressions in (93) and (94)
as \( h^\xi \to 0 \) or \( d^\xi \to 0 \). The following results are useful in this connection: in either case (87) or (90) we have (see (91))

\[
\alpha c^2 + \beta' \text{ is independent of } [h^\xi, d_1^\xi, d_2^\xi],
\]

\[
\lim_{d^\xi \to 0} A' = 0, \quad \lim_{d^\xi \to 0} s' = \infty \quad \text{and} \quad \lim_{d^\xi \to 0} A'(s')^2 \text{ is finite}
\]

\[
\lim_{h^\xi \to 0} \alpha = 0, \quad \lim_{h^\xi \to 0} \beta' = -\infty, \quad \lim_{h^\xi \to 0} c = -\infty \quad \text{and} \quad \lim_{h^\xi \to 0} \alpha c, \lim_{h^\xi \to 0} \alpha \beta' \text{ are finite.}
\]

### C.2 Minimization in \( \xi \in S \)

Our final results are obtained by minimization of \( m_\xi \) with respect to \( \xi \). For Type I polycrystals ((10) and (12)) this final step is trivial, since \( m_\xi \) does not change as the tensor \( \xi \) is rotated by an angle of \( \frac{\pi}{2} \). Thus, in this case, the upper bound is given by

\[
U(\epsilon^0) = m_\xi(\epsilon^0)
\]

for any \( \xi \in S_1 \) with \( \xi \neq 0 \).

For Type II polycrystals, on the other hand, additional work is necessary. For simplicity we consider purely deviatoric or purely hydrostatic eigenstrains only. In the former case we have

\[
h^\xi = 0, \quad d_1^\xi = (2\lambda - 1)D \quad \text{and} \quad d_2^\xi = 0 \quad (0 \leq \lambda \leq 1),
\]

see (11), while in the latter

\[
h^\xi = \lambda H, \quad d_1^\xi = 0 \quad \text{and} \quad d_2^\xi = 0 \quad (0 \leq \lambda \leq 1),
\]

see (13). Since the minimum \( m_\xi \) depends on \( d_1^\xi \) and \( d_2^\xi \) through the quantity \( (d^\xi)^2 \) only, we may assume that \( 0 \leq 2\lambda - 1 \leq 1 \) in (96) so that (96) and (97) can both be written as

\[
h^\xi = \gamma H, \quad d_1^\xi = \gamma D \quad \text{and} \quad d_2^\xi = 0, \quad (0 \leq \gamma \leq 1).
\]

and minimization with respect to \( \xi \) reduces to minimization with respect to \( \gamma \).

Now, from (84), (88) and (89) we have in either the purely deviatoric or hydrostatic case

\[
A' = A_0 \gamma^2
\]

\[
\alpha = \alpha_0 \gamma^2
\]

\[
\beta' = -\beta_0 + \beta_1 \gamma - \beta_2 \gamma^2
\]

\[
c = \frac{c_1}{\gamma} + c_2
\]

\[
s' = \frac{s_0}{\gamma}
\]

50
where the constants \( A_0, s_0, \alpha_0, c_2, \beta_0, \beta_1 \) and \( \beta_2 \) depend on \([h^0, d^0_1, d^0_2]\) and \([H, D, 0]\) and they satisfy
\[
A_0, s_0, \alpha_0, c_2, \beta_0, \beta_1, \beta_2 > 0
\]
Moreover, in view of (95),
\[
\alpha_0 \gamma^2 (\frac{c_1}{\gamma} + c_2)^2 - \beta_0 + \beta_1 \gamma - \beta_2 \gamma^2
\]
is independent of \( \gamma \)
which implies
\[
\beta_1 = 2\alpha_0 c_1 c_2, \quad \beta_2 = \alpha_0 c_2^2.
\]
Finally, the number \( t_{\text{ver}} \) in (92) is given by
\[
t_{\text{ver}} = \frac{A's' + \alpha c}{A' + \alpha} = \frac{(A_0 s_0 + \alpha_0 c_1) - \alpha_0 c_2 \gamma}{(A_0 + \alpha_0) \gamma}
\]
so that
\[
t_{\text{ver}} \geq 0 \iff \gamma \leq \gamma_0 \equiv \frac{A_0 s_0 + \alpha_0 c_1}{\alpha_0 c_2}
\]
\[
t_{\text{ver}} \leq 1 \iff \gamma \geq \gamma_1 \equiv \frac{A_0 s_0 + \alpha_0 c_1}{A_0 + \alpha_0 + \alpha_0 c_2}.
\]
Thus, from (93), (94) and (98) we obtain
\[
\text{for } s_0 \geq \gamma, \quad m_\xi = \begin{cases}
\frac{A_0 \gamma}{(A_0 + \alpha_0)} (s_0 - c_1 + c_2 \gamma)^2 - \beta_0 + \beta_1 \gamma - \beta_2 \gamma^2 & \text{if } \gamma_1 \leq \gamma \leq \gamma_0 \\
A_0 (\gamma - s_0)^2 + \alpha_0 \gamma^2 - 2\alpha_0 (c_1 \gamma - c_2 \gamma^2) + \alpha_0 c_2^2 - \beta_0 & \text{if } \gamma \leq \gamma_1 \\
A_0 s_0^2 + \alpha_0 c_2^2 - \beta_0 & \text{if } \gamma_0 \leq \gamma.
\end{cases}
\]
and
\[
\text{for } s_0 < \gamma, \quad m_\xi = \begin{cases}
\frac{A_0 \gamma}{(A_0 + \alpha_0)} (s_0 - c_1 + c_2 \gamma)^2 - \beta_0 + \beta_1 \gamma - \beta_2 \gamma^2 & \text{if } \frac{c_1 - s_0}{c_2} \leq \gamma \leq \gamma_0 \\
A_0 s_0^2 + \alpha_0 c_2^2 - \beta_0 & \text{if } \gamma_0 \leq \gamma \\
-\beta_0 + \beta_1 \gamma - \beta_2 \gamma^2 & \text{if } \frac{c_1}{c_2 + 1} \leq \gamma \leq \frac{c_1 - s_0}{c_2} \\
\alpha_0 \gamma^2 - 2\alpha_0 (c_1 \gamma - c_2 \gamma^2) + \alpha_0 c_1^2 - \beta_0 & \text{if } \gamma \leq \frac{c_1}{c_2 + 1}.
\end{cases}
\]
since

