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On the computation of crystalline microstructure

Mitchell Luskin *
School of Mathematics
University of Minnesota
Minneapolis, MN 55455, USA
E-mail: luskin@math.umn.edu

Microstructure is a feature of crystals with multiple symmetry-related energy-minimizing states. Continuum models have been developed explaining microstructure as the mixture of these symmetry-related states on a fine scale to minimize energy. This article is a review of numerical methods and the numerical analysis for the computation of crystalline microstructure.

CONTENTS

1. Introduction

Advances in the understanding of material microstructure are playing an important role in the development of many new technologies that depend on material properties such as shape memory, magnetostriction, and ferroelectricity. Microstructure occurs in many materials as the fine-scale spatial oscillation

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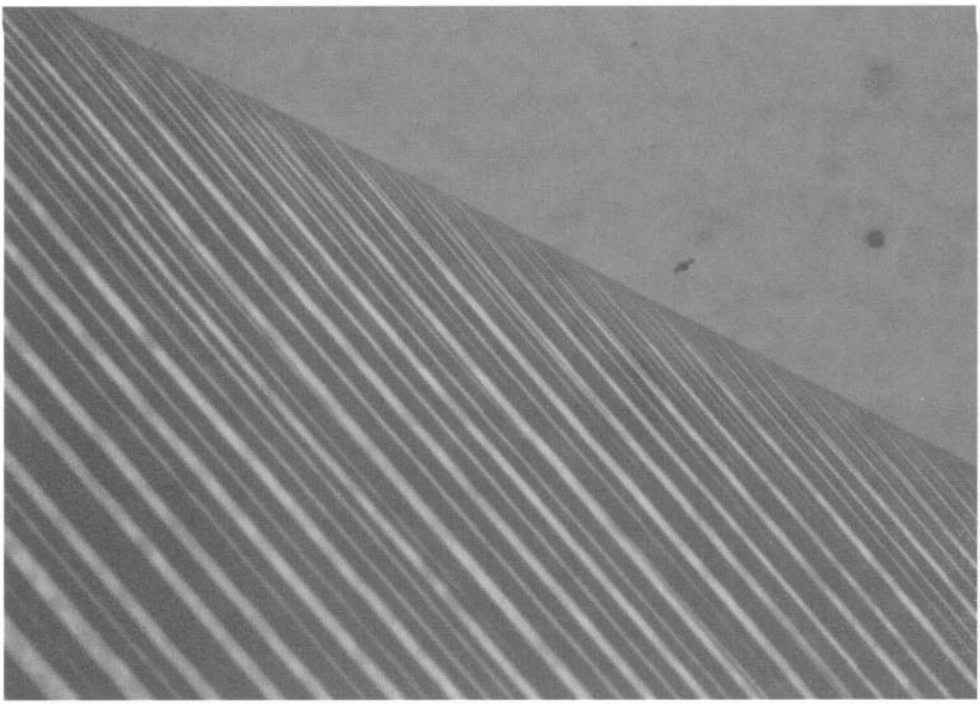

Fig. 1. Photomicrograph of an austenitic-martensitic phase boundary (see Section 3.9) for a single crystal of Cu-14 at.% Al-3.9 at.% Ni from the laboratory of C. Chu and R. James. The martensitic phase is laminated or 'twinned'. (Field of view: 1.25 mm $\times$ 0.86 mm.)

between symmetry-related states. In this article, we survey the recent development of numerical methods and their analysis to compute microstructure in materials. We will be mainly concerned here with the microstructure of martensitic crystals where lattice structure oscillates between 'twinned' states (see Fig. 1 and Fig. 2).

During the past several years a geometrically nonlinear continuum theory for the equilibria of martensitic crystals based on elastic energy minimization has been developed (Ericksen 1986, 1987*a*, 1987*b*, Ball and James 1987, James and Kinderlehrer 1989, Ball and James 1992). The invariance of the energy density with respect to symmetry-related states implies that the elastic energy density is non-convex and must have multiple energy wells. For a large class of boundary conditions, the gradients of energy-minimizing sequences of deformations must oscillate between the energy wells to allow the energy to converge to the lowest possible value. Even though the deformation gradients of such energy-minimizing sequences do not converge pointwise, certain kinds of averages of the deformation gradients converge for a large class of boundary conditions. This convergence has been studied intensively using

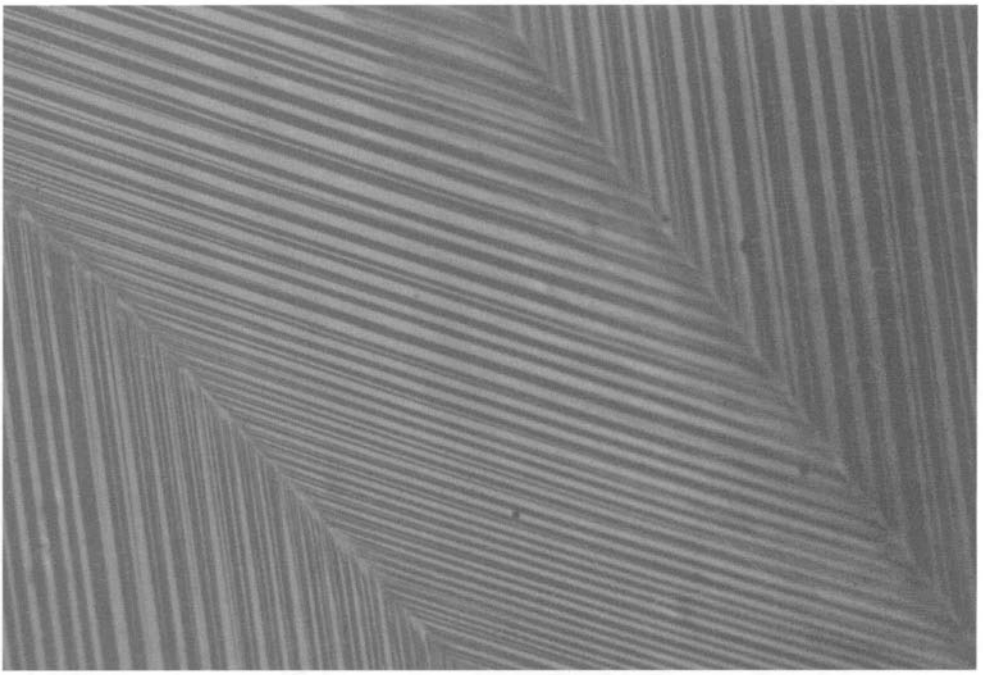

Fig. 2. Photomicrograph of a second-order laminate (see Section 3.10) for a single crystal of Cu-14 at.% Al-3.9 at.% Ni from the laboratory of C. Chu and R. James. (Field of view: 1.25 mm × 0.86 mm.)

the Young measure (Tartar 1984, Kinderlehrer and Pedregal 1991, Ball and James 1992) and the H-measure (Tartar 1990, Kohn 1991).

A geometrically linear theory for the equilibria of martensitic crystals was developed by Eshelby (1961), Khachaturyan (1967, 1983), Khachaturyan and Shatalov (1969), and Roitburd (1969, 1978). This theory is nonlinear, though, because the energy density has local minima at multiple stress-free strains. The relationship between the geometrically linear theory and the geometrically nonlinear theory has been explored by Kohn (1991), Ball and James (1992), and Bhattacharya (1993). Most of the results for the geometrically nonlinear theory that we discuss in this article have related counterparts for the geometrically linear theory.

These theories have presented a major challenge to the development and analysis of numerical methods, since they have features very unlike those of the physical theories usually approximated by numerical methods. The presence of microstructure has motivated the development of numerical methods that can capture macroscopic information without resolving the microstructure on the physical length scale (which can vary from nanometres to millimetres).

Although much progress has been made in the analysis of global minima of models for the energy of martensitic crystals, such crystals typically exhibit

hysteretic behaviour and are usually observed in local minima or in meta-stable states (Burkart and Read 1953, Basinski and Christian 1954, Ball, Chu and James 1994, Ball, Chu and James 1995). Since the analytic study of these local minima is difficult, the computational approach offers an important tool for the exploration of meta-stable states. Thus, a further computational challenge is presented by the multitude of local minima which the numerical models necessarily inherit from the continuum models (Ball, Holmes, James, Pego and Swart 1991), as well as the local minima that occur from representing the same microstructure on the different scales possible for a given grid.

Early three-dimensional computations and numerical algorithms for a geometrically nonlinear model of microstructure in martensitic crystals have been given by Collins and Luskin (1989) for the In-20.7 at.% Tl alloy, and Silling (1989) has reported computations for a two-dimensional model exhibiting microstructure. Later computational results and numerical algorithms for equilibrium problems are given by Collins, Luskin and Riordan (1993) and Collins (1993*a*). Computations and numerical algorithms for geometrically linear models of martensitic crystals have been given by Wen, Khachaturyan and Morris Jr. (1981), Wang, Chen and Khachaturyan (1994), Kartha, Castán, Krumhansl and Sethna (1994) and Kartha, Krumhansl, Sethna and Wickham (1995).

A theory for the numerical analysis of microstructure was proposed by Collins, Kinderlehrer and Luskin (1991*a*) and Collins and Luskin (1991*b*) and extended in Chipot (1991), Chipot and Collins (1992), Gremaud (1994) and Chipot, Collins and Kinderlehrer (1995). This theory has been used to give an analysis of the convergence of numerical methods for three-dimensional, physical models of microstructure in ferromagnetic crystals (Luskin and Ma 1992) and in martensitic crystals with an orthorhombic to monoclinic transformation (Luskin 1996*a*, Luskin 1996*b*) and a cubic to tetragonal transformation (Li and Luskin 1996).

The theory for the numerical analysis of microstructure gives error estimates for the local mixture, rather than the pointwise values, of the deformation gradients; so the representations of the same microstructure on different scales are shown to yield almost identical macroscopic properties. These estimates show that many macroscopic properties converge as the length scale of the underlying microstructure converges to zero, which gives a justification for computing microstructure on a length scale that can be orders of magnitude larger than the physical length scale.

The relaxed energy density for a given deformation gradient $F \in \mathbb{R}^{3\times 3}$ is given by the *infimum* of the average energy of deformations defined on a smooth domain and constrained to be equal to an Fx on the boundary. Under appropriate conditions, the *infimum* of the relaxed energy is attained by deformations that are the limit of energy-minimizing (for the original en-

ergy) sequences of deformations (Ekeland and Temam 1974, Dacorogna 1989). Although an explicit formula or practical computational algorithm for the relaxed energy density (the quasi-convex envelope) is generally not known for the non-convex energies used to model martensitic crystals, representations of the polyconvex and rank-one convex envelopes have been given, which can be numerically approximated to give lower and upper bounds for the relaxed energy density (Dacorogna 1989). These representations, especially that given by Kohn and Strang (1986), have been used in Nicolaides and Walkington (1993), Roubíček (1994), Carstensen and Plecháč (1995), Roubíček (1996*a*), Pedregal (1996), Pedregal (1995) and Kružík (1995).

The computation of the dynamics of the development and propagation of microstructure is important for the modelling and control of materials with microstructure. Swart and Holmes (1992) have studied the 'viscoelastodynamics' of a scalar, two-dimensional model, and Klouček and Luskin (1994*a*) and Klouček and Luskin (1994*b*) have computed the viscoelastodynamics of a three-dimensional model for the In-20.7 at.% Tl alloy.

This article focuses on computational methods for continuum theories for single martensitic crystals. Our bibliography contains references to many topics that we do not consider in detail in the text, such as homogenization, polycrystals, surface energy, and dynamics. We refer the reader to Luskin and Ma (1992, 1993) and Ma (1993) for recent developments in numerical methods and numerical analysis for the computation of the microstructure in the magnetization of ferromagnetic crystals.

2. Continuum theory for martensitic crystals

We give here a brief outline of the geometrically nonlinear continuum theory for martensitic crystals (Ericksen 1986, 1987*a*, 1987*b*; Ball and James 1987, 1992). The crystallographic background for the topics treated in this section will be given in the forthcoming book by Pitteri and Zanzotto (1996*a*). Martensitic crystals have a high-temperature phase known as *austenite*, and a low-temperature, less symmetric phase known as *martensite*. The austenitic phase exists in one variant, but the martensitic phase exists in several symmetry-related variants and can form a microstructure by the fine-scale mixing of the variants.

2.1. The elastic energy and admissible deformations

We use the austenitic phase at the transformation temperature as the reference configuration $\Omega \subseteq \mathbb{R}^3$ of the crystal. We assume that Ω is either a polyhedron or a smooth, bounded domain. We denote deformations by functions $y(x) : \Omega \to \mathbb{R}^3$, and we denote the corresponding deformation gradients by $F(x) = \nabla y(x)$.

We shall denote the elastic energy per unit volume at temperature θ and

deformation gradient $F \in \mathbb{R}^{3\times 3}$ by $\phi(F,\theta)$, which shall always be assumed to be continuous and to satisfy the growth condition

$$\phi(F,\theta) \geq C_1\|F\|^p - C_0 \qquad \text{for all } F \in \mathbb{R}^{3\times 3}, \tag{2.1}$$

where C_0 and C_1 are positive constants independent of $F \in \mathbb{R}^{3\times 3}$, where we assume $p > 3$ to ensure that deformations with finite energy are continuous (see (2.4) below), and where we are using the matrix norm

$$\|F\|^2 \equiv \sum_{i,j=1}^{3} F_{ij}^2 \qquad \text{for } F \in \mathbb{R}^{3\times 3}.$$

It is not realistic to consider deformations with arbitrarily large deformation gradients $F(x) = \nabla y(x)$ within the theory of elasticity (we can expect non-elastic behaviour such as fracture and plasticity to occur at large deformation gradients), so our use of the growth condition (2.1) can be viewed as a mathematical convenience. Also, we will be concerned only with temperatures in a neighbourhood (θ_L, θ_U) of the transformation temperature θ_T, so we need only assume that the growth condition (2.1) is valid uniformly for $\theta \in (\theta_L, \theta_U)$.

We expect that observed deformations $\hat{y}(x)$ are local minima of the total elastic energy

$$\mathcal{E}(\hat{y}) = \int_\Omega \phi(\nabla \hat{y}(x), \theta)\, dx \tag{2.2}$$

among all deformations satisfying appropriate boundary conditions and having finite energy. However, we will see that there generally do not exist energy-minimizing deformations to (2.2) for the non-convex energy densities ϕ that we use to model martensitic crystals, and so we must consider energy-minimizing sequences.

Since $p > 3$ in the growth condition (2.1), we have that the deformations with finite energy are uniformly continuous (Adams 1975), so we can denote the set of deformations of finite energy by

$$W^\phi = \left\{ y \in C(\bar{\Omega}; \mathbb{R}^3) : \int_\Omega \phi(\nabla y(x), \theta)\, dx < \infty \right\}. \tag{2.3}$$

We note that

$$W^\phi \subset W^{1,p}(\Omega; \mathbb{R}^3) \subset C(\bar{\Omega}; \mathbb{R}^3), \tag{2.4}$$

where $W^{1,p}(\Omega; \mathbb{R}^3)$ is the Sobolev space of measurable deformations $y : \Omega \to \mathbb{R}^3$ such that (Adams 1975)

$$\int_\Omega \left[|y(x)|^p + \|\nabla y(x)\|^p\right] dx < \infty.$$

In what follows (and above in the definition of $\mathcal{E}$ and W^ϕ), we shall often

suppress the explicit dependence on temperature where we do not think that there is a danger of misunderstanding.

To model an unconstrained crystal, we define the admissible set of deformations $\mathcal{A}$ to be the set of deformations of finite energy

$$\mathcal{A} = W^{\phi},$$

and we consider energy-minimizing sequences of deformations for the problem

$$\inf_{y \in \mathcal{A}} \mathcal{E}(y). \tag{2.5}$$

For a crystal that is constrained on the entire boundary by the condition

$$y(x) = y_0(x), \qquad \text{for all } x \in \partial\Omega, \tag{2.6}$$

for some $y_0(x) \in W^{\phi}$, we consider energy-minimizing sequences of deformations for the problem (2.5), where the set $\mathcal{A}$ of admissible deformations consists of all deformations of finite energy constrained on the boundary by (2.6), that is,

$$\mathcal{A} = \left\{ y \in W^{\phi} : y(x) = y_0(x), \text{ for } x \in \partial\Omega \right\}.$$

Our model and analysis can also accommodate more general boundary conditions, such as the inclusion of boundary loads.

Admissible deformations should be orientation-preserving isomorphisms, that is, $\det \nabla y(x) > 0$ for all $x \in \Omega$. However, we shall not explicitly impose this constraint since we have found that computed solutions have always satisfied this condition.

2.2. Frame indifference and crystal symmetry

The elastic energy density ϕ is required to be frame-indifferent, that is,

$$\phi(RF, \theta) = \phi(F, \theta) \qquad \text{for all } R \in \mathrm{SO}(3) \text{ and } F \in \mathbb{R}^{3\times 3}, \tag{2.7}$$

where SO(3) denotes the set of orthogonal matrices with determinant equal to 1. We assume that the energy density inherits the symmetry of the more symmetric high temperature phase of the crystal when the domain of the energy density is suitably restricted (Ericksen 1980, Pitteri 1984), so

$$\phi(R_i F R_i^T, \theta) = \phi(F, \theta) \qquad \text{for all } R_i \in \mathcal{G}, \tag{2.8}$$

where $\mathcal{G} = \{R_1, \ldots, R_L\}$ is the symmetry group of the austenite.

2.3. Local minima of the energy density

Near the transformation temperature, we will assume that the energy density $\phi(F, \theta)$ has local minima at the deformation gradients that describe the austenitic and the martensitic phases, and is therefore non-convex. The reference

configuration has been taken to be the austenitic phase at the transformation temperature, so the identity deformation gradient I describes the austenitic phase, and by the frame indifference of the energy density (2.7), every $R \in \mathrm{SO}(3)$ should then be a local minimum of the energy density $\phi(F, \theta)$. We note that for simplicity we have neglected the thermal expansion of the austenite in the above conditions, since the deformations describing the austenitic phase are taken to be independent of temperature.

We shall assume that the energy density $\phi(F, \theta)$ for the temperature θ near the transformation temperature θ_T also has local minima at the set of *variants*

$$\left\{ R_i U_1 R_i^T : R_i \in \mathcal{G} \right\} = \{ U_1, \ldots, U_M \} \tag{2.9}$$

which describe the martensitic phase. Here the $U_i = U_i(\theta)$ are deformation gradients for an unstressed crystal in the low-temperature, martensitic phase. It follows from the symmetry of the energy density (2.8) that

$$\phi(U_1, \theta) = \cdots = \phi(U_M, \theta). \tag{2.10}$$

Since M (defined in (2.9)) is equal to the number of cosets of the subgroup

$$\mathcal{H} = \left\{ R_i \in \mathcal{G} : R_i U_1 R_i^T = U_1 \right\}$$

in $\mathcal{G}$, we have by Lagrange's Theorem (Herstein 1975) that

$$M = \frac{|\mathcal{G}|}{|\mathcal{H}|}.$$

It follows from (2.10) and the frame indifference of the energy density (2.7) that $\phi(F, \theta)$ has local minima at the energy wells of each variant given by

$$\mathcal{U}_i = \mathrm{SO}(3) U_i = \{ R U_i : R \in \mathrm{SO}(3) \} . \tag{2.11}$$

If we denote the union of the energy wells by

$$\mathcal{U} = \mathcal{U}_1 \cup \cdots \cup \mathcal{U}_M,$$

then it follows from the frame indifference (2.7) of the energy density and (2.10) that

$$\phi(U, \theta) = \phi(U_1, \theta) = \cdots = \phi(U_M, \theta) \qquad \text{for all } U \in \mathcal{U}.$$

Also, since admissible deformations are required to be orientation-preserving isomorphisms, we shall always assume that $\det U_1 > 0$, so by (2.9) and (2.11) we have that

$$\det U = \det U_1 > 0 \qquad \text{for all } U \in \mathcal{U}. \tag{2.12}$$

2.4. The orthorhombic to monoclinic transformation

We next present two examples of martensitic phase transformations. First, we describe the symmetry group $\mathcal{G}$ and the corresponding martensitic vari-

ants $\{R_i U_1 R_i^T : R_i \in \mathcal{G}\}$ for one of the orthorhombic to monoclinic transformations (Ball and James 1992). The symmetry group of the orthorhombic (high-temperature) phase is composed of the rotations of π radians about an orthogonal set of axes, so

$$\mathcal{G} = \{ I, -I + 2e_1 \otimes e_1, -I + 2e_2 \otimes e_2, -I + 2e_3 \otimes e_3 \} ,$$

where $\{e_1, e_2, e_3\}$ is an orthonormal basis of $\mathbb{R}^3$. We recall that $v \otimes w \in \mathbb{R}^{3\times 3}$ for $v, w \in \mathbb{R}^3$ is the tensor product defined by $(v \otimes w)_{kl} = v_k w_l$, or, equivalently, $(v \otimes w)u = (w \cdot u)v$ for $u \in \mathbb{R}^3$.