\[ s' \geq c \iff \frac{c_1 - s_0}{c_2} \leq \gamma \]

\[ \frac{c_1 - s_0}{c_2} \leq \gamma_0 \iff 0 \leq s_0(A_0 + \alpha_0) \]

and \( c \leq 1 \iff 0 \leq s_0(A_0 + \alpha_0) \)

and \( c \leq 1 \iff \frac{c_1}{c_2 + 1} \leq \gamma. \)

We can now obtain our results for purely deviatoric and purely hydrostatic Type II polycrystals. First consider purely deviatoric polycrystals \( H = 0. \) Since

\[
\lim_{H \to 0} \alpha_0 = 0, \quad \lim_{H \to 0} \beta_1 = \infty, \quad \lim_{H \to 0} c_1 = \infty, \quad \lim_{H \to 0} \frac{c_1}{c_2} = 0
\]

and \( \lim_{H \to 0} \alpha_0 c_1^2, \lim_{H \to 0} \alpha_0 c_2 \) are finite

equations (99), (100) give

\[
m_\xi = \begin{cases} 
A_0(\gamma - s_0)^2 + 2\alpha_0 c_2 \gamma^2 + \alpha_0 c_1^2 - \beta_0 & \text{if } 0 \leq \gamma \leq \gamma_1 \\
\frac{-\alpha_0 c_2^2}{A_0} \gamma^2 + 2\alpha_0 c_2 s_0 \gamma + \alpha_0 c_1^2 - \beta_0 & \text{if } \gamma_1 \leq \gamma \leq \gamma_0 \\
A_0 s_0^2 + \alpha_0 c_1^2 - \beta_0 & \text{if } \gamma_0 \leq \gamma \leq 1.
\end{cases}
\]  

(First check directly that (99) implies (101). To see that (100) also implies (101) note that, in this case, 1) the last two equations in (100) refer to the vacuous case \( \gamma \leq 0 \) and 2) we have \( \gamma_1 < s_0, \) and thus \( \gamma > \gamma_1. \) Thus, setting

\[ \gamma_{\text{ver}} = \frac{A_0 s_0}{A_0 + 2\alpha_0 c_2} \]

(i.e. the vertex of the first parabola in (101), which, in this purely deviatoric case satisfies

52
\( \gamma_{ver} < \gamma_1 \) it follows

\[
U = \min_{\xi \in \mathcal{D}} \, m_\xi = \min_{0 \leq \gamma \leq 1} \, m_\xi = \begin{cases} \frac{2A_0 \xi_1 \alpha c_2}{A_0 + 2\alpha_0 c_2} + \alpha_0 c_1^2 - \beta_0 & \text{if } \gamma_{ver} \leq 1 \\ A_0 (1 - s_0) + 2\alpha_0 c_2 + \alpha_0 c_1^2 - \beta_0 & \text{if } \gamma_{ver} \geq 1 \end{cases}
\]

Finally, for the purely hydrostatic polycrystal \( D = 0 \) we have

\[
\lim_{D \to 0} A_0 = 0, \quad \lim_{D \to 0} s_0 = \infty,
\]

and \( \lim_{D \to 0} A_0 s_0^2 \) is finite.

and from (99), (100) and a calculation analogous to the one above we obtain

\[
m_\xi = \begin{cases} \alpha_0 (1 + 2c_2) \gamma^2 - 2\alpha_0 c_1 \gamma + A_0 s_0^2 + \alpha_0 c_1^2 - \beta_0 & \text{if } \gamma \leq \gamma_1 \\ -\beta_2 \gamma^2 + \beta_1 \gamma - \beta_0 + A_0 s_0^2 & \text{if } \gamma_1 \leq \gamma \leq \gamma_0 \\ A_0 s_0^2 + \alpha_0 c_1^2 - \beta_0 & \text{if } \gamma_0 \leq \gamma. \end{cases}
\]

To minimize (103) with respect to \( \gamma \) we need to consider separately the cases \( c_1 < 0 \) and \( c_1 \geq 0 \). In the former case

\[
\gamma_0 = \frac{c_1}{c_2} < 0,
\]

\[
\gamma_1 = \frac{c_1}{1 + c_2} < 0
\]

and we thus have, for \( c_1 < 0 \),

\[
U = \min_{\xi \in \mathcal{D}} \, m_\xi = \min_{0 \leq \gamma \leq 1} \, m_\xi = A_0 s_0^2 + \alpha_0 c_1^2 - \beta_0.
\]

Letting

\[
\gamma_{ver} = \frac{c_1}{1 + 2c_2}
\]

denote the vertex of the first parabola in (103) we obtain, for \( c_1 \geq 0 \)

\[
U = \min_{0 \leq \gamma \leq 1} \, m_\xi = \begin{cases} A_0 s_0^2 - \beta_0 + \frac{2\alpha_0 c_1 c_2}{1 + 2c_2} & \text{if } \gamma_{ver} \leq 1 \\ A_0 s_0^2 - \beta_0 + \alpha_0 [(c_1 - 1)^2 + 2c_2] & \text{if } \gamma_{ver} \geq 1. \end{cases}
\]
D  Appendix: Fields in an Infinite Matrix

After a brief discussion of the explicit solution for the circular inclusion problem in §D.1 we calculate, in §D.2, the self and interaction energies associated with a system of $N$ circular grains in an infinite matrix. Because of the algebraic content of these sections we have preferred to use here the symbols $\epsilon^T = [h, d_1, d_2]$ for the hydrostatic and deviatoric components of the transformation strain, instead of the more explicit notations $\epsilon^T = [h^T, d_1^T, d_2^T]$ we have used in the rest of the paper. Also, the parameter $\delta$ does not play any role in these calculations, and it is therefore suppressed throughout the following sections.

D.1  Fields in an Infinite Matrix

Consider a system formed by a circular transforming inclusion $G$ of radius $R$, centered at the origin and confined by an infinite elastic matrix, and assume the elasticity of both matrix and inclusion is described by the same isotropic elastic constants (1). The plane-strain displacement $w$ generated by this transformation is the solution of (18)–(19) (with $\epsilon^T(x) = [h, d_1, d_2]$ within $G$ and $\epsilon^T(x) = 0$ outside $G$) which vanishes at infinity. It follows from consideration of the general solution for two-dimensional elasticity problems in polar coordinates (e.g. Fung (1965)) that the displacement $w = w'$ in the inclusion is given by

\[
\begin{align*}
    w_r' &= \frac{r}{(2+g)} [2h + (1+g)d_1 \cos(2\theta) + (1+g)d_2 \sin(2\theta)] \\
    w_\theta' &= \frac{r(1+g)}{(2+g)} [-d_1 \sin(2\theta) + d_2 \cos(2\theta)],
\end{align*}
\]

(106)

see (9), whereas the matrix displacement $w = w^M$ equals

\[
\begin{align*}
    w_r^M &= \frac{R^2}{r(2+g)} \left[ 2h - \left( \frac{R^2}{r^2} - (2+g) \right) d_2 \sin(2\theta) + \left( -\frac{R^2}{r^2} + (2+g) \right) d_1 \cos(2\theta) \right] \\
    w_\theta^M &= -\frac{R^2}{r(2+g)} \left[ \left( \frac{R^2}{r^2} + g \right) d_1 \sin(2\theta) - \left( \frac{R^2}{r^2} + g \right) d_2 \cos(2\theta) \right].
\end{align*}
\]

(107)
The strains in the inclusion and the matrix can easily be derived from (106), (107) and the relations

\[ \epsilon_{rr} = \frac{\partial w_r}{\partial r} \]

\[ \epsilon_{r \theta} = \frac{1}{2r} \left( \frac{\partial w_r}{\partial \theta} + r \frac{\partial w_\theta}{\partial r} - w_\theta \right) \]

\[ \epsilon_{\theta \theta} = \frac{1}{r} \frac{\partial w_\theta}{\partial \theta} + \frac{1}{r} w_r. \]

We obtain

\[ \epsilon^I_{rr} = \frac{1}{2 + g} \left[ 2h + (1 + g) d_1 \cos(2\theta) + (1 + g) d_2 \sin(2\theta) \right] \]

\[ \epsilon^I_{r \theta} = \frac{1}{2 + g} \left[ (1 + g) d_2 \cos(2\theta) - (1 + g) d_1 \sin(2\theta) \right] \]

\[ \epsilon^I_{\theta \theta} = \frac{1}{2 + g} \left[ 2h - (1 + g) d_2 \sin(2\theta) - (1 + g) d_1 \cos(2\theta) \right] \] (108)

\[ \epsilon^M_{rr} = \frac{R^2}{r^2(2 + g)} \left[ -2h + \left( \frac{3R^2}{r^2} - (2 + g) \right) d_1 \cos(2\theta) + \left( \frac{3R^2}{r^2} - (2 + g) \right) d_2 \sin(2\theta) \right] \]

\[ \epsilon^M_{r \theta} = \frac{R^2}{r^2(2 + g)} \left[ - \left( \frac{3R^2}{r^2} - 2 \right) d_2 \cos(2\theta) + \left( \frac{3R^2}{r^2} - 2 \right) d_1 \sin(2\theta) \right] \]

\[ \epsilon^M_{\theta \theta} = \frac{R^2}{r^2(2 + g)} \left[ 2h - \left( \frac{3R^2}{r^2} - (2 - g) \right) d_2 \sin(2\theta) - \left( \frac{3R^2}{r^2} - (2 - g) \right) d_1 \cos(2\theta) \right]. \]