The variants of the monoclinic (low-temperature) phase can then be given by

$$U_1 = (I - \eta e_2 \otimes e_1)\, D \qquad \text{and} \qquad U_2 = (I + \eta e_2 \otimes e_1)\, D, \tag{2.13}$$

where $\eta > 0$, and where $D \in \mathbb{R}^{3\times 3}$ is the positive diagonal matrix

$$D = d_1 e_1 \otimes e_1 + d_2 e_2 \otimes e_2 + d_3 e_3 \otimes e_3$$

for $d_1, d_2, d_3 > 0$. We note that

$$\left\{ R_i U_1 R_i^T : R_i \in \mathcal{G} \right\} = \{ U_1, U_2 \} .$$

2.5. The cubic to tetragonal transformation

For the more common cubic (high-temperature) to tetragonal (low-temperature) transformation, the group $\mathcal{G}$ is the symmetry group of the cube

$$\mathcal{G} = \{ R_1, \ldots, R_{24} \} , \tag{2.14}$$

which is given by the group of matrices

$$R_i = (-1)^{v(1)} e_{\pi(1)} \otimes e_1 + (-1)^{v(2)} e_{\pi(2)} \otimes e_2 + (-1)^{v(3)} e_{\pi(3)} \otimes e_3,$$

where $v : \{1, 2, 3\} \to \{0, 1\}$; $\pi : \{1, 2, 3\} \to \{1, 2, 3\}$ is a permutation; and $\det R_i = 1$. We also assume as above that $\{e_1, e_2, e_3\}$ is an orthonormal basis of $\mathbb{R}^3$. The variants of the tetragonal phase can be taken to be

$$\begin{aligned} U_1 = \nu_1 I + (\nu_2 - \nu_1) e_1 \otimes e_1, \qquad U_2 = \nu_1 I + (\nu_2 - \nu_1) e_2 \otimes e_2, \\ U_3 = \nu_1 I + (\nu_2 - \nu_1) e_3 \otimes e_3 \end{aligned} \tag{2.15}$$

where $0 < \nu_1$, $0 < \nu_2$, and $\nu_1 \neq \nu_2$. For this transformation,

$$\left\{ R_i U_1 R_i^T : R_i \in \mathcal{G} \right\} = \{ U_1, U_2, U_3 \} .$$

2.6. Global minima of the energy density

The reference configuration has been chosen so that $F = I$ is the deformation gradient for the high-temperature phase at the transformation temperature $\theta = \theta_T$. The elastic energy density should then predict that the

high-temperature phase (represented by $F \in \mathrm{SO}(3)$) is a global minimum for $\theta > \theta_T$ and the low-temperature phase (represented by $U \in \mathcal{U} = \mathcal{U}_1 \cup \cdots \cup \mathcal{U}_M$) is a global minimum for $\theta < \theta_T$. Thus, the elastic energy density should satisfy the conditions that, for $\theta > \theta_T$,

$$\phi(F,\theta) > \phi(R,\theta) \quad \text{for all } F \notin \mathrm{SO}(3),\ R \in \mathrm{SO}(3); \tag{2.16}$$

for $\theta = \theta_T$,

$$\phi(F,\theta_T) > \phi(R,\theta_T) = \phi(U,\theta_T) \quad \text{for all } F \notin \mathrm{SO}(3) \cup \mathcal{U},\ R \in \mathrm{SO}(3),\ U \in \mathcal{U}; \tag{2.17}$$

and for $\theta < \theta_T$,

$$\phi(F,\theta) > \phi(U,\theta) \quad \text{for all } F \notin \mathcal{U},\ U \in \mathcal{U}. \tag{2.18}$$

2.7. The Ericksen–James energy density for the cubic to tetragonal transformation

The development of a computational model for martensitic crystals requires the construction of an energy density $\phi(F,\theta)$ that is frame-indifferent (2.7), has the symmetry group of the crystal (2.8), satisfies the qualitative properties of the first-order phase transition (2.16)–(2.18), and matches available experimental data such as the linear elastic moduli of the pure phases and the dependence of the transformation temperature on stress. The following such energy density for the cubic to tetragonal transformation was developed by Ericksen and James (Ericksen 1986, Ericksen 1987*a*, Collins and Luskin 1989):

$$\begin{aligned}\phi(F,\theta) = {} & \frac{b(\theta)}{6}\left[\left(\frac{3C_{11}}{\operatorname{tr} C}-1\right)^2+\left(\frac{3C_{22}}{\operatorname{tr} C}-1\right)^2+\left(\frac{3C_{33}}{\operatorname{tr} C}-1\right)^2\right] \\ & +\frac{c(\theta)}{2}\left(\frac{3C_{11}}{\operatorname{tr} C}-1\right)\left(\frac{3C_{22}}{\operatorname{tr} C}-1\right)\left(\frac{3C_{33}}{\operatorname{tr} C}-1\right) \\ & +\frac{d(\theta)}{36}\left[\left(\frac{3C_{11}}{\operatorname{tr} C}-1\right)^2+\left(\frac{3C_{22}}{\operatorname{tr} C}-1\right)^2+\left(\frac{3C_{33}}{\operatorname{tr} C}-1\right)^2\right]^2 \\ & +\frac{e}{2}(C_{12}^2+C_{13}^2+C_{23}^2+C_{21}^2+C_{31}^2+C_{32}^2)+f(\operatorname{tr} C-3)^2,\end{aligned} \tag{2.19}$$

where $C = F^T F$ is the right Cauchy–Green strain and $\operatorname{tr} C$ is the trace of C. The energy density (2.19) is frame-indifferent since it is a function of the right Cauchy–Green strain C. Ericksen has also shown that it has the cubic symmetry group, and that the coefficients b, c, d, e, and f can be chosen so that the energy density satisfies the qualitative conditions for the first-order phase transition with

$$\nu_1 = \sqrt{1-\epsilon} \qquad \nu_2 = \sqrt{1+2\epsilon}$$

for $0 < \epsilon < 1$ (Ericksen 1986).

Ericksen and James have also determined moduli that fit experimental data for the In-20.7 at% Tl alloy. These moduli are given by (θ in °C and moduli in gigapascals)

$$b = 0.38 + (1.22 \times 10^{-3})(\theta - \theta_T), \qquad c = -29.23, \qquad d = 562.13$$
$$e = 3.26, \qquad f = 5.25,$$

where the transformation temperature is $\theta_T = 70°\text{C}$. The size of In-20.7 at% Tl crystals used in laboratory experiments is typically on the order of several centimetres in diameter.

An easy calculation establishes that

$$\phi(U(\epsilon), \theta) = b(\theta)\epsilon^2 + c\epsilon^3 + d\epsilon^4,$$

where $U(\epsilon) = \text{diag}(\sqrt{1+2\epsilon}, \sqrt{1-\epsilon}, \sqrt{1-\epsilon})$. Thus $\phi(U(\epsilon), \theta)$ has a local minimum in ϵ corresponding to the austenitic phase at $\epsilon(\theta) = 0$, for all temperatures satisfying $b(\theta) > 0$ (or for $\theta > -240°\text{C}$). Further, there is a local minimum at

$$\epsilon(\theta) = \frac{-3c + \sqrt{9c^2 - 32db(\theta)}}{8d}$$

corresponding to the martensitic phase for $\theta < \theta^*$, where $\theta^* = 108.92°\text{C}$ satisfies $9c^2 - 32db(\theta^*) = 0$. Thus, $\epsilon(\theta_T) = 0.026$.

3. Microstructure

In this section we will describe some examples and properties of microstructures.

3.1. Interfaces and the rank-one property

We first give a necessary and sufficient condition for the existence of a continuous deformation with a planar interface separating two regions with constant deformation gradients $F_0 \in \mathbb{R}^{3\times3}$ and $F_1 \in \mathbb{R}^{3\times3}$.

Lemma 1 Let $n \in \mathbb{R}^3$, $|n| = 1$, and $s \in \mathbb{R}$. There exists a continuous deformation $w(x) \in C(\mathbb{R}^3; \mathbb{R}^3)$ such that

$$\nabla w(x) = \begin{cases} F_0 & \text{for all } x \text{ such that } x \cdot n < s, \\ F_1 & \text{for all } x \text{ such that } x \cdot n > s, \end{cases} \tag{3.1}$$

if and only if there exists $a \in \mathbb{R}^3$ such that

$$F_1 = F_0 + a \otimes n. \tag{3.2}$$

Proof. If $w(x) \in C(\mathbb{R}^3; \mathbb{R}^3)$ satisfies (3.1), then the equality of the directional derivatives of $w(x)$ in directions orthogonal to the normal of the interface implies that

$$F_1 v = F_0 v \qquad \text{for all } v \in \mathbb{R}^3 \text{ such that } v \cdot n = 0.$$

Thus, we have that (3.2) holds with

$$a = F_1 n - F_0 n.$$

Conversely, if (3.2) holds, then the deformation

$$w(x) = \begin{cases} F_0 x & \text{for all } x \text{ such that } x \cdot n < s, \\ F_1 x - sa & \text{for all } x \text{ such that } x \cdot n > s, \end{cases}$$

is continuous and satisfies (3.1). □

Lemma 1 can be strengthened to state that if $w(x)$ is a continuous deformation whose gradient takes constant values $F_0 \in \mathbb{R}^{3\times 3}$ and $F_1 \in \mathbb{R}^{3\times 3}$, with $F_0 \neq F_1$ in two regions separated by a smooth interface, then the interface is planar and (3.2) holds for some a, $n \in \mathbb{R}^3$, $|n| = 1$, with n a normal to the planar interface. A more general result for a deformation with a gradient taking two values can be found in Ball and James (1987). We also note that the condition $|n| = 1$ above is not essential since we can always rewrite $a \otimes n$ by $|n| a \otimes \frac{n}{|n|}$ when $n \neq 0$.

The above lemma motivates the following definition.

Definition 1 We say that $F_0 \in \mathbb{R}^{3\times 3}$ and $F_1 \in \mathbb{R}^{3\times 3}$ are *rank-one connected* if there exist $a \in \mathbb{R}^3$ and $n \in \mathbb{R}^3$, $|n| = 1$, such that

$$F_1 = F_0 + a \otimes n. \tag{3.3}$$

3.2. Laminated microstructure

More generally, if F_0 and F_1 are rank-one connected as in (3.3), then we can construct a continuous deformation having parallel planar interfaces

$$S_i = \{ x \in \Omega : x \cdot n = s_i \}$$

for $s_1 < \cdots < s_m$ with the same normal n separating the layers in which the deformation gradient alternates between F_0 and F_1 by

$$w(x) = F_0 x + \left[\int_0^{x\cdot n} \chi(s)\, \mathrm{d}s \right] a, \tag{3.4}$$

where $\chi(s) : \mathbb{R} \to \mathbb{R}$ is the characteristic function

$$\chi(s) = \begin{cases} 0 & \text{if } x \in (s_{2l}, s_{2l+1}) \text{ for } 0 \leq 2l \leq m \text{ where } l \in \mathbb{Z}, \\ 1 & \text{if } x \in (s_{2l+1}, s_{2l+2}) \text{ for } 1 \leq 2l+1 \leq m \text{ where } l \in \mathbb{Z}, \end{cases}$$

where we take $s_0 = -\infty$ and $s_{m+1} = \infty$. This deformation satisfies the property that

$$\nabla w(x) = F_0 + \chi(x \cdot n) a \otimes n = \begin{cases} F_0 & \text{for all } x \text{ such that } \chi(x \cdot n) = 0, \\ F_1 & \text{for all } x \text{ such that } \chi(x \cdot n) = 1. \end{cases}$$

Deformations $w(x)$ of the form (3.4) with layer thickness $s_{i+1} - s_i$ small for $i = 1, \ldots, m$ are the simplest examples of *microstructure*.

We define $\phi_{\min}(\theta)$ to be the lowest attainable energy at the temperature θ, that is,

$$\phi_{\min}(\theta) = \min_{F \in \mathbb{R}^{3\times 3}} \phi(F, \theta). \tag{3.5}$$

For $\theta \leq \theta_T$ and $F_0,\ F_1 \in \mathcal{U}$, we have that

$$\phi_{\min}(\theta) = \phi(F_0, \theta) = \phi(F_1, \theta).$$

Thus, if $\theta \leq \theta_T$ and $F_0,\ F_1 \in \mathcal{U}$, then the deformation $w(x)$ defined by (3.4) attains the minimum energy, since

$$\mathcal{E}(w) = \int_\Omega \phi(\nabla w(x), \theta)\, \mathrm{d}x = \phi_{\min}(\theta) \operatorname{meas} \Omega.$$

Furthermore, if $\theta > \theta_T$ and $F_0,\ F_1 \in \mathcal{U}$, then the deformations $w(x)$ defined by (3.4) are equilibria, since every $F \in \mathcal{U}$ is a local minimum of $\phi(F, \theta)$ (see Section 2.3), and hence

$$\mathcal{E}(w + z) - \mathcal{E}(w) = \int_\Omega \left[\phi\left(\nabla w(x) + \nabla z(x), \theta\right) - \phi\left(\nabla w(x), \theta\right)\right] \mathrm{d}x \geq 0$$

for all $z \in W^{1,\infty}(\Omega; \mathbb{R}^3)$ such that ess $\sup_{x\in\Omega} \|\nabla z(x)\|$ is sufficiently small.

3.3. Surface energy

The *surface energy* $\mathcal{S}$ associated with all the interfaces S_i can be modelled by

$$\mathcal{S}(w) = \alpha \sum_{i=1}^{m} \operatorname{area} S_i, \tag{3.6}$$

where $\alpha > 0$ is the surface energy density and m is the number of interfaces. For $\theta \leq \theta_T$ and $F_0,\ F_1 \in \mathcal{U}$, the total energy is the sum of the bulk energy and the surface energy given by

$$\mathcal{E}(w) + \mathcal{S}(w) = \phi_{\min}(\theta) \operatorname{meas} \Omega + \alpha \sum_{i=1}^{m} \operatorname{area} S_i, \tag{3.7}$$

which is minimized when the deformation w does not have any interfaces, that is, when $w(x) = F_0 x$ or $w(x) = F_1 x$. So, how do we explain the presence of interfaces in martensitic crystals? We will see later in this section that the constraint of boundary conditions or the constraint of continuity between austenitic and martensitic regions can make deformations with closely spaced interfaces energetically advantageous. The presence of interfaces can also be explained by the meta-stability of such deformations (Abeyaratne, Chu and James 1994, Ball et al. 1995).

For analytical and computational purposes, the surface energy is usually

modelled by a strain gradient term such as

$$\hat{\mathcal{S}}(w) = \hat{\alpha}^2 \int_\Omega \nabla\nabla w(x) \cdot A\nabla\nabla w(x)\,\mathrm{d}x, \tag{3.8}$$

where $\hat{\alpha}$ is the strain gradient coefficient. Here A is a sixth-order tensor such that the surface energy density $\nabla\nabla w(x) \cdot A\nabla\nabla w(x)$ is positive definite, is frame-indifferent, and has the symmetry properties of the crystal (Barsch, Horovitz and Krumhansl 1987, Horovitz, Barsch and Krumhansl 1991).

Kohn and Müller (1992*a*, 1992*b*, 1994) have given an analysis of the relation between (3.6) and (3.8) for some scalar models, and they have presented results for the geometry, energy, and length scale of the microstructure for energy-minimizing deformations. In addition, Müller (1993) has given a detailed study of energy-minimizing deformations for one-dimensional problems with an energy of the form

$$\int_0^1 \left[\left(\frac{dw}{dx}(x) - 1 \right)^2 \left(\frac{dw}{dx}(x) + 1 \right)^2 + w(x)^2 + \hat{\alpha}^2 \left(\frac{d^2w}{dx^2}(x) \right)^2 \right] \mathrm{d}x$$

for the singular limit given by $\hat{\alpha} \to 0$. Müller's work gives rigorous asymptotic results on the periodicity, length scales, and energy of energy-minimizing deformations.

We expect under appropriate conditions that there exist smooth energy-minimizing deformations $w_{\hat{\alpha}}(x)$ to the total energy

$$\int_\Omega \left[\phi(\nabla w(x),\, \theta) + \hat{\alpha}^2 \nabla\nabla w(x) \cdot A\nabla\nabla w(x) \right] \mathrm{d}x,$$

and that the deformations $w_{\hat{\alpha}}(x)$ for $\hat{\alpha} \to 0$ are an energy-minimizing sequence for the elastic energy

$$\int_\Omega \phi(\nabla w(x),\, \theta)\,\mathrm{d}x. \tag{3.9}$$

Now let Ω be a reference configuration and suppose that the deformation $w^{[\hat{\alpha},\, L]}(x) : L\Omega \to \mathbb{R}^3$ is an energy-minimizing deformation defined on the domain $L\Omega = \{Lx : x \in \Omega\}$, with $L > 0$ for the total energy

$$\int_{L\Omega} \left[\phi(\nabla w(x),\, \theta) + \hat{\alpha}^2 \nabla\nabla w(x) \cdot A\nabla\nabla w(x) \right] \mathrm{d}x. \tag{3.10}$$

It can then be seen that

$$w_{\hat{\alpha},\, L}(x) = \frac{1}{L} w^{[\hat{\alpha},\, L]}(Lx) \qquad \text{for all } x \in \Omega$$

is an energy-minimizing deformation on the domain Ω with the total energy

$$L^3 \int_\Omega \left[\phi(\nabla w(x),\, \theta) + \frac{\hat{\alpha}^2}{L^2} \nabla\nabla w(x) \cdot A\nabla\nabla w(x) \right] \mathrm{d}x.$$

Thus, we see that the properties of energy-minimizing deformations for the total energy given by (3.10) for crystals on a domain $L\Omega$ with $L \gg \hat{\alpha}$ can be investigated by considering energy-minimizing sequences of deformations for the elastic energy given by (3.9) on a reference configuration Ω. This approach has been rigorously justified by DeSimone (1993) for the micromagnetics problem (with the exchange energy playing the role of the surface energy).

For those energies that include a surface energy such as (3.7) or (3.8), we see that the surface energy determines the length scale and the geometry of the layers of energy-minimizing deformations, but it often does not influence many of the macroscopic properties of interest (Ball and James 1987, 1992). Also, the length scale at which the surface energy is significant is usually orders of magnitude smaller than our numerical grid scale, and the surface energy is often orders of magnitude smaller than the expected discretization error. For this reason, we shall usually neglect the surface energy in our discussion in this article.

3.4. Classification of interfaces

We give in this subsection a complete description for both the orthorhombic to monoclinic transformation (2.13) and the cubic to tetragonal transformation (2.15) of all interfaces separating two regions with constant deformation gradients in either the martensitic or the austenitic phase (Ball and James 1987).

We start by showing that there does not exist a continuous deformation with a planar interface separating two regions of the austenitic phase (Ball and James 1987).

Lemma 2 There do not exist R_0, $R_1 \in \mathrm{SO}(3)$ with $R_0 \neq R_1$, such that R_0 and R_1 are rank-one connected.