The stresses in the inclusion and matrix (see (18)) are thus given by

\[ \sigma^I_{rr} = \frac{2\mu}{2 + g} \left[ -2h - d_1 \cos(2\theta) - d_2 \sin(2\theta) \right] \]
\[
\sigma_{r\theta}^{I} = \frac{2\mu}{(2 + g)} \left[ -d_2 \cos(2\theta) + d_1 \sin(2\theta) \right]
\]

\[
\sigma_{\theta\theta}^{I} = \frac{2\mu}{(2 + g)} \left[ -2h + d_1 \cos(2\theta) + d_2 \sin(2\theta) \right],
\]

and

\[
\sigma_{rr}^{M} = \frac{2\mu}{(2 + g)} \frac{R^2}{r^2} \left[ -2h + \left( 3\frac{R^2}{r^2} - 4 \right) d_1 \cos(2\theta) + \left( 3\frac{R^2}{r^2} - 4 \right) d_2 \sin(2\theta) \right]
\]

\[
\sigma_{r\theta}^{M} = \frac{2\mu}{(2 + g)} \frac{R^2}{r^2} \left[ - \left( \frac{3R^2}{r^2} - 2 \right) d_2 \cos(2\theta) + \left( \frac{3R^2}{r^2} - 2 \right) d_1 \sin(2\theta) \right]
\]

\[
\sigma_{\theta\theta}^{M} = \frac{2\mu}{(2 + g)} \frac{R^2}{r^2} \left[ 2h - 3\frac{R^2}{r^2} d_1 \cos(2\theta) - 3\frac{R^2}{r^2} d_2 \sin(2\theta) \right]
\]

respectively.

### D.2 Self and Interaction energies

The integrals in (50) can be computed easily. Indeed, suppressing the \( \delta \)-dependence call \( R_k \) the radius of the \( k \)-th grain \( G^{(k)} \), call \( h^{(k)}, d_1^{(k)}, d_2^{(k)} \) the hydrostatic and deviatoric components of the transformation strain in \( G^{(k)} \), and set \( d^{(k)} = \sqrt{(d_1^{(k)})^2 + (d_2^{(k)})^2} \). Then, using the expressions

\[
\varepsilon_{rr}^{T(k)} = h^{(k)} + d_1^{(k)} \cos(2\theta) + d_2^{(k)} \sin(2\theta)
\]

\[
\varepsilon_{r\theta}^{T(k)} = -d_1^{(k)} \sin(2\theta) + d_2^{(k)} \cos(2\theta)
\]

\[
\varepsilon_{\theta\theta}^{T(k)} = h^{(k)} - d_1^{(k)} \cos(2\theta) - d_2^{(k)} \sin(2\theta).
\]
for the polar coordinates of $\epsilon^{(k)}$ and equation (109) we obtain

$$
\int_{G^{(k)}} \sigma^{I}_{ij} \epsilon^{I}_{ij} = -\frac{4 \mu \pi R^2}{2 + g} \left[ 2 \left( h^{(k)} \right)^2 + \left( d^{(k)} \right)^2 \right].
$$

(112)

Thus

$$
W_{self} = \sum_{k=1}^{N} \frac{2 \mu R_k^2}{2 + g} \left[ 2 \left( h^{(k)} \right)^2 + \left( d^{(k)} \right)^2 \right]
$$

(113)

—see (50) and note from (15) that $|B| = \pi$.

The calculation of the quantity $W_{int}$, on the other hand, requires considerable algebra, and we have preferred to use the symbolic manipulator Maple; the calculation will be outlined in what follows. As before, we denote the polar coordinate system centered at the $k$-th grain by $(r, \theta)$, and we call $(\rho, \psi)$ the corresponding polar coordinates sharing a center with the $p$-th grain. The stresses $\sigma_{\rho \rho}(\rho, \psi), \sigma_{\rho \psi}(\rho, \psi), \sigma_{\psi \psi}(\rho, \psi)$ arising from the eigenstrain in the $p$-th grain can be obtained from equations (109), (110) by means of the substitution $\psi \to \theta, \rho \to r$. Denoting by $(x_j, y_j)$ the center of the $j$-th grain, we have the following relations, which are useful in changing between polar coordinate systems:

$$
\rho = \left( (r \cos(\theta) + x_k - x_p)^2 + (r \sin(\theta) + y_k - y_p)^2 \right)^{1/2}
$$

(114)

$$
\cos(\psi) = \frac{r \cos(\theta) + x_k - x_p}{((r \cos(\theta) + x_k - x_p)^2 + (r \sin(\theta) + y_k - y_p)^2)^{1/2}}
$$

$$
\sin(\psi) = \frac{r \sin(\theta) + y_k - y_p}{((r \cos(\theta) + x_k - x_p)^2 + (r \sin(\theta) + y_k - y_p)^2)^{1/2}}
$$

(115)

and

$$
\sigma^{(p)}_{rr} = \sigma_{pp}^{(p)} \cos^2(\theta - \psi) + \sigma_{\rho \psi}^{(p)} \sin^2(\theta - \psi) + 2 \sigma_{\rho \psi}^{(p)} \sin(\theta - \psi) \cos(\theta - \psi)
$$

$$
\sigma^{(p)}_{\theta \theta} = \sigma_{pp}^{(p)} \sin^2(\theta - \psi) + \sigma_{\rho \psi}^{(p)} \cos^2(\theta - \psi) - 2 \sigma_{\rho \psi}^{(p)} \sin(\theta - \psi) \cos(\theta - \psi)
$$

(116)

$$
\sigma^{(p)}_{r \theta} = -\sigma_{pp}^{(p)} \sin(\theta - \psi) \cos(\theta - \psi) + \sigma_{\rho \psi}^{(p)} \sin(\theta - \psi) \cos(\theta - \psi) + \sigma_{\rho \psi}^{(p)} \cos(\theta - \psi) \sin(\theta - \psi)
$$
\[
\sigma^{(p)}_{ijkl}(\cos^2(\theta - \psi) - \sin^2(\theta - \psi)).
\]

Equations (116), (110) and the transformation strains in equation (111) can be used to form the integral of \( \sigma_{ijkl}^{(p)} T^{(k)} \) in the expression for \( W_{int} \). Clearly, this integral is a quadratic form in \( \epsilon^T \) and can therefore be expressed as

\[
-\frac{1}{2|B|} \int_{G^{(k)}} \sigma_{ijkl}^{(p)} \epsilon_{ijkl} \, dx = -\frac{1}{2|B|} \int_0^{R_k} \int_0^{2\pi} \sigma_{ijkl}^{(p)} T^{(k)} \epsilon_{ijkl} \, d\theta \, dr
\]

\[
= \begin{bmatrix}
  h^{(k)} & d_1^{(k)} & d_2^{(k)} \\
  d_1^{(p)} & d_2^{(p)}
\end{bmatrix}
\begin{bmatrix}
  \int_0^{R_k} \int_0^{2\pi} I_{kp}(r, \theta) \, d\theta \, dr \\
  \int_0^{R_k} \int_0^{2\pi} I_{kp}(r, \theta) \, d\theta \, dr
\end{bmatrix}
\]

(117)

for some \( 3 \times 3 \) matrix \( I_{kp}(r, \theta) \). A straightforward calculation gives

\[
I_{kp}(r, \theta) = \frac{2\mu}{\pi(2 + g)} \begin{bmatrix}
  0 & \frac{2R_p^2 \cos(2\psi)}{\rho^2} & \frac{2R_p^2 \sin(2\psi)}{\rho^2} \\
  \frac{2R_p^2 \cos(2\psi)}{\rho^2} & -R_p^2 \cos(4\psi) & -R_p^2 \sin(4\psi) \\
  \frac{2R_p^2 \sin(2\psi)}{\rho^2} & -R_p^2 \sin(4\psi) & R_p^2 \cos(4\psi)
\end{bmatrix}
\]

(118)

where \( \rho = \rho(r, \theta) \) and \( \psi = \psi(r, \theta) \) are given by (114).

In order to compute the integral in (117), let \( \ell_{kp} \) be the distance between the centers of the two particles,

\[
\ell_{kp} = \left( (x_k - x_p)^2 + (y_k - y_p)^2 \right)^{1/2}
\]

(119)

and define the angle \( \eta_{kp} \) as

\[
\eta_{kp} = \tan^{-1} \left( \frac{(y_k - y_p)}{(x_k - x_p)} \right)
\]

so that \( x_k - x_p = \ell_{kp} \cos(\eta_{kp}) \) and \( y_k - y_p = \ell_{kp} \sin(\eta_{kp}) \). Next, introduce a change of variables \( \theta \to z \) where

\[
z = \tan \left( \frac{\theta - \eta_{kp}}{2} \right).
\]

58
Then, using the identities

\[
\cos(\theta) = \frac{(1 - z^2) \cos(\eta_{kp}) - 2z \sin(\eta_{kp})}{1 + z^2} \\
\sin(\theta) = \frac{(1 - z^2) \sin(\eta_{kp}) + 2z \cos(\eta_{kp})}{1 + z^2} \\
d\theta = \frac{2}{1 + z^2} dz
\]

we can rewrite the integral in \( \theta \) as an integral of a rational function of \( z \) for \(-\infty < z < \infty\). This integral can be computed explicitly to yield

\[
-\frac{1}{2|B|} \int_{G^{(e)}} \sigma_{ij}^{(p)} \epsilon_{ij}^{T(k)} \, dx = \begin{bmatrix} h^{(k)} & d_1^{(k)} & d_2^{(k)} \end{bmatrix} \left( \int_0^{R_k} J_{kp}(r) r \, dr \right) \begin{bmatrix} h^{(p)} \\ d_1^{(p)} \\ d_2^{(p)} \end{bmatrix}
\]

(120)

with

\[
J_{kp}(r) = \frac{2\mu R_p^2}{(2 + g)} \begin{bmatrix} 0 & \frac{4 \cos(2\eta_{kp})}{\ell_{kp}^2} & \frac{4 \sin(2\eta_{kp})}{\ell_{kp}^2} \\ \frac{4 \cos(2\eta_{kp})}{\ell_{kp}^2} & -\cos(4\eta_{kp}) & -\sin(4\eta_{kp}) \\ \frac{4 \sin(2\eta_{kp})}{\ell_{kp}^2} & -\sin(4\eta_{kp}) & \cos(4\eta_{kp}) \end{bmatrix}
\]

Finally, integrating in \( r \) we obtain

\[
-\frac{1}{2|B|} \int_{G^{(e)}} \sigma_{ij}^{(p)} \epsilon_{ij}^{T(k)} \, dx = \begin{bmatrix} h^{(k)} & d_1^{(k)} & d_2^{(k)} \end{bmatrix} M_{kp} \begin{bmatrix} h^{(p)} \\ d_1^{(p)} \\ d_2^{(p)} \end{bmatrix}
\]