Proof. If $R_0 \in \mathrm{SO}(3)$ and $R_1 \in \mathrm{SO}(3)$ are rank-one connected, then

$$R_1 = R_0 + a \otimes n$$

for $a \in \mathbb{R}^3$ and $n \in \mathbb{R}^3$, $|n| = 1$. Thus,

$$R_0^{-1} R_1 = I + R_0^{-1} a \otimes n.$$

Hence

$$R_0^{-1} R_1 v = v$$

for all v in the two-dimensional subspace $\{v \in \mathbb{R}^3 : n \cdot v = 0\}$. Since $R_0^{-1} R_1 \in \mathrm{SO}(3)$, we obtain $R_1 = R_0$, which proves the lemma. □

The following four lemmas (Ball and James 1987) show that for the orthorhombic to monoclinic transformation (2.13) and the cubic to tetragonal

transformation (2.15) each $F_0 \in \mathcal{U}_i$ is not rank-one connected to any $F_1 \in \mathcal{U}_i$ with $F_0 \neq F_1$, but that every $F_0 \in \mathcal{U}_i$ is rank-one connected to two distinct $F_1 \in \mathcal{U}_j$ for all $j \neq i$, $j \in \{1, \cdots, M\}$.

Lemma 3 If $F_0 \in \mathcal{U}_i$ for some $i \in \{1, \cdots, M\}$, then there does not exist $F_1 \in \mathcal{U}_i$ with $F_0 \neq F_1$, such that F_0 and F_1 are rank-one connected.

Proof. If $F_0 = R_0 U_i \in \mathcal{U}_i$ and $F_1 = R_1 U_i \in \mathcal{U}_i$ are rank-one connected where R_0, $R_1 \in \mathrm{SO}(3)$, then

$$R_1 U_i = R_0 U_i + a \otimes n$$

for $a \in \mathbb{R}^3$ and $n \in \mathbb{R}^3$, $|n| = 1$. So,

$$R_1 = R_0 + a \otimes U_i^{-T} n. \tag{3.11}$$

It then follows from (3.11) and Lemma 2 that $R_1 = R_0$ which proves the lemma. □

The following lemma will allow us to reduce the problem of determining the rank-one connections for the orthorhombic to monoclinic transformation (2.13) and the cubic to tetragonal transformation (2.15) to a two-dimensional problem.

Lemma 4 Suppose that U_1, $U_2 \in \mathcal{U}$ satisfy the conditions

$$U_1 e_3 = U_1^T e_3 = U_2 e_3 = U_2^T e_3 = \hat{\nu} e_3 \tag{3.12}$$

for $\hat{\nu} \neq 0$. If there exists $R \in \mathrm{SO}(3)$, $a \in \mathbb{R}^3$, and $n \in \mathbb{R}^3$ with $|n| = 1$, such that

$$R U_2 = U_1 + a \otimes n, \tag{3.13}$$

then $a \cdot e_3 = n \cdot e_3 = 0$ and $R = R(\sigma e_3)$ is the rotation matrix of angle σ about the axis e_3, which satisfies

$$R(\sigma e_3) U_2 v = U_1 v \tag{3.14}$$

for $v \in \mathbb{R}^3$ satisfying $v \cdot n = v \cdot e_3 = 0$, $v \neq 0$.

Conversely, if (3.14) holds for some $v \in \mathbb{R}^3$ satisfying $v \cdot e_3 = 0$, $v \neq 0$, then (3.13) holds for $R = R(\sigma e_3)$, $n \in \mathbb{R}^3$ satisfying $n \cdot e_3 = n \cdot v = 0$, $|n| = 1$, and $a = (R U_2 - U_1) n$.

Proof. We suppose that (3.13) holds. It then follows that

$$R U_2 = U_1 + a \otimes n = (I + a \otimes U_1^{-T} n) U_1, \tag{3.15}$$

so, since $\det U_1 = \det U_2 \neq 0$ by (2.12), we have that

$$\det U_1 = \det(R U_2) = \det(I + a \otimes U_1^{-T} n) \det U_1 = \left(1 + a \cdot U_1^{-T} n\right) \det U_1.$$

Hence, it follows that

$$a \cdot U_1^{-T} n = 0. \tag{3.16}$$

We have by (3.15) that

$$RU_2U_1^{-1} = I + a \otimes U_1^{-T}n, \tag{3.17}$$

so we have for

$$C \equiv \left(RU_2U_1^{-1}\right)^T \left(RU_2U_1^{-1}\right) = \left(U_2U_1^{-1}\right)^T \left(U_2U_1^{-1}\right) \tag{3.18}$$

that

$$C = \left(I + U_1^{-T}n \otimes a\right)\left(I + a \otimes U_1^{-T}n\right). \tag{3.19}$$

Now it follows from (3.12) and (3.18) that

$$Ce_3 = e_3 \tag{3.20}$$

and from (3.19) that

$$Ce_3 = e_3 + (U_1^{-T}n \cdot e_3)a + \left[a \cdot e_3 + |a|^2(U_1^{-T}n \cdot e_3)\right] U_1^{-T}n. \tag{3.21}$$

Since a and $U_1^{-T}n$ are linearly independent by (3.16), it follows from (3.20) and (3.21) that

$$U_1^{-T}n \cdot e_3 = 0 \qquad \text{and} \qquad a \cdot e_3 = 0. \tag{3.22}$$

Next, we have by (3.12) and (3.22) that

$$n \cdot e_3 = n \cdot \left(\hat{\nu}U_1^{-1}e_3\right) = \hat{\nu}U_1^{-T}n \cdot e_3 = 0. \tag{3.23}$$

We then obtain from (3.12), (3.13), and (3.23) that

$$\hat{\nu}Re_3 = RU_2e_3 = (U_1 + a \otimes n)\, e_3 = U_1e_3 = \hat{\nu}e_3. \tag{3.24}$$

We have that $Re_3 = e_3$ by (3.24), so we can conclude that

$$R = R(\sigma e_3),$$

where $R(\sigma e_3)$ is a rotation matrix of angle σ about the axis e_3. The result (3.14) now follows by (3.13) for $v \in \mathbb{R}^3$ satisfying $v \cdot n = v \cdot e_3 = 0$, $v \neq 0$.

Conversely, if (3.14) holds, then it is easy to check that (3.13) holds for $R = R(\sigma e_3)$, $n \in \mathbb{R}^3$ satisfying $n \cdot e_3 = n \cdot v = 0$ with $|n| = 1$, and $a = (RU_2 - U_1)n$. □

Lemma 5 We consider the orthorhombic–monoclinic transformation (2.13). If $F_0 \in \mathcal{U}_i$ for $i \in \{1, 2\}$, then for $j \neq i$, $j \in \{1, 2\}$, there exist two distinct $F_1 \in \mathcal{U}_j$ such that F_0 and F_1 are rank-one connected.

Proof. Without loss of generality we may assume that $F_0 = U_1$, and we show that there exist two distinct $R \in \mathrm{SO}(3)$ such that

$$RU_2 = U_1 + a \otimes n \tag{3.25}$$

for some a, $n \in \mathbb{R}^3$, $|n| = 1$. Since (3.12) holds with $\hat{\nu} = 1$, by Lemma 4 it is

sufficient to determine all $\sigma \in \mathbb{R}$ and $v \in \text{Span}\{e_1, e_2\}$, $v \neq 0$, such that

$$R(\sigma e_3)U_2 v = U_1 v. \tag{3.26}$$

Now there exist $\sigma \in \mathbb{R}$ and $v \in \text{Span}\{e_1, e_2\}$, $v \neq 0$, such that

$$R(\sigma e_3)U_2 v = U_1 v$$

if and only if there exists $v \in \text{Span}\{e_1, e_2\}$, $v \neq 0$, such that

$$|U_1 v| = |U_2 v|. \tag{3.27}$$

For $v = v_1 e_1 + v_2 e_2$ where $v_1, v_2 \in \mathbb{R}$, we have that

$$|U_1 v| = |U_2 v| \tag{3.28}$$

if and only if

$$v_1 v_2 = 0.$$

The solution to (3.28) given by $v_1 = 0$ or $v = e_2$ corresponds to the obvious solution

$$U_2 = U_1 + 2\eta d_1 e_2 \otimes e_1$$

to (3.25) given by $n = e_1$ and $\sigma = 0$. The solution to (3.28) given by $v_2 = 0$ or $v = e_1$ corresponds to the solution to (3.25) given by

$$n = e_2, \qquad \cos\sigma = \frac{U_1 v \cdot U_2 v}{|U_1 v||U_2 v|} = \frac{d_1^2 - \eta^2 d_2^2}{d_1^2 + \eta^2 d_2^2} \quad \text{for } -\pi < \sigma < 0.$$

We note that solutions v and $-v$ to (3.28) give the same solutions to (3.25). □

Lemma 6 We consider the cubic to tetragonal transformation (2.15). If $F_0 \in \mathcal{U}_i$ for some $i \in \{1, 2, 3\}$, then for any $j \neq i$, $j \in \{1, 2, 3\}$, there exist two distinct $F_1 \in \mathcal{U}_j$ such that F_0 and F_1 are rank-one connected.

Proof. Without loss of generality we again assume that $F_0 = U_1$ and $j = 2$, and we show that there exist two distinct $R \in \text{SO}(3)$ such that

$$RU_2 = U_1 + a \otimes n \tag{3.29}$$

for some $a, n \in \mathbb{R}^3$, $|n| = 1$. Since (3.12) holds with $\hat{\nu} = \nu_1$, by Lemma 4 it is sufficient to determine all $\sigma \in \mathbb{R}$ and $v \in \text{Span}\{e_1, e_2\}$, $v \neq 0$, such that

$$R(\sigma e_3)U_2 v = U_1 v. \tag{3.30}$$

Again, there exist $\sigma \in \mathbb{R}$ and $v \in \text{Span}\{e_1, e_2\}$, $v \neq 0$, such that

$$R(\sigma e_3)U_2 v = U_1 v$$

if and only if there exists $v \in \text{Span}\{e_1, e_2\}$, $v \neq 0$, such that

$$|U_1 v| = |U_2 v|. \tag{3.31}$$

For $v = v_1 e_1 + v_2 e_2$ where $v_1,\ v_2 \in \mathbb{R}$, we have that

$$|U_1 v| = |U_2 v| \tag{3.32}$$

if and only if

$$v_1^2 = v_2^2.$$

We have for the solution to (3.32) given by $v = e_1 - e_2$ the corresponding solution to (3.29) given by

$$n = \frac{1}{\sqrt{2}}(e_1 + e_2)$$

and

$$\cos\sigma = \frac{U_1 v \cdot U_2 v}{|U_1 v||U_2 v|} = \frac{2\nu_1\nu_2}{\nu_1^2 + \nu_2^2}$$

where

$$\begin{aligned} 0 < \sigma < \frac{\pi}{2} \quad &\text{if} \quad \nu_2 > \nu_1, \\ -\frac{\pi}{2} < \sigma < 0 \quad &\text{if} \quad \nu_1 > \nu_2. \end{aligned}$$

We also have for the solution $v = e_1 + e_2$ of (3.32) the corresponding solution to (3.29) given by

$$n = \frac{1}{\sqrt{2}}(e_1 - e_2)$$

and

$$\cos\sigma = \frac{U_1 v \cdot U_2 v}{|U_1 v||U_2 v|} = \frac{2\nu_1\nu_2}{\nu_1^2 + \nu_2^2}$$

where

$$\begin{aligned} 0 < \sigma < \frac{\pi}{2} \quad &\text{if} \quad \nu_1 > \nu_2, \\ -\frac{\pi}{2} < \sigma < 0 \quad &\text{if} \quad \nu_2 > \nu_1. \end{aligned}$$

Thus, the solutions to (3.29) give two distinct families of parallel interfaces corresponding to

$$n = \frac{1}{\sqrt{2}}(e_1 + e_2) \quad \text{and} \quad n = \frac{1}{\sqrt{2}}(e_1 - e_2).$$

It follows from symmetry that there are four additional distinct families of parallel interfaces corresponding to

$$n = \frac{1}{\sqrt{2}}(e_1 + e_3), \qquad n = \frac{1}{\sqrt{2}}(e_1 - e_3),$$

and

$$n = \frac{1}{\sqrt{2}}(e_2 + e_3), \qquad n = \frac{1}{\sqrt{2}}(e_2 - e_3).$$

□

The homogeneous austenitic phase can be separated from the homogeneous martensitic phase by a planar interface with normal n if and only if there exist a rotation $R \in \mathrm{SO}(3)$ and vectors $a \in \mathbb{R}^3$ and $n \in \mathbb{R}^3$, $|n| = 1$, such that

$$RU_i = I + a \otimes n$$

for some $i \in \{1, \ldots, M\}$, where U_i is one of the variants defined by (2.9). The following theorem gives a necessary and sufficient condition for (3.33) to have a solution.

Lemma 7 We consider the cubic to tetragonal transformation (2.15). If $\nu_1 \neq 1$, then there does not exist a rotation $R \in \mathrm{SO}(3)$ and vectors $a \in \mathbb{R}^3$ and $n \in \mathbb{R}^3$, $|n| = 1$, such that

$$RU_i = I + a \otimes n \tag{3.33}$$

for any $i \in \{1, 2, 3\}$. If $\nu_1 = 1$, then

$$U_i = I + (\nu_2 - 1)e_i \otimes e_i \tag{3.34}$$

for any $i \in \{1, 2, 3\}$.

Proof. We first assume that $\nu_1 \neq 1$ and $\nu_2 = 1$ and that there exist a rotation $R \in \mathrm{SO}(3)$ and vectors $a \in \mathbb{R}^3$ and $n \in \mathbb{R}^3$, $|n| = 1$, such that (3.33) holds for some $i \in \{1, 2, 3\}$. We have that $|RU_i v| = |v|$ if and only if v lies in the one-dimensional subspace spanned by e_i. However, $|(I + a \otimes n)v| = |v|$ for all v in the two-dimensional subspace for which $v \cdot n = 0$, which contradicts (3.33).

We next assume that $\nu_1 \neq 1$ and $\nu_2 \neq 1$. By multiplying (3.33) by its transpose, we have

$$U_i^2 = (RU_i)^T RU_i = (I + n \otimes a)(I + a \otimes n), \tag{3.35}$$

since $U_i^T = U_i$ and $R^T = R^{-1}$ because $R \in \mathrm{SO}(3)$. Further, a is nonzero, because otherwise (3.33) implies that $U_i \in \mathrm{SO}(3)$. Now $a \times n$ is an eigenvector of $(I + n \otimes a)(I + a \otimes n)$ with eigenvalue 1, so we have reached a contradiction, since 1 is not an eigenvalue of U_i^2 in this case.

The proof of the result (3.34) follows directly from the definition of the U_i given in (2.15). □

Bhattacharya (1992) has shown that martensitic crystals exhibiting the shape-memory phenomenon that is important for many technological applications can be expected to have a transformation that is approximately volume preserving, that is, $\det U_i = \det I$ or $\nu_1^2 \nu_2 = 1$. Hence, we do not expect to

observe the homogeneous austenitic phase separated from the homogeneous martensitic phase by a smooth interface in martensitic crystals exhibiting the shape-memory phenomena. We shall see in Section 3.9 that if

$$\nu_1 < 1 < \nu_2 \quad \text{and} \quad \frac{1}{\nu_1^2} + \frac{1}{\nu_2^2} < 2,$$

$$\text{or} \quad \nu_2 < 1 < \nu_1 \quad \text{and } \nu_1^2 + \nu_2^2 < 2,$$

then the homogeneous austenitic phase can be separated by a planar interface from a martensitic phase that is composed of a fine-scale laminate of two martensitic variants.

3.5. Boundary constraints and fine-scale laminates

We can construct energy-minimizing deformations w with arbitrarily fine-scale oscillations from energy-minimizing deformation gradients $F_0 \in \mathcal{U}$ and $F_1 \in \mathcal{U}$ that are rank-one connected as in (3.3). To construct a laminated microstructure having deformation gradient F_0 for volume fraction $1-\lambda$ (where $0 < \lambda < 1$) and having deformation gradient F_1 for volume fraction λ, we construct the continuous deformation $w_\gamma(x)$ with layer thickness $\gamma > 0$ by

$$w_\gamma(x) = \gamma w\left(\frac{x}{\gamma}\right), \tag{3.36}$$

where

$$w(x) = F_0 x + \left[\int_0^{x\cdot n} \chi(s)\, ds\right] a$$

and where $\chi(s) : \mathbb{R} \to \mathbb{R}$ is the characteristic function with period 1 defined by

$$\chi(s) = \begin{cases} 0 & \text{for all} \quad 0 \le s \le 1-\lambda, \\ 1 & \text{for all} \quad 1-\lambda < s < 1. \end{cases}$$

Now

$$\begin{aligned} |w_\gamma(x) - F_\lambda(x)| \quad &= \gamma\left|w(x/\gamma) - F_\lambda(x/\gamma)\right| \quad = \gamma\left|\int_0^{x\cdot n/\gamma} (\chi(s) - \lambda)\, ds\, a\right| \\ &\le \lambda(1-\lambda)|a|\gamma \end{aligned} \tag{3.37}$$

where

$$F_\lambda = (1-\lambda)F_0 + \lambda F_1 = F_0 + \lambda a \otimes n.$$

We also have

$$\nabla w_\gamma(x) = F_0 + \chi\left(\frac{x\cdot n}{\gamma}\right) a \otimes n, \qquad \text{for almost all } x \in \Omega,$$

so

$$\nabla w_\gamma(x) = \begin{cases} F_0 & \text{if } j\gamma < x \cdot n < (j+1-\lambda)\gamma \quad \text{for some } j \in \mathbb{Z}, \\ F_1 & \text{if } (j+1-\lambda)\gamma < x \cdot n < (j+1)\gamma \quad \text{for some } j \in \mathbb{Z}. \end{cases} \tag{3.38}$$

The deformations $w_\gamma(x)$ converge uniformly to $F_\lambda x$ as $\gamma \to 0$ by (3.37), but the deformation gradients oscillate between F_0 in layers of thickness $(1-\lambda)\gamma$ and F_1 in layers of thickness $\lambda\gamma$. In the laboratory, we do not observe laminates with arbitrarily small layer thickness γ. Laminates with arbitrarily small layer thickness exist in our model because we neglect surface energy. However, even with the inclusion of surface energy in the total energy, the constraint of boundary conditions makes the formation of layers of finite thickness with a deformation gradient oscillating between F_0 and F_1 energetically advantageous.

The *infimum* of the energy with respect to deformations constrained by the boundary condition

$$y(x) = Fx \qquad \text{for all } x \in \partial\Omega \tag{3.39}$$

for a fixed $F \in \mathbb{R}^{3\times 3}$ has been the subject of much research, since it gives the minimum energy attainable by a microstructure with average deformation gradient F. The value of this *infimum* is called the *relaxation* of ϕ at F and is discussed further in Section 7 and in more detail in Ekeland and Temam (1974) and Dacorogna (1989). For the boundary condition (3.39), we denote the set of admissible deformations by

$$W_F^\phi = \left\{ v \in W^\phi : v(x) = Fx \text{ for } x \in \partial\Omega \right\}.$$

We know from (3.5) that

$$\inf_{z \in W_F^\phi} \mathcal{E}(z) \geq \phi_{\min}(\theta)\text{meas}(\Omega)$$

for all $F \in \mathbb{R}^{3\times 3}$. The following theorem shows that the *infimum* of the total energy over deformations constrained by the boundary condition

$$y(x) = F_\lambda x = [(1-\lambda)F_0 + \lambda F_1]\, x \qquad \text{for all } x \in \partial\Omega,$$

where $F_0 \in \mathcal{U}$ and $F_1 \in \mathcal{U}$ are rank-one connected as in (3.3) and $\theta \leq \theta_T$, is equal to the lowest energy attainable for deformations that are not constrained on the boundary. The proof of the following theorem also shows that an energy-minimizing sequence can be constructed which is equal to the laminate $w_\gamma(x)$ except for a boundary layer whose thickness converges to zero as $\gamma \to 0$.

Theorem 1 If $F_0 \in \mathcal{U}$ and $F_1 \in \mathcal{U}$ are rank-one connected as in (3.3) and $\theta \leq \theta_T$, then there exist deformations $\hat{w}_\gamma \in W^{\phi}_{F_\lambda}$ defined for $\gamma > 0$ such that

$$\det(\nabla \hat{w}_\gamma(x)) > 0, \qquad \text{for almost all } x \in \Omega$$

and

$$\lim_{\gamma \to 0} \mathcal{E}(\hat{w}_\gamma) = \phi_{\min}(\theta)\text{meas}(\Omega).$$

Proof. The deformation $\hat{w}_\gamma(x)$ that we construct is equal to $w_\gamma(x)$ as defined in (3.36) in the subset

$$\Omega^1_\gamma \equiv \{\, x \in \Omega : \text{dist}(x, \partial\Omega) > \upsilon\gamma \,\},$$

where $\upsilon > 0$ is a constant to be determined to ensure that $\det(\nabla \hat{w}_\gamma(x)) > 0$; $\hat{w}_\gamma(x)$ is equal to $F_\lambda x$ on $\partial\Omega$, and it interpolates between $w_\gamma(x)$ and $F_\lambda x$ on $\Omega \setminus \Omega^1_\gamma$. To construct the interpolation, we define the scalar-valued function $\psi_\gamma(x) : \Omega \to \mathbb{R}$ by

$$\psi_\gamma(x) = \begin{cases} 1 & \text{for all } x \in \Omega^1_\gamma, \\ (\upsilon\gamma)^{-1}\text{dist}(x, \partial\Omega) & \text{for all } x \in \Omega \setminus \Omega^1_\gamma. \end{cases}$$

The function $\psi_\gamma(x)$ is easily seen to satisfy the following properties:

$$\begin{aligned} 0 \leq \psi_\gamma(x) \leq 1 \qquad & \text{for all } x \in \Omega, \\ \psi_\gamma(x) = 1 \qquad & \text{for all } x \in \Omega^1_\gamma, \\ \psi_\gamma(x) = 0 \qquad & \text{for all } x \in \partial\Omega, \\ |\nabla \psi_\gamma(x)| \leq (\upsilon\gamma)^{-1} \qquad & \text{for almost all } x \in \Omega. \end{aligned} \tag{3.40}$$

We define the deformation $\hat{w}_\gamma(x) : \Omega \to \mathbb{R}^3$ by

$$\hat{w}_\gamma(x) \equiv \psi_\gamma(x) w_\gamma(x) + (1 - \psi_\gamma(x)) F_\lambda x \qquad \text{for all } x \in \Omega, \tag{3.41}$$

so we have for $x \in \Omega$ that

$$\nabla \hat{w}_\gamma(x) = (w_\gamma(x) - F_\lambda x) \otimes \nabla \psi_\gamma(x) + \psi_\gamma(x) \nabla w_\gamma(x) + (1 - \psi_\gamma(x))\, F_\lambda.$$

It then follows from (3.37), (3.38), and (3.40) that

$$\begin{aligned} |\hat{w}_\gamma(x) - F_\lambda x| = \psi_\gamma(x)\, |w_\gamma(x) - F_\lambda x| \leq \lambda(1-\lambda)|a|\gamma, \qquad & x \in \Omega, \\ \nabla \hat{w}_\gamma(x) = \nabla w_\gamma(x) \in \{\, F_0,\, F_1 \,\} \subset \mathcal{U}, \qquad & x \in \Omega^1_\gamma, \\ \|\nabla \hat{w}_\gamma(x)\| \leq C, \qquad & \text{almost all } x \in \Omega, \\ \hat{w}_\gamma(x) = F_\lambda x, \qquad & x \in \partial\Omega, \end{aligned} \tag{3.42}$$

where $C > 0$ above and in what follows denotes a generic constant that is independent of γ.

Since ϕ is continuous, it is bounded on bounded sets in $\mathbb{R}^{3\times 3}$. Thus, it

follows from (3.5) and (3.42) that for $\theta \le \theta_T$

$$\begin{aligned}\left|\int_\Omega [\phi(\nabla \hat{w}_\gamma(x),\theta) - \phi_{\min}(\theta)]\,dx\right| &= \int_\Omega [\phi(\nabla \hat{w}_\gamma(x),\theta) - \phi_{\min}(\theta)]\,dx \\ &= \int_{\Omega\setminus\Omega^1_\gamma} [\phi(\nabla \hat{w}_\gamma(x),\theta) - \phi_{\min}(\theta)]\,dx + \int_{\Omega^1_\gamma} [\phi(\nabla \hat{w}_\gamma(x),\theta) - \phi_{\min}(\theta)]\,dx \\ &= \int_{\Omega\setminus\Omega^1_\gamma} [\phi(\nabla \hat{w}_\gamma(x),\theta) - \phi_{\min}(\theta)]\,dx \\ &\le C\gamma \end{aligned} \tag{3.43}$$

since $\text{meas}\,(\Omega \setminus \Omega^1_\gamma) \le C\gamma$.

We next show that

$$\det(\nabla \hat{w}_\gamma(x)) > 0, \qquad \text{for almost all } x \in \Omega, \tag{3.44}$$

for all $\upsilon > 0$ sufficiently large. Since F_0 and F_1 are rank-one connected as in (3.3), we have for any ξ satisfying $0 \le \xi \le 1$ that

$$F_\xi = (1-\xi)F_0 + \xi F_1 = F_0 + \xi a \otimes n = \left(I + \xi a \otimes F_0^{-T} n\right) F_0. \tag{3.45}$$

Hence, we have by (3.45) that

$$\det F_\xi = \left(1 + \xi a \cdot F_0^{-T} n\right) \det F_0 \tag{3.46}$$

for all $0 \le \xi \le 1$. Since F_0, $F_1 \in \mathcal{U}$, it follows from (2.12) that

$$\det F_0 = \det F_1 > 0,$$

so we have from (3.46) that

$$a \cdot F_0^{-T} n = 0, \tag{3.47}$$

and

$$\det F_\xi = \det F_0 \tag{3.48}$$

for all $0 \le \xi \le 1$.

Now, by (3.40) and (3.42),

$$\|(w_\gamma(x) - F_\lambda x) \otimes \nabla \psi_\gamma(x)\| \le C\upsilon^{-1} \qquad \text{for almost all } x \in \Omega, \tag{3.49}$$

and

$$\psi_\gamma(x)\nabla w_\gamma(x) + (1 - \psi_\gamma(x))\,F_\lambda = F_{\xi(x)} \tag{3.50}$$

where

$$\xi(x) = \begin{cases} (1-\psi_\gamma(x))\lambda & \text{if } \nabla w_\gamma(x) = F_0, \\ \psi_\gamma(x) + (1-\psi_\gamma(x))\lambda & \text{if } \nabla w_\gamma(x) = F_1. \end{cases}$$

So, (3.44) follows from (3.49), (3.48), and (3.50) for $\upsilon > 0$ sufficiently large. □

The results of Kohn and Müller (1992*a*, 1992*b* and 1994) for scalar problems with strain gradient surface energies of the form (3.8) show that we can expect the energy-minimizing deformations to have layers that branch in the neighbourhood of the boundary to form infinitesimally small layers, so that the deformation is compatible with the boundary conditions. However, these layers are usually several orders of magnitude smaller than our numerical grid, so the effect of the surface energy is often negligible on macroscopic properties. Our results in Section 6 show that we can approximate the macroscopic properties of energy-minimizing microstructures for the energy (2.2) by solutions obtained on a grid of finite mesh size.

There are affine boundary conditions

$$y(x) = Fx \qquad \text{for all } x \in \partial\Omega$$

for which energy minimization requires a construction more complicated than first-order laminates of the form $w_\gamma(x)$. Higher-order laminates than the first-order laminates $w_\gamma(x)$ are commonly observed (Arlt 1990) and can be constructed from layers of compatible laminates (Bhattacharya 1991, Pedregal 1993, Kohn 1991, Bhattacharya 1992). We shall give a construction of a second-order laminate in Section 3.10. Furthermore, Šverák (1992) has given an energy density for which the *infimum* may only be attained by a microstructure that is not even one of these higher-order laminates, although it is not yet known whether such a property holds for the energy densities used to model martensitic crystals.

3.6. The Young measure and macroscopic densities

The Young measure is a useful device for calculating macroscopic densities from microscopic densities and for describing the pointwise volume fractions of the mixture of the gradient of sequences of energy-minimizing deformations (Tartar 1984, Chipot and Kinderlehrer 1988, Kinderlehrer and Pedregal 1991, Ball and James 1992). We will give a description of the Young measure following most closely the viewpoint of Ball (1989).

We suppose that $\{y_k\} \subset W^\phi$ is a sequence of deformations having uniformly bounded energy $\mathcal{E}(y_k) \leq C$, and enjoying the property that, for any $f \in C(\mathbb{R}^{3\times 3}, \mathbb{R})$ such that $f(F) = o(\|F\|)\|F\|^p$ as $\|F\| \to \infty$, there exists $\tilde{f} \in L^1(\Omega, \mathbb{R})$ so that

$$\lim_{k\to\infty} \int_\omega f(\nabla y_k(x))\,\mathrm{d}x = \int_\omega \tilde{f}(x)\,\mathrm{d}x \tag{3.51}$$

for every measurable set $\omega \subset \Omega$. It can then be shown that there exists a family μ_x of probability measures on $\mathbb{R}^{3\times 3}$, depending measurably on $x \in \Omega$, such that $\tilde{f}(x)$ is given by the formula

$$\tilde{f}(x) = \int_{\mathbb{R}^{3\times 3}} f(F)\,\mathrm{d}\mu_x(F). \tag{3.52}$$

The family of probability measures μ_x is the *Young measure* associated with the sequence y_k. In the above, we note that it follows from the growth condition (2.1) that

$$\int_\Omega \|\nabla v(x)\|^p \, dx \leq C_1^{-1} \int_\Omega \phi(\nabla v(x), \theta) \, dx + C_1^{-1} C_0 \operatorname{meas} \Omega \qquad \text{for all } v \in W^\phi.$$

If a sequence of deformations $y_k \in W^\phi$ with uniformly bounded energy has a Young measure and if for some $y \in W^\phi$ we have that

$$\nabla y_k(x) \to \nabla y(x) \qquad \text{for almost all } x \in \Omega,$$

then we have by (3.51) and the Lebesgue dominated convergence theorem (Rudin 1987) that

$$\lim_{k \to \infty} \int_\omega f(\nabla y_k(x)) \, dx = \int_\omega f(\nabla y(x)) \, dx$$

for all measurable sets $\omega \subset \Omega$ and for all deformations $f \in C_c(\mathbb{R}^{3\times 3}; \mathbb{R})$ where $C_c(\mathbb{R}^{3\times 3}; \mathbb{R})$ denotes the set of continuous deformations $f(F) \in C(\mathbb{R}^{3\times 3}; \mathbb{R})$ with compact support. Thus, it follows from the representation (3.52) that

$$\mu_x = \delta_{\nabla y(x)} \qquad \text{for almost all } x \in \Omega.$$

It can be shown by a compactness argument that every sequence has at least one subsequence with the property that, for every $f \in C(\mathbb{R}^{3\times 3}, \mathbb{R})$ such that $f(F) = o(\|F\|)\|F\|^p$ as $\|F\| \to \infty$, there exists a $\tilde{f} \in L^1(\Omega, \mathbb{R})$ such that (3.51) holds. Thus, every bounded sequence of deformations in W^ϕ contains a subsequence with a Young measure.

The thermodynamic properties of materials, such as energy density and stress, depend nonlinearly on the deformation gradient and can be described by densities $f(F) \in C(\mathbb{R}^{3\times 3}; \mathbb{R})$ (the dependence of f on temperature is suppressed in this paragraph). We can identify $f(\nabla y_k(x))$ with a *microscopic* density and $\tilde{f}(x)$ with the corresponding *macroscopic* density. We observe that the microscopic density $f(\nabla y_k(x))$ can be oscillatory, while the corresponding macroscopic density $\tilde{f}(x)$ is smooth. For example, we have for the energy-minimizing sequence $\hat{w}_{\gamma_k}(x)$ defined by (3.41) that the macroscopic density

$$\tilde{f}(x) = (1 - \lambda) f(F_0) + \lambda f(F_1)$$

is constant for every $f \in C(\mathbb{R}^{3\times 3}, \mathbb{R})$ such that $f(F) = o(\|F\|)\|F\|^p$ as $\|F\| \to \infty$ even though $f(\nabla \hat{w}_{\gamma_k}(x))$ is oscillatory.

For any deformation $y \in W^\phi$, $x \in \Omega$, and $R > 0$, we can define a probability measure on the Borel sets $\Upsilon \subset \mathbb{R}^{3\times 3}$ by

$$\mu_{x,R,\nabla y}(\Upsilon) = \frac{\operatorname{meas} \{\tilde{x} \in B_R(x) : \nabla y(\tilde{x}) \in \Upsilon\}}{\operatorname{meas} B_R(x)} \tag{3.53}$$

where

$$B_R(x) = \{\, \tilde{x} \in \Omega : |\tilde{x} - x| < R\} \,.$$

The probability measure $\mu_{x,R,\nabla y}(\Upsilon)$ gives the volume fraction for which $\nabla y(\tilde{x}) \in \Upsilon$, where $\tilde{x} \in B_R(x)$. We can easily check that

$$\int_{\mathbb{R}^{3\times 3}} f(F)\, \mathrm{d}\mu_{x,R,\nabla y}(F) = \frac{1}{\operatorname{meas} B_R(x)} \int_{B_R(x)} f\left(\nabla y(\tilde{x})\right)\, \mathrm{d}\tilde{x} \tag{3.54}$$

for $f(F) \in C_c(\mathbb{R}^{3\times 3}; \mathbb{R})$, so

$$\mu_{x,R,\nabla y} = \frac{1}{\operatorname{meas} B_R(x)} \int_{B_R(x)} \delta_{\nabla y(\tilde{x})}\, \mathrm{d}\tilde{x}.$$

If y_k is a bounded sequence of deformations in W^{ϕ} with Young measure μ_x, so that (3.51) holds for every $f(F) \in C_c(\mathbb{R}^{3\times 3}; \mathbb{R})$ for $\tilde{f}$ given by (3.52); then it follows from (3.54) that

$$\lim_{k\to\infty} \int_{\mathbb{R}^{3\times 3}} f(F)\, \mathrm{d}\mu_{x,R,\nabla y_k}(F) = \operatorname{meas} B_R(x)^{-1} \int_{B_R(x)} \int_{\mathbb{R}^{3\times 3}} f(F)\, \mathrm{d}\mu_{\tilde{x}}(F)\, \mathrm{d}\tilde{x} = \int_{\mathbb{R}^{3\times 3}} f(F)\, \mathrm{d}\mu_{x,R}(F) \tag{3.55}$$

where

$$\mu_{x,R} \equiv \frac{1}{\operatorname{meas} B_R(x)} \int_{B_R(x)} \mu_{\tilde{x}}\, \mathrm{d}\tilde{x}. \tag{3.56}$$

The result (3.55) can be restated as

$$\mu_{x,R,\nabla y_k} \overset{*}{\rightharpoonup} \mu_{x,R} \qquad \text{as } n \to \infty,$$

where the limit is understood to be in the sense of measures (weak-* convergence). It further follows from (3.56) and the Lebesgue differentiation theorem (Ball 1989) that

$$\mu_{x,R} \overset{*}{\rightharpoonup} \mu_x \qquad \text{as } R \to 0, \text{ for almost all } x \in \Omega.$$

We can thus characterize the Young measure by the result that

$$\lim_{R\to 0} \lim_{k\to\infty} \mu_{x,R,\nabla y_k} = \mu_x.$$

3.7. Computation of the Young measure for a first-order laminate

We next compute the Young measure of the sequence of first-order laminates constructed in Section 3.5. For the energy-minimizing sequence of first-order laminates $\hat{w}_\gamma$ defined by (3.41), we have that if $\Upsilon \subset \mathbb{R}^{3\times 3}$ is an open set with smooth boundary, such that

$$F_0 \notin \Upsilon, \qquad F_1 \notin \Upsilon;$$

then we have by the above construction that

$$\mu_{x,R,\nabla\hat{w}_\gamma}(\Upsilon) \leq \min\left\{\frac{\gamma}{R}, 1\right\}.$$

(In fact, if $B_R(x) \subset \Omega^1_\gamma$, then we have that $\mu_{x,R,\nabla\hat{w}_\gamma}(\Upsilon) = 0$.) Also, if $\Upsilon \subset \mathbb{R}^{3\times 3}$ is an open set with smooth boundary, such that

$$F_0 \in \Upsilon, \qquad F_1 \notin \Upsilon,$$

then

$$\left|\mu_{x,R,\nabla\hat{w}_\gamma}(\Upsilon) - (1-\lambda)\right| \leq \min\left\{\frac{\gamma}{R}, 1\right\};$$

and if $\Upsilon \subset \mathbb{R}^{3\times 3}$ is an open set with smooth boundary such that

$$F_1 \in \Upsilon, \qquad F_0 \notin \Upsilon,$$

then we have that

$$\left|\mu_{x,R,\nabla\hat{w}_\gamma}(\Upsilon) - \lambda\right| \leq \min\left\{\frac{\gamma}{R}, 1\right\}.$$

Thus, we can conclude that for any open set $\Upsilon \subset \mathbb{R}^{3\times 3}$ with smooth boundary $\Upsilon \subset \mathbb{R}^{3\times 3}$, we have that

$$\left|\mu_{x,R,\nabla\hat{w}_\gamma}(\Upsilon) - [(1-\lambda)\delta_{F_0}(\Upsilon) + \lambda\delta_{F_1}(\Upsilon)]\right| \leq \min\left\{\frac{\gamma}{R}, 1\right\} \tag{3.57}$$

where $\delta_F(\Upsilon)$ is the Dirac measure of unit mass at $F \in \mathbb{R}^{3\times 3}$.

It follows from (3.57) that we have for any sequence $\gamma_k \to 0$ that

$$\mu_{x,R} = \lim_{\gamma_k \to 0} \mu_{x,R,\nabla\hat{w}_{\gamma_k}} = (1-\lambda)\delta_{F_0} + \lambda\delta_{F_1}.$$

Hence, we have that the Young measure for the energy-minimizing sequence $\hat{w}_{\gamma_k}(x)$ defined by (3.41) satisfies

$$\mu_x = \lim_{R\to 0} \mu_{x,R} = (1-\lambda)\delta_{F_0} + \lambda\delta_{F_1}.$$

We note that in this special case the Young measure μ_x is independent of $x \in \Omega$, although in general the Young measure depends on $x \in \Omega$.

3.8. The failure of the direct method of the calculus of variations to give an energy-minimizing deformation

The direct method of the calculus of variations is widely used to construct energy-minimizers to variational problems (2.5) by taking the limit of energy-minimizing sequences of deformations (Dacorogna 1989). On the other hand, if $(1-\lambda)F_0 + \lambda F_1 \notin \mathcal{U}$, then we cannot use this technique to construct an energy-minimizing deformation for our models of martensitic crystals, since

we have by (3.43) and (2.18) that

$$\lim_{\gamma\to 0}\int_\Omega \phi\left(\nabla\hat{w}_\gamma(x)\right)\,\mathrm{d}x = \phi_{\min}\mathrm{meas}\,(\Omega) < \phi((1-\lambda)F_0+\lambda F_1)\mathrm{meas}\,(\Omega)$$

$$= \int_\Omega \phi\left(\nabla(F_\lambda x)\right)\,\mathrm{d}x = \int_\Omega \phi(\nabla\left(\lim_{\gamma\to 0}\hat{w}_\gamma(x)\right)\,\mathrm{d}x.$$

This result, together with the fact that $\nabla\hat{w}_\gamma$ converges weakly to F_λ, shows that the functional $\mathcal{E}(y)$ is not *weakly lower semi-continuous* (Dacorogna 1989).