(121)
where

\[
M_{kp} = \frac{2\mu R_k^2 R_p^2}{(2 + g)} \begin{bmatrix}
0 & \frac{2\cos(2\eta_{kp})}{\ell_{kp}^2} & \frac{2\sin(2\eta_{kp})}{\ell_{kp}^2} \\
\frac{2\cos(2\eta_{kp})}{2\sin(2\eta_{kp})} & \cos(4\eta_{kp}) \left( \frac{3R_p^2 + 3R_k^2 - 2\ell_{kp}^2}{\ell_{kp}^2} \right) & \sin(4\eta_{kp}) \left( \frac{3R_p^2 + 3R_k^2 - 2\ell_{kp}^2}{\ell_{kp}^2} \right) \\
\frac{2\sin(2\eta_{kp})}{2\sin(2\eta_{kp})} & \sin(4\eta_{kp}) \left( \frac{3R_p^2 + 3R_k^2 - 2\ell_{kp}^2}{\ell_{kp}^2} \right) & \cos(4\eta_{kp}) \left( \frac{3R_p^2 + 3R_k^2 - 2\ell_{kp}^2}{\ell_{kp}^2} \right)
\end{bmatrix}.
\]

Calling

\[
M_{ii} = \frac{2\mu R_k^2}{2 + g} \begin{bmatrix}
2 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{bmatrix},
\]

\[
M = \begin{bmatrix}
M_{11} & M_{12} & \cdots & M_{1N} \\
M_{21} & M_{22} & \cdots & M_{2N} \\
\vdots & \vdots & \ddots & \vdots \\
M_{N1} & M_{N2} & \cdots & M_{NN}
\end{bmatrix},
\]

and \( e \) the row-vector

\[
e = \left( h^{(1)}, d_1^{(1)}, d_2^{(1)}, h^{(2)}, d_1^{(2)}, d_2^{(2)}, \ldots, h^{(N)}, d_1^{(N)}, d_2^{(N)} \right)
\]

the sum \( W_{self} + W_{int} \) is given by the quadratic form

\[
W_{self} + W_{int} = eM e^t.
\]