The following lemmas show that $(1-\lambda)F_0+\lambda F_1 \notin \mathcal{U}$ for $0<\lambda<1$ in the orthorhombic to monoclinic case (2.13) and the cubic to tetragonal case (2.15).

Lemma 8 If $F_0 \in \mathcal{U}$ and $F_1 \in \mathcal{U}$ with $F_0 \neq F_1$ are rank-one connected and

$$\left\{ R_iU_1R_i^T : R_i \in \mathcal{G}\right\} = \{U_1, U_2\}\ ,$$

then

$$(1-\lambda)F_0+\lambda F_1 \notin \mathcal{U}$$

for $0<\lambda<1$.

Proof. We prove the result by contradiction, so we assume that $F_0 \in \mathcal{U}$ and $F_1 \in \mathcal{U}$ are rank-one connected and that

$$(1-\lambda)F_0+\lambda F_1 \in \mathcal{U} \tag{3.58}$$

for some $0<\lambda<1$. It follows by Lemma 3 that we may assume that

$$F_0 = R_0U_1 \quad \text{and} \quad F_1 = R_1U_2 \tag{3.59}$$

for R_0, $R_1 \in \mathrm{SO}(3)$ and that we may assume by (3.58) that

$$(1-\lambda)F_0+\lambda F_1 = QU_1 \tag{3.60}$$

for $Q \in \mathrm{SO}(3)$. Since $F_0 \in \mathcal{U}$ and $F_1 \in \mathcal{U}$ are rank-one connected, we have by (3.3) that there exist $a \in \mathbb{R}^3$ and $n \in \mathbb{R}^3$, $|n| = 1$, such that

$$(1-\lambda)F_0+\lambda F_1 = F_0 + \lambda a \otimes n. \tag{3.61}$$

It follows from (3.59)–(3.61) that

$$QU_1 = R_0U_1 + \lambda a \otimes n, \tag{3.62}$$

so it follows from Lemma 3 that $Q = R_0$. Since $0<\lambda<1$, it follows from (3.62) that $a = 0$ and $F_0 = F_1$, which is a contradiction with the hypothesis of the lemma. □

Lemma 9 For the cubic to tetragonal transformation (2.15), if $F_0 \in \mathcal{U}$ and $F_1 \in \mathcal{U}$ are rank-one connected, then

$$(1-\lambda)F_0+\lambda F_1 \notin \mathcal{U}$$

for $0 < \lambda < 1$.

Proof. If $F_0 \in \mathcal{U}$ and $F_1 \in \mathcal{U}$ are rank-one connected, then it follows from Lemma 3 that we may assume without loss of generality that

$$F_1 = RU_2, \qquad F_0 = U_1,$$

for $R \in \mathrm{SO}(3)$, and by Lemma 6 that

$$RU_2 = U_1 + a \otimes n \tag{3.63}$$

where

$$n = \frac{1}{\sqrt{2}}(e_1 + e_2) \quad \text{or} \quad n = \frac{1}{\sqrt{2}}(e_1 - e_2). \tag{3.64}$$

We suppose that $(1-\lambda)F_0 + \lambda F_1 \in \mathcal{U}$. It then follows from the proof of Lemma 8 that

$$(1-\lambda)F_0 + \lambda F_1 \notin \mathcal{U}_1 \cup \mathcal{U}_2,$$

so we conclude that

$$(1-\lambda)F_0 + \lambda F_1 = QU_3 \tag{3.65}$$

for $Q \in \mathrm{SO}(3)$. We next obtain from (3.63) and (3.65) that

$$U_1 + \lambda a \otimes n = QU_3. \tag{3.66}$$

We have thus reached a contradiction with (3.64) since Lemma 6 implies the relation

$$n = \frac{1}{\sqrt{2}}(e_1 \pm e_3)$$

for any solution to (3.66). □

The following result shows that for the orthorhombic to monoclinic case (2.13) and for the cubic to tetragonal case (2.15) there does not exist an energy-minimizing deformation (Ball and James 1992).

Theorem 2 For the orthorhombic to monoclinic case (2.13) and for the cubic to tetragonal case (2.15) there does not exist a deformation $y(x) \in W^{\phi}_{F_\lambda}$ such that

$$\mathcal{E}(y) = \inf_{z \in W^{\phi}_{F_\lambda}} \mathcal{E}(z). \tag{3.67}$$

Proof. We give a proof that covers both the orthorhombic to monoclinic case (2.13) and the cubic to tetragonal case (2.15). We assume that (3.67) holds, so by Theorem 1 (which holds for both the orthorhombic to monoclinic case (2.13) and the cubic to tetragonal case (2.15)) and (3.67) we have that

$$\mathcal{E}(y) = \int_\Omega \phi(\nabla y, \theta)\, \mathrm{d}x = \phi_{\min}(\theta) \mathrm{meas}\, \Omega. \tag{3.68}$$

Since (3.67) holds, we can conclude from Theorem 7 in Section 6 (which also holds for both the orthorhombic to monoclinic case (2.13) and the cubic to tetragonal case (2.15)) that for all $x \in \Omega$ and $R > 0$ we have that

$$\begin{aligned} \text{meas } \{\tilde{x} \in B_R(x) : \nabla y(x) = F_0\} &= (1-\lambda)\,\text{meas } B_R(x), \\ \text{meas } \{\tilde{x} \in B_R(x) : \nabla y(x) = F_1\} &= \lambda\,\text{meas } B_R(x). \end{aligned} \tag{3.69}$$

It then follows from (3.69) that

$$\frac{1}{\text{meas } B_R(x)} \int_{B_R(x)} \nabla y(\tilde{x})\,\mathrm{d}\tilde{x} = (1-\lambda)F_0 + \lambda F_1 = F_\lambda. \tag{3.70}$$

Now y is an element of W^ϕ, so the Lebesgue differentiation theorem (Rudin 1987) implies that

$$\lim_{R\to 0} \frac{1}{\text{meas } B_R(x)} \int_{B_R(x)} \nabla y(\tilde{x})\,\mathrm{d}\tilde{x} = \nabla y(x), \tag{3.71}$$

for almost all $x \in \Omega$. Hence, we can conclude from (3.70), (3.71), and (3.68) that

$$\phi((1-\lambda)F_0 + \lambda F_1, \theta) = \phi_{\min}(\theta),$$

which is a contradiction, since $(1-\lambda)F_0 + \lambda F_1 \notin \mathcal{U}$ by Lemma 8. □

3.9. The austenitic–martensitic interface

Microstructure is observed in phase transformations between the austenitic and the martensitic phases (see Fig. 1). A phase boundary is observed to separate a homogeneous austenitic region from a microstructured martensitic region (Basinski and Christian 1954, Burkart and Read 1953). Ball and James (1987) have shown that this phenomenon can be explained by the geometrically nonlinear continuum theory and Chu and James (1995) have used this theory to explain the austenitic–martensitic phase boundary presented in Fig. 1. The kinematic condition that the martensitic phase be compatible with the austenitic phase imposes a boundary condition similar to that of (3.39).

For the cubic to tetragonal case (2.15), Ball and James (1987) have shown that if

$$\begin{aligned} &\nu_1 < 1 < \nu_2 \text{ and } \tfrac{1}{\nu_1^2} + \tfrac{1}{\nu_2^2} < 2, \\ \text{or } &\nu_2 < 1 < \nu_1 \text{ and } \nu_1^2 + \nu_2^2 < 2, \end{aligned}$$

then the continuum theory predicts that there are fine-scale mixtures of any two variants of the martensite that can be separated from a homogeneous austenitic phase by a planar interface. For example, we can construct the *mixture w_γ using $F_0 = U_1$ and $F_1 = RU_2$ where RU_2 and U_1 are as defined*

in (3.29). By (3.37), $w_\gamma \to F_\lambda x$ uniformly as $\gamma \to 0$. It turns out that for the volume fraction $0 < \lambda^* < 1/2$ given by

$$\lambda^* = \frac{1}{2}\left[1 - \left(2(\nu_2^2 - 1)(\nu_1^2 - 1)(\nu_1^2 + \nu_2^2)(\nu_2^2 - \nu_1^2)^{-2} + 1\right)^{1/2}\right],$$

there exists a continuous deformation with deformation $F_{\lambda^*}x$ on one side of a planar interface with normal m, and the homogeneous austenitic deformation Qx, where $Q \in \mathrm{SO}(3)$, on the opposite side. Here we have used the fact that there is a $Q \in \mathrm{SO}(3)$ and corresponding b, $m \in \mathbb{R}^3$, with $|m| = 1$, such that

$$F_{\lambda^*} = (1 - \lambda^*)U_1 + \lambda^* R U_2 = Q(I + b \otimes m) \tag{3.72}$$

where in the orthonormal basis $\{e_1, e_2, e_3\}$

$$b = (1 + \chi^2 + \tau^2)\,(-\zeta(\chi + \tau),\ \zeta(\chi - \tau),\ \beta)\,,$$
$$m = (1 + \chi^2 + \tau^2)^{-1}\,(-(\chi + \tau),\ (\chi - \tau),\ 1)\,,$$

with

$$\chi = \tfrac{1}{2}\left[(\nu_2^2 + \nu_1^2 - 2)(1 - \nu_1^2)^{-1}\right]^{1/2},$$
$$\tau = \tfrac{1}{2}\left[(2\nu_1^2\nu_2^2 - \nu_1^2 - \nu_2^2)(1 - \nu_1^2)^{-1}\right]^{1/2},$$
$$\zeta = (1 - \nu_1^2)(1 + \nu_2)^{-1},$$
$$\beta = \nu_2(\nu_1^2 - 1)(1 + \nu_2)^{-1}.$$

All of the remaining austenitic–martensitic interfaces can be obtained from (3.72) by symmetry considerations, and we obtain that there are 24 distinct ways a parallel, planar interface can separate the homogeneous austenitic phase from a microstructured martensitic phase.

We say (3.72) represents an austenitic–martensitic interface because Ball and James (1987) have constructed an energy-minimizing sequence u_γ of continuous deformations such that

$$\int_\Omega \phi(\nabla u_\gamma(x), \theta_T)\,dx \to \phi_{\min}(\theta_T)\,\mathrm{meas}\,\Omega \tag{3.73}$$

and $u_\gamma(x) \to u(x)$ uniformly as $\gamma \to 0$, where

$$u(x) = \begin{cases} Qx & \text{for } x \cdot m < 0, \\ F_{\lambda^*}x & \text{for } x \cdot m > 0. \end{cases}$$

We note that

$$\phi_{\min}(\theta_T) = \phi(Q, \theta_T) = \phi(RU_2, \theta_T) = \phi(U_1, \theta_T).$$

We can construct $u_\gamma(x)$ by

$$u_\gamma(x) = \begin{cases} Qx & \text{for } x \cdot m < 0, \\ \psi_\gamma(x)w_\gamma(x) + (1 - \psi_\gamma(x))F_{\lambda^*}x & \text{for } x \cdot m > 0, \end{cases}$$

where $w_\gamma(x)$ is the first-order laminate defined by (3.36), and where

$$\psi_\gamma(x) = \begin{cases} \gamma^{-1} x \cdot m & \text{if } 0 < x \cdot m < \gamma, \\ 1 & \text{if } x \cdot m > \gamma. \end{cases}$$

It is easy to check that $u_\gamma(x)$ satisfies the scaling $u_\gamma(x) = \gamma u_1(\gamma^{-1}x)$ for $\gamma > 0$ and $x \in \mathbb{R}^3$. We also note that we can ensure that $\det \nabla u_\gamma(x) > 0$ almost everywhere by replacing $\psi_\gamma(x)$ by $\psi_\gamma(v^{-1}x)$ in the definition of $u_\gamma(x)$ if the constant $v > 0$ is sufficiently large (*cf.* Theorem 1).

Then $u_\gamma(x)$ satisfies

$$\nabla u_\gamma(x) = \begin{cases} Q & \text{if } x \cdot m < 0, \\ U_1 & \text{if } x \cdot m > \gamma \text{ and } j\gamma \le x \cdot n \le (j + 1 - \lambda^*)\gamma \\ & \quad \text{for some } j \in \mathbb{Z}, \\ RU_2 & \text{if } x \cdot m > \gamma \text{ and } (j + 1 - \lambda^*)\gamma < x \cdot n < (j+1)\gamma \\ & \quad \text{for some } j \in \mathbb{Z}\,, \end{cases}$$

and

$$\begin{aligned} \|\nabla u_\gamma(x)\| &\le C \qquad \text{for almost all } x \in \Omega, \\ |u_\gamma(x) - u(x)| &\le C\gamma, \qquad x \in \Omega, \\ u_\gamma(x) &\in C(\mathbb{R}^3; \mathbb{R}^3). \end{aligned}$$

The estimate (3.73) now follows by the argument (3.43).

The microstructure represented by the deformations $u_\gamma(x)$ for $\gamma \to 0$ is austenite for $x \cdot m < 0$, and is finely twinned martensite for $x \cdot m > 0$ with volume fraction $1 - \lambda^*$ of the deformation gradient U_1 and volume fraction λ^* of the deformation gradient RU_2. The plane of the interface satisfies $x \cdot m = 0$. It is easily checked that any sequence of deformations $u_{\gamma_k}(x)$ with $\gamma_k \to 0$ has the Young measure

$$\mu_x = \begin{cases} \delta_Q & \text{if } x \cdot m < 0, \\ (1 - \lambda^*)\delta_{U_1} + \lambda^* \delta_{RU_2} & \text{if } x \cdot m > 0. \end{cases}$$

Note that $u(x)$ is not an energy-minimizing deformation, since by Lemma 9

$$\phi((1 - \lambda^*)U_1 + \lambda^* RU_2, \theta_T) > \phi(U_1, \theta_T) = \phi(RU_2, \theta_T).$$

The austenitic–martensitic phase transformation has been the subject of many numerical studies (Collins and Luskin 1989, Klouček and Luskin 1994*a*, Klouček and Luskin 1994*b*) since it is one of the primary mechanisms for the creation of microstructure. These numerical studies have been three-dimensional since the following lemma does not seem to allow for an adequate two-dimensional model. Two-dimensional models (Collins et al. 1993) usually represent the martensitic variants by $\mathrm{SO}(2)U_i$ where the eigenvalues $\tilde{\nu}_1^2$, $\tilde{\nu}_2^2$ of $U_i^T U_i$ satisfy $0 < \tilde{\nu}_1^2 \le 1$ and $\tilde{\nu}_2^2 \ge 1$, so the following lemma shows that these variants have a rank-one connection to the matrices $\mathrm{SO}(2)$, which represent the austenitic phase.

Lemma 10 If $U \in \mathbb{R}^{2\times 2}$ and the eigenvalues $\tilde{\nu}_1^2$, $\tilde{\nu}_2^2$ of U^TU satisfy $0 < \tilde{\nu}_1^2 \leq 1$ and $\tilde{\nu}_2^2 \geq 1$, then there exist a rotation $R \in \mathrm{SO}(2)$ and vectors $a \in \mathbb{R}^2$ and $n \in \mathbb{R}^2$, $|n| = 1$, such that

$$RU = I + a \otimes n. \tag{3.74}$$

Proof. Since $U^TU \in \mathbb{R}^{2\times 2}$ has eigenvalues $\tilde{\nu}_1^2$, $\tilde{\nu}_2^2$ such that $0 < \tilde{\nu}_1^2 \leq 1$ and $\tilde{\nu}_2^2 \geq 1$, there exists a $v \in \mathbb{R}^2$, $v \neq 0$, such that

$$|Uv| = |v|.$$

So, there exists $R \in \mathrm{SO}(2)$ such that

$$RUv = v.$$

Hence, for $n \in \mathbb{R}^2$ satisfying $n \cdot v = 0$ and $|n| = 1$, we have that (3.74) holds with $a = RUn - n$. □

3.10. Higher-order laminates

Higher-order laminates of layers within layers are common in martensitic materials. For example, the photomicrograph in Fig. 2 shows a second-order laminate that has been explained by Chu and James (1995) using the geometrically nonlinear continuum theory. More general treatments of higher-order laminates can be found in Kohn and Strang (1986), Kohn (1991) and Pedregal (1993).

Collins (1993*a*) has reported computational results for affine boundary conditions that have a second-order laminate as an optimal microstructure, but do not have a first-order laminate as an optimal laminate. He reported that his algorithm computed a first-order laminate until the mesh was sufficiently fine. He explained this by an argument that the energy associated with the lack of compatibility of the first-order laminate with the boundary conditions is less than the additional energy associated with the additional interfaces needed to represent the second-order laminate until the mesh is sufficiently fine.

We will construct a second-order laminate by layering two first-order laminates. To construct the first-order laminates, we assume that F_{00}, $F_{01} \in \mathcal{U}$ and F_{10}, $F_{11} \in \mathcal{U}$ are pairs of rank-one connected matrices, that is, we assume that there exist a_0, $n_0 \in \mathbb{R}^3$, $|n_0| = 1$, and a_1, $n_1 \in \mathbb{R}^3$, $|n_1| = 1$, such that

$$\begin{aligned} F_{01} &= F_{00} + a_0 \otimes n_0, \\ F_{11} &= F_{10} + a_1 \otimes n_1. \end{aligned}$$

We can construct first-order laminates with layer thickness $\gamma_1 > 0$ and a mixture of F_{i0} with volume fraction $1 - \lambda_i$ and F_{i1} with volume fraction λ_i

following (3.36) by

$$w_{\gamma_1}^{[i]}(x) = \gamma_1 w^{[i]}\left(\frac{x}{\gamma_1}\right) \qquad \text{for all } x \in \mathbb{R}^3$$

where

$$w^{[i]}(x) = F_{i0}x + \left[\int_0^{x\cdot n_i} \chi_i(s)\, \mathrm{d}s\right] a_i \qquad \text{for all } x \in \mathbb{R}^3$$

for $i = 0$, 1 and where $\chi_i(s) : \mathbb{R} \to \mathbb{R}$ is the characteristic function with period 1 defined by

$$\chi_i(s) = \begin{cases} 0 & \text{for all } \ 0 \le s \le 1 - \lambda_i, \\ 1 & \text{for all } \ 1 - \lambda_i < s < 1. \end{cases}$$

We recall that by (3.37) we have that

$$|w_{\gamma_1}^{[i]}(x) - F_{i\lambda_i}x| = \gamma_1 \left| w^{[i]}\left(\frac{x}{\gamma_1}\right) - F_{i\lambda_i}\left(\frac{x}{\gamma_1}\right)\right| \le \lambda_i(1-\lambda_i)|a_i|\gamma_1 \qquad (3.75)$$

for all $x \in \mathbb{R}^3$ where

$$F_{i\lambda_i} = (1-\lambda_i)F_{i0} + \lambda_i F_{i1} = F_{i0} + \lambda_i a_i \otimes n_i$$

for $i = 0, 1$.

We can construct a second-order laminate from the first-order laminates $w_{\gamma_1}^{[i]}(x)$ if there exist $0 \le \lambda_0$, $\lambda_1 \le 1$ such that $F_{0\lambda_0} \in \mathbb{R}^{3\times 3}$ and $F_{1\lambda_1} \in \mathbb{R}^{3\times 3}$ are rank-one connected, that is, there exist a, $n \in \mathbb{R}^3$, $|n| = 1$, such that

$$F_{1\lambda_1} = F_{0\lambda_0} + a \otimes n. \qquad (3.76)$$

If (3.76) holds, then for $2\gamma_1 < \min\{1-\lambda, \lambda\}$ we can construct a second-order laminate for any $0 < \lambda < 1$ by the periodic extension to $\mathbb{R}^3$ of the continuous deformation

$$w_{\gamma_1}(x) = \begin{cases} \psi_{\gamma_1}(x) w_{\gamma_1}^{[0]}(x) + (1 - \psi_{\gamma_1}(x))F_{0\lambda_0}x & \text{for } 0 < x\cdot n < 1-\lambda, \\ \psi_{\gamma_1}(x) w_{\gamma_1}^{[1]}(x) + (1 - \psi_{\gamma_1}(x))F_{1\lambda_1}x & \text{for } 1-\lambda < x\cdot n < 1, \end{cases}$$

where $w_{\gamma_1}^{[i]}(x)$ is the first-order laminate defined by (3.75), and where

$$\psi_{\gamma_1}(x) = \begin{cases} {\gamma_1}^{-1} x\cdot n & \text{if } \ 0 < x\cdot n < \gamma_1, \\ 1 & \text{if } \ \gamma_1 < x\cdot n < 1-\lambda-\gamma_1, \\ {\gamma_1}^{-1}|x\cdot n - (1-\lambda)| & \text{if } \ |x\cdot n - (1-\lambda)| < \gamma_1, \\ 1 & \text{if } \ 1-\lambda+\gamma_1 < x\cdot n < 1-\gamma_1, \\ (\gamma_1)^{-1}|x\cdot n - 1| & \text{if } \ 1-\gamma_1 < x\cdot n < 1. \end{cases}$$

We can scale the second-order laminate $w_{\gamma_1}(x)$ by $\gamma_2 > 0$ to obtain the second-order laminate $w_{\gamma_1\gamma_2}(x)$ defined by

$$w_{\gamma_1\gamma_2}(x) = \gamma_2 w_{\gamma_1}\left(\frac{x}{\gamma_2}\right) \qquad \text{for all } x \in \mathbb{R}^3.$$

As $\gamma_1 \to 0$, the second-order laminate $w_{\gamma_1\gamma_2}(x)$ converges to a mixture with layer thickness γ_2 of the first-order laminate $w_{\gamma_1}^{[0]}(x)$ with volume fraction $1-\lambda$ and of the first-order laminate $w_{\gamma_1}^{[1]}(x)$ with volume fraction λ. The analysis in Section 3.5 can then be used to prove that

$$\left|w_{\gamma_1\gamma_2}(x) - \hat{F}_\lambda x\right| \leq \max\{\lambda_1(1-\lambda_1)|a_1|,\ \lambda_2(1-\lambda_2)|a_2|\}\ \gamma_1\gamma_2$$

for all $x \in \mathbb{R}^3$ where

$$\hat{F}_\lambda = (1-\lambda)F_{0\lambda_0} + \lambda F_{1\lambda_1}.$$

We can check that

$$\|\nabla w_{\gamma_1\gamma_2}(x)\| \leq C \qquad \text{for almost all } x \in \mathbb{R}^3, \tag{3.77}$$

and that

$$\nabla w_{\gamma_1\gamma_2}(x) \in \{F_{00},\ F_{01},\ F_{10},\ F_{11}\} \subset \mathcal{U} \qquad \text{for all } x \in \mathbb{R}^3 \setminus \hat{\Omega}_{\gamma_2} \tag{3.78}$$

where

$$\hat{\Omega}_{\gamma_2} = \bigcup_{j\in\mathbb{Z}} \left\{ x \in \mathbb{R}^3 : |x\cdot n - j\gamma_2| \leq \gamma_1\gamma_2 \text{ or } |x\cdot n - (j+1-\lambda)\gamma_2| \leq \gamma_1\gamma_2 \right\}.$$

Since $\Omega \subset \mathbb{R}^3$ is a bounded domain,

$$\operatorname{meas}(\Omega \cap \hat{\Omega}_{\gamma_2}) \leq C\gamma_1, \tag{3.79}$$

because $\Omega \cap \hat{\Omega}_{\gamma_2}$ is the union of $\mathcal{O}(\gamma_2^{-1})$ non-empty planar layers of thickness $\gamma_1\gamma_2$. (Note that only $\mathcal{O}(\gamma_2^{-1})$ of the sets in the definition of $\hat{\Omega}_{\gamma_2}$ have a non-empty intersection with Ω.) We thus have from (3.77)–(3.79) that for $\theta \leq \theta_T$

$$\begin{aligned}\int_\Omega \phi(\nabla w_{\gamma_1\gamma_2}(x),\theta)\,dx &= \int_{\Omega\setminus\hat{\Omega}_{\gamma_2}} \phi(\nabla w_{\gamma_1\gamma_2}(x),\theta)\,dx + \int_{\Omega\cap\hat{\Omega}_{\gamma_2}} \phi(\nabla w_{\gamma_1\gamma_2}(x),\theta)\,dx \\ &\leq \phi_{\min}(\theta)\operatorname{meas}\Omega + C\gamma_1.\end{aligned}$$

It can also be shown that for any pair of sequences such that $\gamma_{1k} \to 0$ and $\gamma_{2k} \to 0$ as $k \to \infty$ we have that the sequence of deformations $w_{\gamma_{1k}\gamma_{2k}}(x)$ has the Young measure

$$(1-\lambda)(1-\lambda_0)\delta_{F_{00}} + (1-\lambda)\lambda_0\delta_{F_{01}} + \lambda(1-\lambda_1)\delta_{F_{10}} + \lambda\lambda_1\delta_{F_{11}}.$$

Higher-order laminates than second-order can be constructed by iterating the above construction.

4. Finite element methods

We wish to compute an approximation to the microstructure defined by energy-minimizing sequences of deformations to the problem

$$\inf_{y\in\mathcal{A}} \int_\Omega \phi\,(\nabla y(x),\theta)\ \mathrm{d}x, \tag{4.1}$$

where $\mathcal{A}$ denotes a set of admissible deformations. The most accurate finite element method depends on the scale of the microstructure relative to the scale of the mesh and whether it is possible to align the mesh with the microstructure.

4.1. Conforming finite elements

The most commonly used finite element spaces in solid mechanics are conforming spaces that approximate the admissible set of deformations $\mathcal{A}$ by a finite-dimensional subset $\mathcal{A}_h \subset \mathcal{A}$ of continuous deformations which are piecewise polynomials with respect to a finite element mesh. We can compute approximations to energy-minimizing sequences of deformations for problem (4.1) by computing energy-minimizing deformations of the problem

$$\min_{y_h\in\mathcal{A}_h} \int_\Omega \phi\,(\nabla y_h(x),\theta)\ \mathrm{d}x. \tag{4.2}$$

We note that, since $\mathcal{A}_h$ is finite-dimensional and the energy

$$\mathcal{E}(y_h) = \int_\Omega \phi\,(\nabla y_h(x),\theta)\ \mathrm{d}x$$

is continuous, the *infimum* of the energy $\mathcal{E}(y_h)$ is attained for at least one finite element deformation $y_h \in \mathcal{A}_h$, since it follows from the growth property (2.1) that $\phi(F,\theta) \to \infty$ as $\|F\| \to \infty$. The lack of attainment of the *infimum* for the continuous problem (4.1) is the result of the development of arbitrarily fine oscillations by the gradient of energy-minimizing sequences of deformations. The restriction of the admissible deformations to a finite element space limits the possible fineness of the oscillations to the scale of the mesh; therefore, the *infimum* of the energy is attained among deformations which are constrained to lie in the finite element space.

Since deformations with microstructure are typically approximately piecewise linear, the use of piecewise linear or piecewise trilinear elements is a good choice of finite element space for the approximation of microstructure. Although these spaces of continuous finite elements effectively approximate microstructure with layers that are parallel to the planes across which the finite element deformation gradients can be discontinuous, they have difficulty approximating microstructure on the scale of the mesh when the layers are not oriented with respect to the mesh. Computational experiments with the continuous, piecewise linear element for a two-dimensional model have shown

that numerical solutions for microstructure given by conforming spaces have a layer thickness that depends on the orientation of the microstructure with respect to the mesh; see Fig. 3 (below) and Collins (1994).

However, we proved in Section 3 that the number of families of parallel planes (the 'twin planes') across which the deformation gradients of energy-minimizing deformations can be discontinuous is finite, so it is possible for many problems to orient the mesh to the possible twin planes. (By Lemma 5 there are two families of twin planes for the orthorhombic to monoclinic transformation (2.13) and by Lemma 6 there are six families of twin planes for the cubic to tetragonal transformation (2.15).)

Luskin (1996*a*, 1996*b*) has given the use of conforming methods a theoretical validation by giving error estimates for the convergence of the conforming finite element approximation of a laminated microstructure for the rotationally invariant, double well problem ($\mathcal{U} = \mathcal{U}_1 \cup \mathcal{U}_2$), and Li and Luskin (1996) have given error estimates for the finite element approximation of a laminated microstructure for the cubic to tetragonal transformation (2.15). We will give error estimates for this convergence in Section 6.

4.2. Optimization and local minima

It would be most correct to pose the problem of interest as the computation of local minima of the non-convex energy $\mathcal{E}(y) = \int_\Omega \phi(\nabla y(x), \theta)\, dx$ which represent physically observable equilibrium states. The continuous problem (4.1) can be expected to have multiple local minima (Ball et al. 1991, Truskinovsky and Zanzotto 1995, Truskinovsky and Zanzotto 1996), only some of which represent states that can be observed in the laboratory. However, the restriction of our computational interest to global minima is not appropriate, since martensitic crystals typically exhibit hysteresis and meta-stability (Abeyaratne et al. 1994, Ball et al. 1995).

In addition to the local minima which the finite-dimensional problem (4.2) inherits from the continuous problem, there are also local minima created by the numerical discretization, which are the representation of the same microstructure on different length scales and which give the same macroscopic properties.

Gradient iterative methods, which reduce the energy at each iteration, can be used to compute the local minimum corresponding to the energy well of the initial state. Conjugate gradient and other accelerations can be used to develop more efficient iterative methods (Collins and Luskin 1989, Collins 1993*a*, Collins et al. 1993). Since the iterates of gradient methods remain in the energy well of the initial state, the addition of random perturbations to an initial state can be used to explore new local minima (Collins 1993*a*, Collins et al. 1993).

The addition of random perturbations to the initial states for gradient methods suggests the use of more systematic Monte Carlo techniques. Luskin and Ma (1993) used a variant of the simulated annealing algorithm to compute microstructures of fine domains in ferromagnetic crystals. They constructed a discrete set of magnetizations that were close to the set of local minima and then utilized a gradient method to compute the optimal solution within the energy well they had computed with the simulated annealing. The key to the generalization of this algorithm to the case of martensitic crystals is the construction of a discrete set of deformations that represent the energy wells of the martensitic crystal. Kartha et al. (1994) have used a Monte Carlo method to investigate the properties of a two-dimensional model of martensite, and Gremaud (1995) has developed a Monte Carlo method to compute global minima of two-dimensional variational problems with local minima.

To ensure that one computes physically observed states in a quasi-static or dynamical process, one should start with a physically observed state and then compute the change in the state as environmental conditions such as boundary conditions or temperature are varied. For quasi-static processes, continuation methods can be used. For example, Kinderlehrer and Ma (1994*a*, 1994*b*) have used a continuation method to compute hysteresis in the response of a ferromagnetic crystal to changes in the applied magnetic field. The techniques reported in Klouček and Luskin (1994*a*, 1994*b*) for the computation of the dynamics of martensitic crystals offer another possibility for exploring physically observed local minima and hysteretic phenomena by computing the physical dynamics of the response of the crystal to changes in its environment.

4.3. Rotation of the coordinate system

We discussed in Section 4.1 that it can be advantageous to orient the mesh with respect to the planes across which the gradients of energy-minimizing deformations are allowed to be discontinuous. This can often be achieved by rotating the coordinate system describing the reference domain with the mesh fixed in the coordinate system. It is also convenient to rotate the coordinate system with the mesh fixed in the coordinate system to test the effect of the orientation of the finite element mesh with respect to the microstructure.

If we rotate the coordinate system of the reference domain by the rotation $\hat{R}^T$ where $\hat{R} \in \mathrm{SO}(3)$, then the energy density for the crystal in the rotated coordinate system is given by

$$\hat{\phi}(F, \theta) = \phi(F\hat{R}, \theta).$$

For the transformed energy density $\hat{\phi}(F, \theta)$, it follows from (2.18) that for $\theta < \theta_T$ we have that $\hat{\phi}_{\min}(\theta) = \phi_{\min}(\theta)$ and that

$$\hat{\phi}(F, \theta) = \hat{\phi}_{\min}(\theta) \quad \text{if and only if} \quad F \in \mathrm{SO}(3)\hat{U}_1 \cup \cdots \cup \mathrm{SO}(3)\hat{U}_M$$

where

$$\hat{U}_i = \hat{R}U_i\hat{R}^T \qquad \text{for } i = 1, \ldots, M.$$

We also note that we have that

$$QU_i = U_j + a \otimes n \quad \text{if and only if} \quad \hat{Q}\hat{U}_i = \hat{U}_j + \hat{a} \otimes \hat{n}$$

for $Q \in \mathrm{SO}(3)$, $a \in \mathbb{R}^3$, and $n \in \mathbb{R}^3$, where

$$\hat{Q} = \hat{R}Q\hat{R}^T, \quad \hat{a} = \hat{R}a, \quad \hat{n} = \hat{R}n.$$

Hence, it follows that $\hat{n} = \hat{R}n$ is the normal to a plane across which the gradient of an energy-minimizing deformation for the energy density $\hat{\phi}(F, \theta)$ can be discontinuous if and only if n is the normal to a plane across which the gradient of an energy-minimizing deformation for the energy density $\phi(F, \theta)$ can be discontinuous.

4.4. Visualization techniques

The development of techniques to visualize the results of the computation of microstructure has been important to the study of microstructure. It is possible to visualize the deformation by displaying the transformation of the finite element mesh (Collins and Luskin 1989). However, it is generally easier to study microstructure by displaying the deformation gradient.

Several techniques have been developed to visualize the deformation gradient. Collins and Luskin (1989) developed the technique of colouring elements according to the closest energy well to the deformation gradient. They assigned the martensitic variant U_l to a given element K with right Cauchy–Green strain $C(x) = (\nabla y(x))^T \nabla y(x)$ if and only if

$$|C - C_l|_K = \min\{|C - C_1|_K, \ldots, |C - C_M|_K, |C - I|_K, \tau\},$$

where $C_i = U_i^T U_i$, where $\tau > 0$ is a user-supplied sensitivity, and where the matrix norm $|C|_K$ is defined by

$$|C|_K = \left[\frac{1}{\operatorname{meas} K}\int_K \|C(x)\|^2 \, \mathrm{d}x\right]^{1/2}.$$

They assigned the austenitic phase I to the element K if and only if

$$|C - I|_K = \min\{|C - C_1|_K, \ldots, |C - C_M|_K, |C - I|_K, \tau\}.$$

Finally, they assigned the 'unidentified phase' to the element K if it is not assigned to the austenitic or martensitic phases by the above formulae. The different variants of martensite and austenite are then represented by distinct colours or shades of grey. Collins and Luskin (1989) visualized the gradients of three-dimensional deformations by displaying the gradients on a series of parallel cross-sections.

We know from Ball and James (1992), Luskin (1996*a*) and Li and Luskin

(1996) or Theorem 7 that the microstructure which minimizes the energy among deformations constrained on the boundary by the condition

$$y(x) = [(1-\lambda)F_0 + \lambda F_1]\, x \qquad \text{for all } x \in \partial\Omega$$

is a mixture only of the deformation gradients F_0 and F_1 for the orthorhombic to monoclinic transformation (2.13) and for the cubic to tetragonal transformation (2.15) when F_0 and F_1 are rank-one connected, F_0, $F_1 \in \mathcal{U}$, and $\theta < \theta_T$. Thus, for this problem Collins, Luskin and Riordan (1991*b*) and Collins et al. (1993) displayed the interpolant of the function

$$\psi(F)_K = \frac{|F^TF - F_0^TF_0|_K}{|F^TF - F_0^TF_0|_K + |F^TF - F_1^TF_1|_K}$$

defined at the centre of gravity of the elements K to display the proximity of the deformation gradient to the energy wells corresponding to F_0 (where $\psi = 0$) and to F_1 (where $\psi = 1$). They represented the function ψ by a map of $(0,1)$ into colour space or into a grey scale. Other useful variants of the function ψ are given by

$$\tilde{\psi}(F)_K = \frac{|F^TF - F_0^TF_0|_K^2}{|F^TF - F_0^TF_0|_K^2 + |F^TF - F_1^TF_1|_K^2}, \tag{4.3}$$

which increases the range of deformations that are represented to be nearly in the energy wells of F_0 and F_1, and

$$\hat{\psi}(F)_K = \frac{|F - F_0|_K}{|F - F_0|_K + |F - F_1|_K}, \tag{4.4}$$

which measures the proximity of the deformation gradient to F_0 and F_1 rather than to their respective energy wells.

The use of isosurfaces of the energy density and surface energy density was developed and used in Klouček and Luskin (1994*a*, 1994*b*) to identify the austenitic–martensitic interface.

4.5. Numerical experiments for the continuous, piecewise linear approximation of a two-dimensional model

We can investigate the computation of a simple laminated microstructure by a two-dimensional model (Collins and Luskin 1990, Collins et al. 1991*b*, Collins 1993*a*, Collins et al. 1993, Collins 1994). For the two-dimensional model, we have that the reference configuration $\Omega \subset \mathbb{R}^2$, the deformation $y(x) : \mathbb{R}^2 \to \Omega$, and the energy density $\phi(F) : \mathbb{R}^{2\times 2} \to \mathbb{R}$ (where we suppress the dependence of the energy density on temperature). We present in Figs 3 and 4 the results of two-dimensional computations by C. Collins using the continuous, piecewise linear finite element for the problem that will next be described.

The three-dimensional orthorhombic to monoclinic problem (2.13) can be modelled in two dimensions by the energy density

$$\phi(F) = \kappa_1 \left(C_{11} - (1+\eta^2)\right)^2 + \kappa_2 (C_{22} - 1)^2 + \kappa_3 (C_{12}^2 - \eta^2)^2, \tag{4.5}$$

where $C = F^T F$ is the right Cauchy–Green strain and where η, κ_1, κ_2, κ_3 are positive constants. It can then be checked that

$$\phi(F) \geq 0 \qquad \text{for all } F \in \mathbb{R}^{2\times 2},$$

and

$$\phi(F) = 0 \quad \text{if and only if} \quad F \in \mathrm{SO}(2)U_1 \cup \mathrm{SO}(2)U_2 \tag{4.6}$$

where

$$U_1 = I - \eta e_2 \otimes e_1 \qquad \text{and} \qquad U_2 = I + \eta e_2 \otimes e_1$$

for $e_1 \in \mathbb{R}^2$ and $e_2 \in \mathbb{R}^2$ given by the canonical basis

$$e_1 = (1, 0) \qquad \text{and} \qquad e_2 = (0, 1).$$

The proof of Lemma 5 can be used to show that there exists a continuous deformation with a linear interface with normal n separating two regions with constant deformation gradients $F_0 \in \mathrm{SO}(2)U_1$ and $F_1 \in \mathrm{SO}(2)U_2$ if and only if $n = e_1$ or $n = e_2$. It can be checked that the energy density (4.5) does not have a local minimum at deformations $F \in \mathrm{SO}(2)$ representing the austenitic phase. This is a desired property for a two-dimensional model, since otherwise, by Lemma 10, there would be rank-one connections between stress-free deformation gradients representing the martensitic and austenitic phases.

To allow for interfaces with arbitrary orientation with respect to a fixed mesh or coordinate system (see Section 4.3), we define for the rotation $\hat{R} \in \mathrm{SO}(2)$ the energy density

$$\hat{\phi}(F) = \phi(F\hat{R}) \qquad \text{for all } F \in \mathbb{R}^{2\times 2}. \tag{4.7}$$

For this energy density, it follows from (4.6) that

$$\hat{\phi}(F) = 0 \quad \text{if and only if} \quad F \in \mathrm{SO}(2)\hat{U}_1 \cup \mathrm{SO}(2)\hat{U}_2$$

where

$$\hat{U}_1 = I - \eta \hat{e}_2 \otimes \hat{e}_1 \qquad \text{and} \qquad \hat{U}_2 = I + \eta \hat{e}_2 \otimes \hat{e}_1$$

for

$$\hat{e}_1 = \hat{R}e_1 \qquad \text{and} \qquad \hat{e}_2 = \hat{R}e_2.$$

It follows by the above that there exists a continuous deformation with a linear interface with normal $\hat{n}$ separating two regions with constant deformation gradients $F_0 \in \mathrm{SO}(2)\hat{U}_1$ and $F_1 \in \mathrm{SO}(2)\hat{U}_2$ if and only if $\hat{n} = \hat{e}_1 = \hat{R}e_1$ or $\hat{n} = \hat{e}_2 = \hat{R}e_2$.