**References**


61


<table>
<thead>
<tr>
<th>#</th>
<th>Author/s</th>
<th>Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>1302</td>
<td>J. Zhang</td>
<td>A nonlinear nonlocal multi-dimensional conservation law</td>
</tr>
<tr>
<td>1303</td>
<td>M.E. Taylor</td>
<td>Estimates for approximate solutions to acoustic inverse scattering problems</td>
</tr>
<tr>
<td>1304</td>
<td>J. Kim &amp; D. Sheen</td>
<td>A priori estimates for elliptic boundary value problems with nonlinear boundary conditions</td>
</tr>
<tr>
<td>1305</td>
<td>B. Engquist &amp; E. Luo</td>
<td>New coarse grid operators for highly oscillatory coefficient elliptic problems</td>
</tr>
<tr>
<td>1306</td>
<td>A. Boutet de Monvel &amp; I. Egorova</td>
<td>On the almost periodicity of solutions of the nonlinear Schrödinger equation with the cantor type spectrum</td>
</tr>
<tr>
<td>1307</td>
<td>A. Boutet de Monvel &amp; V. Georgescu</td>
<td>Boundary values of the resolvent of a self-adjoint operator: Higher order estimates</td>
</tr>
<tr>
<td>1308</td>
<td>S.K. Patch</td>
<td>Diffuse tomography modulo Graßmann and Laplace</td>
</tr>
<tr>
<td>1309</td>
<td>A. Friedman &amp; J.J.L. Velázquez</td>
<td>Liouville type theorems for fourth order elliptic equations in a half plane</td>
</tr>
<tr>
<td>1310</td>
<td>T. Aktosun, M. Klaus &amp; C. van der Mee</td>
<td>Recovery of discontinuities in a nonhomogeneous medium</td>
</tr>
<tr>
<td>1311</td>
<td>V. Bondarevsky</td>
<td>On the global regularity problem for 3-dimensional Navier-Stokes equations</td>
</tr>
<tr>
<td>1312</td>
<td>M. Cheney &amp; D. Isaacson</td>
<td>Inverse problems for a perturbed dissipative half-space</td>
</tr>
<tr>
<td>1313</td>
<td>B. Cockburn, D.A. Jones &amp; E.S. Titi</td>
<td>Determining degrees of freedom for nonlinear dissipative equations</td>
</tr>
<tr>
<td>1314</td>
<td>B. Engquist &amp; E. Luo</td>
<td>Convergence of a multigrid method for elliptic equations with highly oscillatory coefficients</td>
</tr>
<tr>
<td>1315</td>
<td>L. Pastur &amp; M. Shcherbina</td>
<td>Universality of the local eigenvalue statistics for a class of unitary invariant random matrix ensembles</td>
</tr>
<tr>
<td>1316</td>
<td>V. Jakšić, S. Molchanov &amp; L. Pastur</td>
<td>On the propagation properties of surface waves</td>
</tr>
<tr>
<td>1317</td>
<td>J. Nečas, M. Ružička &amp; V. Šverák</td>
<td>On self-similar solutions of the Navier-Stokes equations</td>
</tr>
<tr>
<td>1318</td>
<td>S. Stojanović</td>
<td>Remarks on $W^{2,p}$-solutions of bilateral obstacle problems</td>
</tr>
<tr>
<td>1319</td>
<td>E. Luo &amp; H-O. Kreiss</td>
<td>Pseudospectral vs. Finite difference methods for initial value problems with discontinuous coefficients</td>
</tr>
<tr>
<td>1320</td>
<td>V.E. Grikuro</td>
<td>Soliton's rebuilding in one-dimensional Schrödinger model with polynomial nonlinearity</td>
</tr>
<tr>
<td>1321</td>
<td>J.M. Harrison &amp; R.J. Williams</td>
<td>A multiclass closed queueing network with unconventional heavy traffic behavior</td>
</tr>
<tr>
<td>1322</td>
<td>M.E. Taylor</td>
<td>Microlocal analysis on Morrey spaces</td>
</tr>
<tr>
<td>1323</td>
<td>C. Huang</td>
<td>Homogenization of biharmonic equations in domains perforated with tiny holes</td>
</tr>
<tr>
<td>1324</td>
<td>C. Liu</td>
<td>An inverse obstacle problem: A uniqueness theorem for spheres</td>
</tr>
<tr>
<td>1325</td>
<td>M. Luskin</td>
<td>Approximation of a laminated microstructure for a rotationally invariant, double well energy density</td>
</tr>
<tr>
<td>1326</td>
<td>Rakesh &amp; P. Sacks</td>
<td>Impedance inversion from transmission data for the wave equation</td>
</tr>
<tr>
<td>1327</td>
<td>O. Lafitte</td>
<td>Diffraction for a Neumann boundary condition</td>
</tr>
<tr>
<td>1328</td>
<td>E. Sobel, K. Lange, J.R. O'Connell &amp; D.E. Weeks</td>
<td>Haplotype algorithms</td>
</tr>
<tr>
<td>1329</td>
<td>B. Cockburn, D.A. Jones &amp; E.S. Titi</td>
<td>Estimating the number of asymptotic degrees of freedom for nonlinear dissipative systems</td>
</tr>
<tr>
<td>1330</td>
<td>T. Aktosun</td>
<td>Inverse Schrödinger scattering on the line with partial knowledge of the potential</td>
</tr>
<tr>
<td>1331</td>
<td>T. Aktosun &amp; C. van der Mee</td>
<td>Partition of the potential of the one-dimensional Schrödinger equation</td>
</tr>
<tr>
<td>1332</td>
<td>B. Engquist &amp; E. Luo</td>
<td>Convergence of the multigrid method with a wavelet coarse grid operator</td>
</tr>
<tr>
<td>1333</td>
<td>V. Jakšić &amp; C.-A. Pillet</td>
<td>Ergodic properties of the Spin-Boson system</td>
</tr>
<tr>
<td>1334</td>
<td>S.K. Patch</td>
<td>Recursive solution for diffuse tomographic systems of arbitrary size</td>
</tr>
<tr>
<td>1335</td>
<td>J.C. Bronski</td>
<td>Semiclassical eigenvalue distribution of the non self-adjoint Zakharov-Shabat eigenvalue problem</td>
</tr>
<tr>
<td>1336</td>
<td>J.C. Cockburn,</td>
<td>Bidirectional structured interpolation theory</td>
</tr>
<tr>
<td>1337</td>
<td>S. Kichenassamy</td>
<td>The blow-up problem for exponential nonlinearities</td>
</tr>
<tr>
<td>1338</td>
<td>F.A. Grünbaum &amp; S.K. Patch</td>
<td>How many parameters can one solve for in diffuse tomography?</td>
</tr>
<tr>
<td>1339</td>
<td>R. Lipton</td>
<td>Reciprocal relations, bounds and size effects for composites with highly conducting interface</td>
</tr>
<tr>
<td>1340</td>
<td>H.A. Levine &amp; J. Serrin</td>
<td>A global nonexistence theorem for quasilinear evolution equations with dissipation</td>
</tr>
<tr>
<td>1341</td>
<td>A. Boutet de Monvel &amp; R. Purice</td>
<td>The conjugate operator method: Application to DIRAC operators and to stratified media</td>
</tr>
<tr>
<td>1342</td>
<td>G. Michele Graf</td>
<td>Stability of matter through an electrostatic inequality</td>
</tr>
<tr>