We now give computational results for the approximations to the energy-minimizing microstructure for the energy

$$\int_\Omega \hat{\phi}(\nabla y(x))\,\mathrm{d}x \tag{4.8}$$

for the reference configuration $\Omega = (0, 1) \times (0, 1)$ where the deformation $y(x)$ is constrained on the boundary by

$$y(x) = \left[\frac{1}{2}\hat{U}_1 + \frac{1}{2}\hat{U}_2\right] x, \qquad x \in \partial\Omega. \tag{4.9}$$

All of the results in Section 6 hold for the two-dimensional problem (4.7)–(4.9), so we can conclude that the gradients of energy-minimizing sequences of deformations to the two-dimensional problem (4.7)–(4.9) computed using the continuous, piecewise linear finite element approximation on a uniform mesh converge to the Young measure

$$\nu_x = \frac{1}{2}\delta_{\hat{U}_1} + \frac{1}{2}\delta_{\hat{U}_2}.$$

In Fig. 3, we present Collins' numerical results for the approximation of an energy-minimizing microstructure to the problem (4.7)–(4.9) with $\hat{R} = R(45°)$ (where $R(\theta)$ denotes the rotation matrix of θ degrees) by the piecewise linear finite element approximation on a uniform mesh of size $h = 1/N$ where $N = 16, 32, 64$. Thus, we have that the lines that can separate regions with constant deformation gradients $\hat{U}_1$ and $\hat{U}_2$ have normal

$$\hat{n} = \hat{e}_1 = \frac{1}{\sqrt{2}}(e_1 + e_2),$$

and are parallel to lines along which the gradients of deformations in the finite element space are allowed to be discontinuous.

The optimization problem was solved by the Polak–Ribière conjugate gradient method (Polak 1971, Glowinski 1984) with initial data

$$y_{init}(x) = \left[\frac{1}{2}\hat{U}_1 + \frac{1}{2}\hat{U}_2\right] x + \frac{1}{2}\eta h r(x) \qquad \text{for all } x \in \Omega, \tag{4.10}$$

where h is the mesh size and where $r(x) = (r_1(x), r_2(x))$ was obtained by getting values for $r_i(x)$ on the interior vertices from a random number generator for the interval $(-1, 1)$ and then extending $r_i(x)$ to all of Ω by interpolation. We note that $\|\nabla[\eta h r(x)]\| = \mathcal{O}(1)$, so the deformation gradients of the initial state need not be close to the energy wells.

To visualize the results of the computations of microstructure, we use the function $\hat{\psi}$ defined by (4.4) with $F_0 = U_1$ and $F_1 = U_2$ and enhanced by the continuous function

$$g(\varsigma) = \begin{cases} \frac{1}{2}(2\varsigma)^2 & \text{for } 0 \le \varsigma < \frac{1}{2}, \\ 1 - \frac{1}{2}(2(1-\varsigma))^2 & \text{for } \frac{1}{2} \le \varsigma \le 1. \end{cases}$$

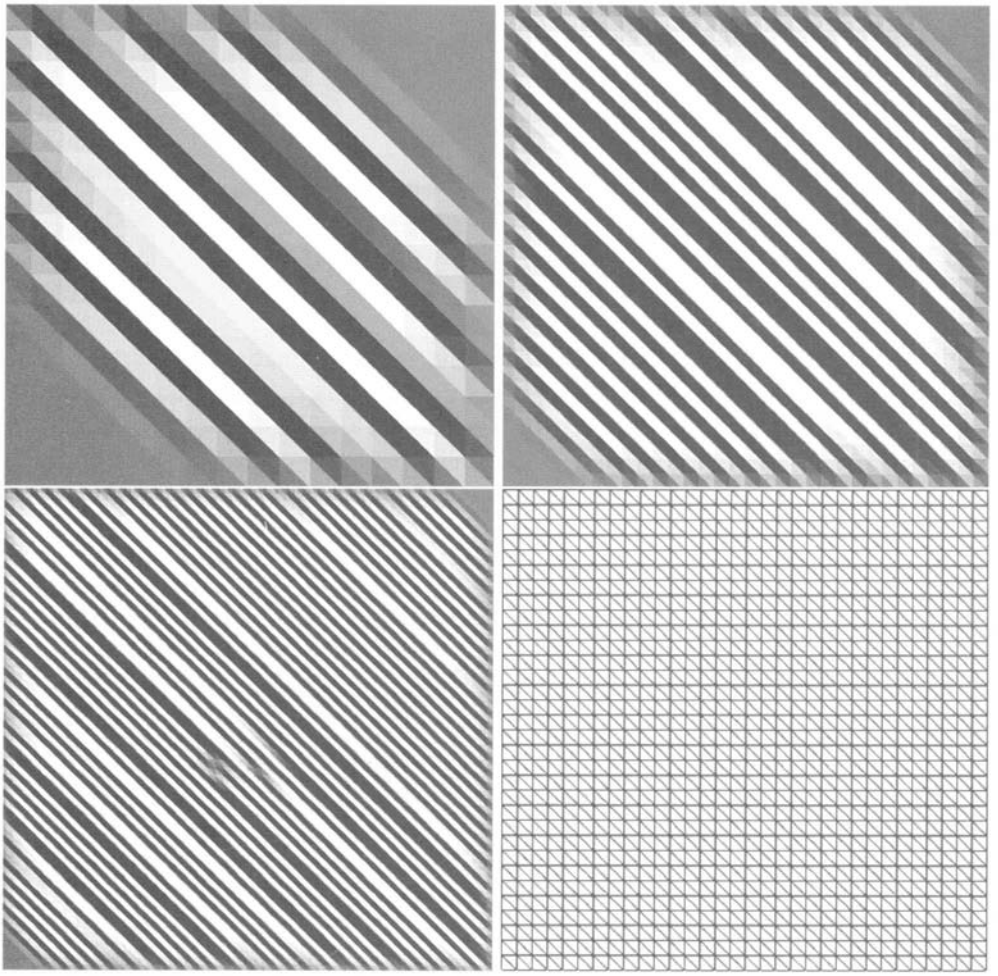

Fig. 3. Deformation gradients for the problem (4.7)–(4.9) with $\eta = .1$ and $\hat{R} = R(45°)$ computed by continuous, piecewise linear finite elements for a uniform finite element mesh of size $h = 1/N$ with $N = 16, 32, 64$. The finite element mesh for $N = 32$ is shown. Courtesy of C. Collins.

We display a map from $g(\hat{\psi}(F))$ into a grey scale so that elements are coloured white if $g(\hat{\psi}(F)) = 0$ (corresponding to $F = U_1$) and elements are coloured black if $g(\hat{\psi}(F)) = 1$ (corresponding to $F = U_2$).

We see in Fig. 3 that microstructure has been obtained on the scale of each successively refined mesh. Since the computed microstructure shown in Fig. 3 is not completely regular, a local minimum of the finite element optimization problem has been computed and not a global minimum. However, the energy of the computed local minimum is close enough to that of a global minimum to give the microstructure and the macroscopic properties of a global minimum.

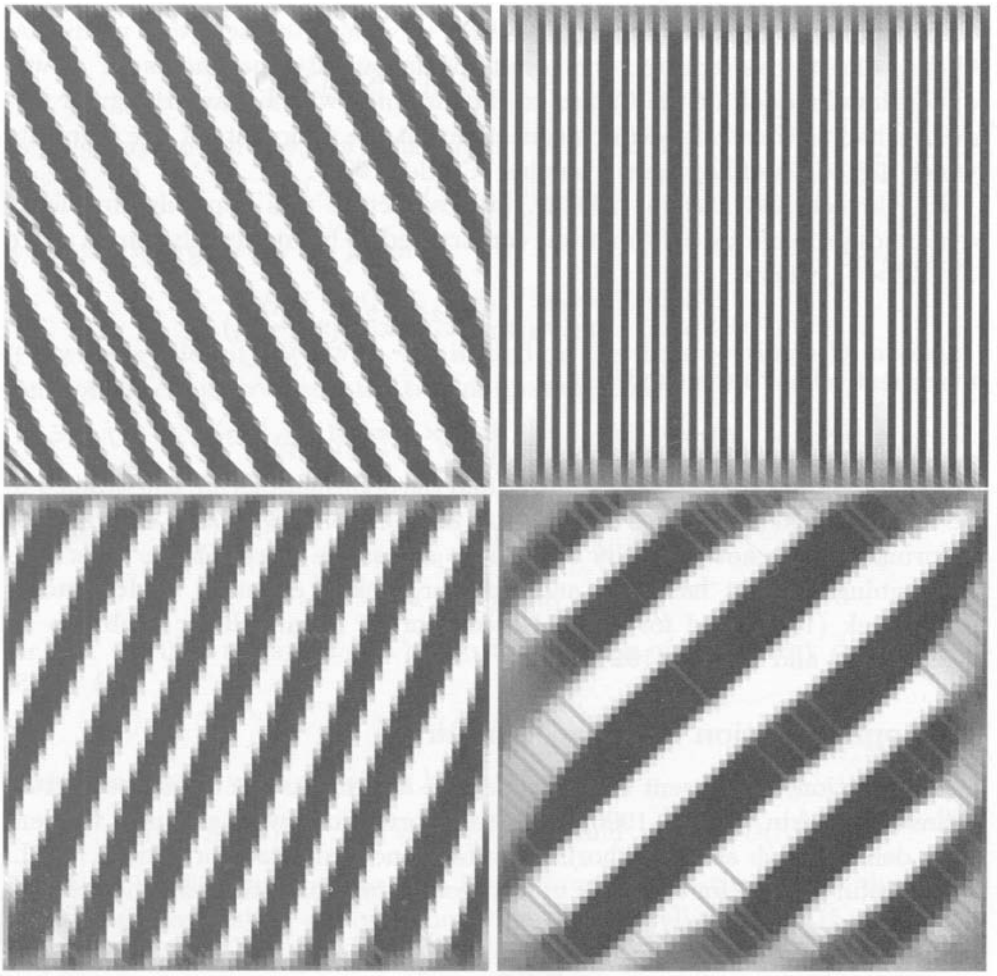

Fig. 4. Deformation gradients for the problem (4.7)–(4.9) with $\eta = .5$ and the mesh $N = 64$ for the orientation defined by $\hat{R} = R(\theta)$ with $\theta = 25°, 0°, -25°, -45°$. Courtesy of C. Collins.

The results in Fig. 4 illustrate the effect of mesh orientation with respect to the lines of discontinuity of the deformation gradient. We see that the layers are several mesh widths thick when they are not oriented with respect to the mesh.

4.6. Nonconforming finite elements

An alternative approach is that given by the use of non-conforming finite elements (Ciarlet 1978, Quarteroni and Valli 1994), that is, $\mathcal{A}_h \not\subset \mathcal{A}$. The use of non-conforming finite elements is intuitively appealing for problems with microstructure because the admissible finite element deformations should

then have more flexibility to approximate oscillatory deformation gradients. Collins (1994) has reported the results of numerical experiments for a two-dimensional model for the Crouzeix–Raviart piecewise linear, triangular element which is constrained to be continuous at the midpoints of line segments which are edges of adjacent triangles (Ciarlet 1978).

In Klouček and Luskin (1994*a*), microstructure was approximated for a dynamics problem by deformations constrained to be in the polynomial space $\mathcal{P} \times \mathcal{P} \times \mathcal{P}$, where

$$\mathcal{P} = \text{Span}\,\{\,1, x_1, x_2, x_3, (x_1^2 - x_2^2), (x_1^2 - x_3^2)\,\}$$

when restricted to the subdomains

$$\Omega_{ijk} = ((i-1)h_1, ih_1) \times ((j-1)h_2, jh_2) \times ((k-1)h_3, kh_3), \qquad i, j, k \in \mathbb{Z},$$

where h_1, h_2, h_3 are the mesh lengths, and the deformations are constrained to be continuous at the centres of gravity of the faces of Ω_{ijk}. These approximate deformations are not generally continuous across the faces of Ω_{ijk}. This non-conforming element has been analysed for Stokes' equation by Rannacher and Turek (1992) and for general second-order linear elliptic problems by Klouček, Li and Luskin (1996).

5. Approximation of microstructure

In this section, we present estimates for the approximation of microstructure following Luskin (1996*a*, 1996*b*) (for transformations with a double well energy density, such as the orthorhombic to monoclinic transformation) and Li and Luskin (1996) (for the cubic to tetragonal transformation) for the problem

$$\inf_{v \in W^{\phi}_{F_\lambda}} \mathcal{E}(v), \tag{5.1}$$

where we recall that

$$W^{\phi}_{F_\lambda} = \left\{ v \in W^{\phi} : v(x) = F_\lambda x \text{ for } x \in \partial\Omega \right\}$$

for $F_\lambda = (1-\lambda)F_0 + \lambda F_1$ and where $F_0 \in \mathcal{U}$ and $F_1 \in \mathcal{U}$ satisfy the rank-one condition that there exist $a \in \mathbb{R}^3$ and $n \in \mathbb{R}^3$, $|n| = 1$, such that

$$F_1 = F_0 + a \otimes n. \tag{5.2}$$

We will assume in this section that $\theta < \theta_T$ and that the energy density $\phi(F, \theta)$ is minimized either on two rotationally invariant energy wells (such as given by the orthorhombic to monoclinic transformation (2.13)) or on the three rotationally invariant wells of the cubic to tetragonal transformation (2.15). The proofs of the main results in this section are given in Luskin (1996*a*) and Li and Luskin (1996).

We recall that if the energy density $\phi(F, \theta)$ is minimized on two rotationally

invariant wells (the double well case), then

$$\left\{ R_i U_1 R_i^T : R_i \in \mathcal{G} \right\} = \{ U_1, U_2 \} , \tag{5.3}$$

so the energy density $\phi(F, \theta)$ has minima at $F \in \mathcal{U}$ for

$$\mathcal{U} = \mathcal{U}_1 \cup \mathcal{U}_2$$

where the energy wells are given by

$$\mathcal{U}_1 = \mathrm{SO}(3) U_1 \quad \text{and} \quad \mathcal{U}_2 = \mathrm{SO}(3) U_2.$$

If the energy density $\phi(F, \theta)$ is minimized on the three rotationally invariant wells of the cubic to tetragonal transformation, then

$$\left\{ R_i U_1 R_i^T : R_i \in \mathcal{G} \right\} = \{ U_1, U_2, U_3 \}$$

where

$$\begin{aligned} U_1 = \nu_1 I + (\nu_2 - \nu_1) e_1 \otimes e_1, \qquad U_2 = \nu_1 I + (\nu_2 - \nu_1) e_2 \otimes e_2, \\ U_3 = \nu_1 I + (\nu_2 - \nu_1) e_3 \otimes e_3 \end{aligned} \tag{5.4}$$

for $0 < \nu_1$, $0 < \nu_2$, and $\nu_1 \neq \nu_2$, so the minima of the energy density are $F \in \mathcal{U}$ for

$$\mathcal{U} = \mathcal{U}_1 \cup \mathcal{U}_2 \cup \mathcal{U}_3$$

where the energy wells are given by

$$\mathcal{U}_1 = \mathrm{SO}(3) U_1, \quad \mathcal{U}_2 = \mathrm{SO}(3) U_2, \quad \text{and} \quad \mathcal{U}_3 = \mathrm{SO}(3) U_3.$$

All of the results given in Sections 5 and 6 on error estimates for the finite element approximation apply to both the double well problem (5.3) and to the cubic to tetragonal problem (5.4).

Since $F_0 \in \mathcal{U}$ and $F_1 \in \mathcal{U}$ satisfy the rank-one condition (5.2), it follows from Lemma 3, Lemma 5, and Lemma 6 that we may assume without loss of generality for both the double well problem (5.3) and the cubic to tetragonal problem (5.4) that

$$F_0 \in \mathcal{U}_1 \qquad \text{and} \qquad F_1 \in \mathcal{U}_2.$$

We will also assume in this section without loss of generality that

$$\phi_{\min}(\theta) = 0 \tag{5.5}$$

(by replacing $\phi(F, \theta)$ by $\phi(F, \theta) - \phi_{\min}(\theta)$). Also, in what follows we shall not explicity denote the dependence of ϕ, $\mathcal{E}$, and $\mathcal{U}_i$ on the temperature θ.

The results in this section give a bound for $v \in W^{\phi}_{F_\lambda}$ in terms of $\mathcal{E}(v) = \int_\Omega \phi(\nabla v(x)\, \theta)\, dx$. Since we proved in Theorem 1 that

$$\inf_{v \in W^{\phi}_{F_\lambda}} \mathcal{E}(v) = 0,$$

all of the results in this section give related results for the convergence of energy-minimizing sequences. In Section 6 we will give an estimate for

$$\inf_{v_h \in \mathcal{A}_{h,F_\lambda}} \mathcal{E}(v_h),$$

where $\mathcal{A}_{h,F_\lambda}$ is a conforming finite element approximation to $W^\phi_{F_\lambda}$, which is then used to give estimates for the finite element approximation of microstructure.

We shall also assume that ϕ grows quadratically away from the energy wells, that is, we shall assume that there exists $\kappa > 0$ such that

$$\phi(F) \geq \kappa \|F - \pi(F)\|^2 \qquad \text{for all } F \in \mathbb{R}^{3\times 3} \tag{5.6}$$

where $\pi : \mathbb{R}^{3\times 3} \to \mathcal{U}$ is a Borel measurable projection defined by

$$\|F - \pi(F)\| = \min_{U \in \mathcal{U}} \|F - U\|.$$

The projection π exists since $\mathcal{U}$ is compact, although the projection is not uniquely defined at $F \in \mathbb{R}^{3\times 3}$ where the minimum above is attained at more than one $U \in \mathcal{U}$. We also define the Borel measurable projection $\pi_{1,2} : \mathbb{R}^{3\times 3} \to \mathcal{U}_1 \cup \mathcal{U}_2$ by

$$\|F - \pi_{1,2}(F)\| = \min_{U \in \mathcal{U}_1 \cup \mathcal{U}_2} \|F - U\|. \tag{5.7}$$

We note that $\pi = \pi_{1,2}$ in the double well case (5.3), but that $\pi \neq \pi_{1,2}$ in the cubic to tetragonal case (5.4) since $\mathcal{U} \neq \mathcal{U}_1 \cup \mathcal{U}_2$. We shall also find it useful to utilize the operators $R(F) : \mathbb{R}^{3\times 3} \to \mathrm{SO}(3)$ and $\Pi : \mathbb{R}^{3\times 3} \to \{F_0, F_1\}$, which are defined by the relation

$$\pi_{1,2}(F) = R_{1,2}(F)\Pi_{1,2}(F) \qquad \text{for all } F \in \mathbb{R}^{3\times 3}. \tag{5.8}$$

The following theorem demonstrates that the directional derivatives orthogonal to n (where $F_1 = F_0 + a \otimes n$) of sequences of energy-minimizing deformations converge strongly in L^2. It is crucial to the proof of all of the other results.

Theorem 3 If $w \in \mathbb{R}^3$ satisfies $w \cdot n = 0$, then there exists a positive constant C such that

$$\int_\Omega |(\nabla v(x) - F_\lambda)w|^2 \, \mathrm{d}x \leq C\mathcal{E}(v)^{1/2} + C\mathcal{E}(v) \qquad \text{for all } v \in W^\phi_{F_\lambda}. \tag{5.9}$$

Proof. See Luskin (1996*a*) for the case of two rotationally invariant energy wells (5.3) and Li and Luskin (1996) for the case of three rotationally invariant energy wells given by the cubic to tetragonal transformation (5.4). □

It follows from the convergence of the directional derivatives orthogonal to n of energy-minimizing sequences of deformations and the Poincaré inequality (Wloka 1987) that energy-minimizing sequences of deformations converge in L^2.