<td>1343</td>
<td>G. Avalos</td>
<td>Sharp regularity estimates for solutions of the wave equation and their traces with prescribed Neumann data</td>
</tr>
<tr>
<td>1344</td>
<td>G. Avalos</td>
<td>The exponential stability of a coupled hyperbolic/parabolic system arising in structural acoustics</td>
</tr>
<tr>
<td>1345</td>
<td>G. Avalos &amp; I. Lasiecka</td>
<td>A differential Riccati equation for the active control of a problem in structural acoustics</td>
</tr>
<tr>
<td>1346</td>
<td>G. Avalos</td>
<td>Well-posedness for a coupled hyperbolic/parabolic system seen in structural acoustics</td>
</tr>
<tr>
<td>1347</td>
<td>G. Avalos &amp; I. Lasiecka</td>
<td>The strong stability of a semigroup arising from a coupled hyperbolic/parabolic system</td>
</tr>
<tr>
<td>1348</td>
<td>A.V. Fursikov</td>
<td>Certain optimal control problems for Navier-Stokes system with distributed control function</td>
</tr>
<tr>
<td>1349</td>
<td>F. Gesztesy, R. Nowell &amp; W. Pöttz</td>
<td>One-dimensional scattering theory for quantum systems with nontrivial spatial asymptotics</td>
</tr>
<tr>
<td>1350</td>
<td>F. Gesztesy &amp; H. Holden</td>
<td>On trace formulas for Schrödinger-type operators</td>
</tr>
</tbody>
</table>
1351 X. Chen, Global asymptotic limit of solutions of the Cahn-Hilliard equation
1352 X. Chen, Lorenz equations, Part I: Existence and nonexistence of homoclinic orbits
1353 X. Chen, Lorenz equations Part II: "Randomly" rotated homoclinic orbits and chaotic trajectories
1354 X. Chen, Lorenz equations, Part III: Existence of hyperbolic sets
1355 R. Abeyaratne, C. Chu & R.D. James, Kinetics of materials with wiggly energies: Theory and application to the evolution of twinning microstructures in a Cu-Al-Ni shape memory alloy
1356 C. Liu, The Helmholtz equation on Lipschitz domains
1357 G. Avalos & I. Lasiecka, Exponential stability of a thermoelastic system without mechanical dissipation
1358 R. Lipton, Heat conduction in fine scale mixtures with interfacial contact resistance
1359 V. Odisharia & J. Peradze, Solvability of a nonlinear problem of Kirchhoff shell
1360 P.J. Olver, G. Sapiro & A. Tannenbaum, Affine invariant edge maps and active contours
1361 R.D. James, Hysteresis in phase transformations
1362 A. Sei & W. Symes, A note on consistency and adjointness for numerical schemes
1363 A. Friedman & B. Hu, Head-media interaction in magnetic recording
1364 A. Friedman & J.J.L. Velázquez, Time-dependent coating flows in a strip, part I: The linearized problem
1365 X. Ren & M. Winter, Young measures in a nonlocal phase transition problem
1366 K. Bhattacharya & R.V. Kohn, Elastic energy minimization and the recoverable strains of polycrystalline shape-memory materials
1367 G.A. Chechkin, Operator pencil and homogenization in the problem of vibration of fluid in a vessel with a fine net on the surface
1368 M. Carme Calderer & B. Mukherjee, On Poiseuille flow of liquid crystals
1369 M.A. Pinsky & M.E. Taylor, Pointwise Fourier inversion: A wave equation approach
1370 D. Brandon & R.C. Rogers, Order parameter models of elastic bars and precursor oscillations
1371 H.A. Levine & B.D. Sleeman, A system of reaction diffusion equations arising in the theory of reinforced random walks
1373 B. Li & M. Luskin, Finite element analysis of microstructure for the cubic to tetragonal transformation
1374 M. Luskin, On the computation of crystalline microstructure
1375 J.P. Matos, On gradient young measures supported on a point and a well
1376 M. Nitsche, Scaling properties of vortex ring formation at a circular tube opening
1377 J.L. Bona & Y.A. Li, Decay and analyticity of solitary waves
1378 V. Isakov, On uniqueness in a lateral cauchy problem with multiple characteristics
1379 M.A. Kouritzin, Averaging for fundamental solutions of parabolic equations
1380 T. Aktosun, M. Klaus & C. van der Mee, Integral equation methods for the inverse problem with discontinuous wavespeed
1381 P. Morin & R.D. Spies, Convergent spectral approximations for the thermomechanical processes in shape memory alloys
1382 D.N. Arnold & X. Liu, Interior estimates for a low order finite element method for the Reissner-Mindlin plate model
1383 D.N. Arnold & R.S. Falk, Analysis of a linear-linear finite element for the Reissner-Mindlin plate model
1384 D.N. Arnold, R.S. Falk & R. Winther, Preconditioning in H(div) and applications
1385 M. Lavrentiev, Nonlinear parabolic problems possessing solutions with unbounded gradients
1386 O.P. Bruno & P. Laurence, Existence of three-dimensional toroidal MHD equilibria with nonconstant pressure
1387 O.P. Bruno, F. Reitich, & P.H. Leo, The overall elastic energy of polycrystalline martensitic solids
1388 M. Fila & H.A. Levine, On critical exponents for a semilinear parabolic system coupled in an equation and a boundary condition
1390 J.M. Berg & H.G. Kwatny, Unfolding the zero structure of a linear control system
1391 A. Sei, High order finite-difference approximations of the wave equation with absorbing boundary conditions: A stability analysis
1392 A.V. Coward & Y.Y. Renardy, Small amplitude oscillatory forcing on two-layer plane channel flow
1393 V.A. Pliss & G.R. Sell, Approximation dynamics and the stability of invariant sets
1394 J.G. Cao & P. Roblin, A new computational model for heterojunction resonant tunneling diode
1395 C. Liu, Inverse obstacle problem: Local uniqueness for rougher obstacles and the identification of a ball
1396 K.A. Pericak-Spector & S.J. Spector, Dynamic cavitation with shocks in nonlinear elasticity
1397 G. Avalos & I. Lasiecka, Exponential stability of a thermoelastic system without mechanical dissipation II: The case of simply supported boundary conditions
1398 B. Brighi & M. Chipot, Approximation of infima in the calculus of variations