Corollary 1 There exists a positive constant C such that

$$\int_\Omega |v(x) - F_\lambda x|^2 \, dx \leq C\mathcal{E}(v)^{1/2} + C\mathcal{E}(v) \qquad \text{for all } v \in W^\phi_{F_\lambda}. \tag{5.10}$$

For the double well case (5.3), it follows trivially from the quadratic growth of the energy density away from the energy wells (5.6) that the deformation gradients of energy-minimizing sequences converge to the union of the energy wells $\mathcal{U} = \mathcal{U}_1 \cup \mathcal{U}_2$. However, for the cubic to tetragonal case (5.4) the proof of this result relies on the bound for the directional derivatives orthogonal to n given by Theorem 3. We state this result in the following Theorem.

Theorem 4 For the double well case (5.3) we have the estimate

$$\int_\Omega \|\nabla v(x) - \pi_{1,2}(\nabla v(x))\|^2 \, dx \leq \kappa^{-1}\mathcal{E}(v) \qquad \text{for all } v \in W^\phi_{F_\lambda}.$$

For the cubic to tetragonal transformation (5.4), there exists a positive constant C such that

$$\int_\Omega \|\nabla v(x) - \pi_{1,2}(\nabla v(x))\|^2 \, dx \leq C\mathcal{E}^{1/2}(v) + C\mathcal{E}(v) \qquad \text{for all } v \in W^\phi_{F_\lambda}.$$

Proof. The proof for the double well case (5.3) follows trivially from the quadratic growth of the energy density away from the energy wells (5.6). See Li and Luskin (1996) for the proof in the cubic to tetragonal case (5.4). □

The next theorem shows that the gradients of energy-minimizing sequences of deformations converge weakly to F_λ. It is a consequence of the convergence of the deformations in L^2.

Theorem 5 If $\omega \subset \Omega$ is a smooth domain, then there exists a positive constant C such that

$$\left\| \int_\omega (\nabla v(x) - F_\lambda) \, dx \right\| \leq C\mathcal{E}(v)^{1/8} + C\mathcal{E}(v)^{1/2} \qquad \text{for all } v \in W^\phi_{F_\lambda}.$$

Proof. The proof for the double well case (5.3) is given in Luskin (1996*a*), and the proof for the cubic to tetragonal transformation (5.4) is given in Li and Luskin (1996). □

The following theorem shows that the gradients of energy-minimizing sequences converge to the set $\{F_0, F_1\}$. The proof relies on the bound for the directional derivatives orthogonal to n given in Theorem 3.

Theorem 6 We have the estimate

$$\int_\Omega \|\nabla v(x) - \Pi_{1,2}(\nabla v(x))\|^2 \, dx \leq C\mathcal{E}(v)^{1/2} + C\mathcal{E}(v) \qquad \text{for all } v \in W^\phi_{F_\lambda}.$$

Proof. See Luskin (1996*a*) for the case of two rotationally invariant energy wells (5.3) and Li and Luskin (1996) for the case of three rotationally invariant energy wells given by the cubic to tetragonal transformation (5.4). □

The next theorem states that in any smooth domain $\omega \subset \Omega$ and for any energy-minimizing sequence the volume fraction that $\nabla v(x)$ is near F_0 converges to $1 - \lambda$ and the volume fraction that $\nabla v(x)$ is near F_1 converges to λ. This result follows from the weak convergence of the deformation gradients (see Theorem 5) and the convergence of the deformation gradients to the set $\{F_0, F_1\}$ (see Theorem 6). We recall from Theorem 2 that the result of the following theorem implies that there does not exist an energy-minimizing deformation $y \in W^{\phi}_{F_\lambda}$ to the problem (5.1).

To make the result of the following theorem precise, we define for any smooth domain $\omega \subset \Omega$, $\rho > 0$, and $v \in W^{\phi}_{F_\lambda}$, the sets

$$\omega^0_\rho = \omega^0_\rho(v) = \{ x \in \omega : \Pi_{1,2}(\nabla v(x)) = F_0 \text{ and } \|F_0 - \nabla v(x)\| < \rho \} ,$$
$$\omega^1_\rho = \omega^1_\rho(v) = \{ x \in \omega : \Pi_{1,2}(\nabla v(x)) = F_1 \text{ and } \|F_1 - \nabla v(x)\| < \rho \} .$$

We can then use Theorem 5 and Theorem 6 to prove the following theorem which describes the convergence of the microstructure (or Young measure) of the deformation gradients of energy minimizing sequences.

Theorem 7 For any smooth domain $\omega \subset \Omega$ and any $\rho > 0$ we have that

$$\left| \frac{\text{meas } \omega^0_\rho(v)}{\text{meas } \omega} - (1 - \lambda) \right| \leq C\mathcal{E}(v)^{1/8} + C\mathcal{E}(v)^{1/2}, \tag{5.11}$$

$$\left| \frac{\text{meas } \omega^1_\rho(v)}{\text{meas } \omega} - \lambda \right| \leq C\mathcal{E}(v)^{1/8} + C\mathcal{E}(v)^{1/2} \tag{5.12}$$

for all $v \in W^{\phi}_{F_\lambda}$. The constants C in the estimates (5.11) and (5.12) are independent of $v \in W^{\phi}_{F_\lambda}$, but they depend on ω and ρ.

Proof. The proof for the double well case (5.3) is given in Luskin (1996*a*), and the proof for the cubic to tetragonal transformation (5.4) is given in Li and Luskin (1996). □

We have by the compactness of $\text{SO}(3)U_1$ and $\text{SO}(3)U_2$ that there exists a positive constant ρ_0 such that

$$\text{dist}\,(\text{SO}(3)U_1, \text{SO}(3)U_2) = \rho_0 > 0 \tag{5.13}$$

where

$$\text{dist}\,(\text{SO}(3)U_1, \text{SO}(3)U_2) = \min \{ \|V_1 - V_2\| : V_1 \in \text{SO}(3)U_1, V_2 \in \text{SO}(3)U_2 \}.$$

By the definition of $\pi_{1,2}$ (see (5.7)) and the definition of $\Pi_{1,2}$ (see (5.8)), we have for $0 < \rho < \rho_0/2$ that

$$\|F_i - F\| < \rho \qquad \text{implies that} \qquad \Pi_{1,2}(F) = F_i$$

for all $F \in \mathbb{R}^{3\times 3}$ and $i \in \{0, 1\}$. Thus, for any $0 < \rho < \rho_0/2$, any smooth

domain $\omega \subset \Omega$, any $v \in W^{\phi}$, and any $i \in \{0, 1\}$ we have that

$$\omega_{\rho}^{i}(v) = \{ x \in \omega : \nabla v(x) \in \mathcal{B}_{\rho}(F_i) \} ,$$

where the set $\mathcal{B}_{\rho}(F)$ for $\rho > 0$ and $F \in \mathbb{R}^{3\times 3}$ is defined by

$$\mathcal{B}_{\rho}(F) = \left\{ G \in \mathbb{R}^{3\times 3} : \|G - F\| < \rho \right\} .$$

Hence, it follows from the definition of the probability measure $\mu_{x,R,\nabla v}(\Upsilon)$ given by (3.53) that we have for $x \in \Omega$, $R > 0$, $v \in W^{\phi}$, and $0 < \rho < \rho_0/2$ that

$$\mu_{x,R,\nabla v}\left(\mathcal{B}_{\rho}(F_i)\right) = \frac{\operatorname{meas} \omega_{\rho}^{i}(v)}{\operatorname{meas} \omega} \tag{5.14}$$

for $\omega = B_R(x)$.

The following corollary is a direct consequence of Theorem 7 and the identity (5.14) and implies the result on the uniqueness of the Young measure for energy-minimizing sequences of the problem (5.1) that was given by Ball and James (1992).

Corollary 2 If $x \in \Omega$, $R > 0$, and $\rho < \rho_0/2$, where ρ_0 is given by (5.13), then there exists a positive constant C such that

$$|\mu_{x,R,\nabla v}\left(\mathcal{B}_{\rho}(F_0)\right) - (1 - \lambda)| \leq C\mathcal{E}(v)^{1/8} + C\mathcal{E}(v)^{1/2},$$
$$|\mu_{x,R,\nabla v}\left(\mathcal{B}_{\rho}(F_1)\right) - \lambda| \leq C\mathcal{E}(v)^{1/8} + C\mathcal{E}(v)^{1/2}$$

for all $v \in W_{F_\lambda}^{\phi}$.

Next, we show that the estimates for the weak convergence of the deformation gradients (see Theorem 5) and the convergence of the deformation gradients to the set $\{F_0, F_1\}$ (see Theorem 6) can be used to give estimates for the nonlinear integrals of $\nabla v(x)$ that approximate macroscopic densities.

For linear transformations $\mathcal{L} : \mathbb{R}^{3\times 3} \to \mathbb{R}$ we define the operator norm

$$|\mathcal{L}| = \max_{\|F\|=1} |\mathcal{L}(F)|,$$

and for uniformly Lipschitz functions $g(F) : \mathbb{R}^{3\times 3} \to \mathbb{R}$ we define the function norm

$$\left\| \frac{\partial g}{\partial F} \right\|_{L^{\infty}} = \operatorname{ess\,sup}_{B \in \mathbb{R}^{3\times 3}} \left\| \frac{\partial g}{\partial F}(B) \right\| .$$

We will give estimates of nonlinear integrals of $\nabla v(x)$ for the Sobolev space $\mathcal{V}$ of measurable functions $f(x, F) : \Omega \times \mathbb{R}^{3\times 3} \to \mathbb{R}$ such that

$$\int_{\Omega} \left[\left\| \frac{\partial f}{\partial F}(x, \cdot) \right\|_{L^{\infty}}^{2} + |\nabla G(x) \cdot n|^2 + G(x)^2 \right] \mathrm{d}x < \infty$$

where

$$G(x) = f(x, F_1) - f(x, F_0).$$

We note that if $f(x,F) \in \mathcal{V}$, then $f(x,F)$ is Lipschitz continuous as a function of $F \in \mathbb{R}^{3\times 3}$ for almost all $x \in \Omega$.

Theorem 8 We have for all $v \in W^{\phi}_{F_\lambda}$ and all functions $f(x,F) \in \mathcal{V}$ that

$$\left| \int_\Omega f\left(x, \nabla v(x)\right) - \left[(1-\lambda) f(x,F_0) + \lambda f(x,F_1)\right] \, \mathrm{d}x \right| \leq$$

$$C \left\{ \int_\Omega \left\| \frac{\partial f}{\partial F}(x,\cdot) \right\|^2_{L^\infty} + |\nabla G(x) \cdot n|^2 + G(x)^2 \, \mathrm{d}x \right\}^{1/2} \left(\mathcal{E}(v)^{1/4} + \mathcal{E}(v)^{1/2} \right)$$

where

$$G(x) = f(x,F_1) - f(x,F_0).$$

Proof. See Luskin (1996*a*) for the case of two rotationally invariant energy wells (5.3) and Li and Luskin (1996) for the case of three rotationally invariant energy wells given by the cubic to tetragonal transformation (5.4). □

6. Numerical analysis of microstructure

We shall give in this section error estimates for the finite element approximation of a laminated microstructure for rotationally invariant, double well energy densities (Luskin 1996*a*, 1996*b*) and for energy densities for the cubic to tetragonal transformation (Li and Luskin 1996). These error estimates follow directly from the approximation theory given in Section 5 and the theorem proved in this section for the *infimum* of the energy

$$\inf_{v_h \in \mathcal{A}_{h,F_\lambda}} \mathcal{E}(v_h)$$

where $\mathcal{A}_{h,F_\lambda}$ is a conforming finite element space. We shall assume that all of the assumptions described in Section 5 hold.

6.1. Properties of the conforming finite element approximation

We now define the properties of conforming finite element spaces required for our analysis of microstructure in Section 6. We assume that τ_h for $0 < h < h_0$ is a family of decompositions of Ω into polyhedra $\{K\}$ such that (Quarteroni and Valli 1994):

1 $\bar{\Omega} = \cup_{K\in\tau_h} K$;
2 interior $K_1 \cap$ interior $K_2 = \emptyset$ if $K_1 \neq K_2$ for $K_1,\ K_2 \in \tau_h$;
3 if $S = K_1 \cap K_2 \neq \emptyset$ for $K_1 \neq K_2,\ K_1,\ K_2 \in \tau_h$, then S is a common face, edge, or vertex of K_1 and K_2;
4 diam $K \leq h$ for all $K \in \tau_h$.

The admissible deformations have finite energy and are constrained on the part of the boundary where the deformation of the crystal is given. Hence, we

have by (2.4) that our family of conforming finite element spaces, $\mathcal{A}_h$, defined for mesh diameters in the range $0 < h < h_0$, satisfies

$$\mathcal{A}_h \subset \mathcal{A} \subset W^{\phi} \subset W^{1,p}(\Omega;\mathbb{R}^3) \subset C(\bar{\Omega};\mathbb{R}^3)$$

for $0 < h < h_0$.

We assume that there exists an interpolation operator $\mathcal{I}_h : W^{1,\infty}(\Omega;\mathbb{R}^3) \to \mathcal{A}_h$ such that

$$\operatorname{ess\,sup}_{x\in\Omega}\|\nabla \mathcal{I}_h v(x)\| \leq C \operatorname{ess\ sup}_{x\in\Omega}\|\nabla v(x)\| \tag{6.1}$$

for all $v \in W^{1,\infty}(\Omega;\mathbb{R}^3)$, where the constant C in (6.1) and below will always denote a generic positive constant independent of h. We also assume for $v \in W^{1,\infty}(\Omega;\mathbb{R}^3)$ that

$$\mathcal{I}_h v(x)|_K = v(x)|_K \text{ for any } K \in \tau_h \text{ such that } v(x)|_K \in \left\{P^1(K)\right\}^3 \tag{6.2}$$

where $\left\{P^1(K)\right\}^3 \equiv P^1(K) \times P^1(K) \times P^1(K)$ and $P^1(K)$ denotes the space of linear polynomials defined on K.

We denote the finite element space of admissible functions satisfying the boundary condition

$$v_h(x) = Fx \qquad \text{for all } x \in \partial\Omega$$

for $F \in \mathbb{R}^{3\times 3}$ by

$$\mathcal{A}_{h,F} = \mathcal{A}_h \cap W^{\phi}_F = \{\, v_h \in \mathcal{A}_h : v_h(x) = Fx \text{ for } x \in \partial\Omega\} \,,$$

and we further assume that the interpolation operator $\mathcal{I}_h$ satisfies the property that

$$\mathcal{I}_h v \in \mathcal{A}_{h,F} \qquad \text{if} \qquad v \in W^{\phi}_F. \tag{6.3}$$

The most widely used conforming finite element methods based on continuous, piecewise polynomial spaces have interpolation operators $\mathcal{I}_h$ satisfying (6.1) (for quasi-regular meshes), (6.2), and (6.3) (see Ciarlet 1978, Quarteroni and Valli 1994). In particular, (6.1)–(6.3) are valid for trilinear elements defined on rectangular parallelepipeds as well as for linear elements defined on tetrahedra.

6.2. Approximation of the infimum of the energy

Our analysis of the approximation of microstructure begins with an estimate on the minimization of the energy over deformations $v_h \in \mathcal{A}_h$ that are constrained to satisfy the boundary condition

$$v_h(x) = [(1-\lambda)F_0 + \lambda F_1]\, x = F_\lambda x \qquad \text{for all } x \in \partial\Omega \tag{6.4}$$

for $F_0 \in \mathcal{U}$ and $F_1 \in \mathcal{U}$ rank-one connected as in (3.3) and $\theta < \theta_T$. We recall by (2.18) and (5.5) that

$$\phi_{\min}(\theta) = \phi(F_0, \theta) = \phi(F_1, \theta) = 0 \tag{6.5}$$

if F_0, $F_1 \in \mathcal{U}$ and $\theta < \theta_T$. The following estimate is an extension of similar results in Gremaud (1994), Chipot et al. (1995) and Luskin (1996*a*). We note that improved estimates for all of the results in this section can be obtained for finite element meshes that are aligned with the microstructure.

Theorem 9 If $F_0 \in \mathcal{U}$ and $F_1 \in \mathcal{U}$ are rank-one connected as in (3.3) and $\theta < \theta_T$, then

$$\inf_{v_h \in \mathcal{A}_{h,F_\lambda}} \mathcal{E}(v_h) \leq Ch^{1/2} \qquad \text{for all } 0 < h < h_0 \tag{6.6}$$

Proof. By (6.3), we can define the deformation $v_h(x) \in \mathcal{A}_{h,F_\lambda}$ by

$$v_h(x) = \mathcal{I}_h\left(\hat{w}_\gamma(x)\right)$$

for $\gamma = h^{1/2}$ where $\hat{w}_\gamma(x) \in W^\phi_{F_\lambda}$ is defined by (3.41) in Theorem 1. It follows from property (6.2) of the interpolation operator $\mathcal{I}_h$ that

$$v_h(x) = \hat{w}_\gamma(x) = w_\gamma(x) \qquad \text{for all } x \in \Omega_h \tag{6.7}$$

for (recalling that $|n|=1$)

$$\Omega_h = \Omega_h^2 \setminus \Lambda_h$$

where

$$\Omega_h^2 = \left\{ x \in \Omega : \operatorname{dist}(x, \partial\Omega) > vh^{1/2} + h \right\},$$

$$\Lambda_h = \bigcup_{j \in \mathbb{Z}} \left\{ x \in \Omega_h^2 : |x \cdot n - jh^{1/2}| \leq h \text{ or } |x \cdot n - (j + 1 - \lambda)h^{1/2}| \leq h \right\}.$$

Now $\operatorname{meas}(\Omega \setminus \Omega_h^2) \leq Ch^{1/2}$, since $\Omega \setminus \Omega_h^2$ is a layer of width $vh^{1/2} + h$ around the boundary of Ω, and $\operatorname{meas}(\Lambda_h) \leq Ch^{1/2}$, since Λ_h is the union of $\mathcal{O}(h^{-1/2})$ planar layers of thickness h. (Note that only $\mathcal{O}(h^{-1/2})$ of the sets in the definition of Λ_h are non-empty.) So, since $\Omega \setminus \Omega_h = \{\Omega \setminus \Omega_h^2\} \cup \Lambda_h$, we have that

$$\operatorname{meas}(\Omega \setminus \Omega_h) \leq Ch^{1/2}, \tag{6.8}$$

and we have by (6.1), (3.38), and (6.7) that

$$\begin{aligned} \nabla v_h(x) &\in \{F_0, F_1\} \subset \mathcal{U}, \quad \text{for almost all } x \in \Omega_h, \\ \|\nabla v_h(x)\| &\leq C, \qquad \text{for almost all } x \in \Omega. \end{aligned} \tag{6.9}$$

Since ϕ is continuous, it is bounded on bounded sets in $\mathbb{R}^{3\times 3}$. Thus, it follows from (6.5), (6.8) and (6.9) that

$$\int_\Omega \phi\left(\nabla v_h(x)\right) = \int_{\Omega \setminus \Omega_h} \phi\left(\nabla v_h(x)\right) \, dx \leq C \operatorname{meas}(\Omega \setminus \Omega_h) \leq Ch^{1/2}.$$

□

We have seen in Section 4.2 that we generally expect to compute local minima of the problem

$$\inf_{v_h \in \mathcal{A}_{h,F_\lambda}} \mathcal{E}(v_h)$$

rather than global minima. The local minima that we compute often represent the energy-minimizing microstructure on a length scale $2h$ rather than h. So, it is reasonable to give error estimates for finite element approximations $u_h \in \mathcal{A}_{h,F_\lambda}$ satisfying the quasi-optimality condition

$$\mathcal{E}(u_h) \leq C \inf_{v_h \in \mathcal{A}_{h,F_\lambda}} \mathcal{E}(v_h) \tag{6.10}$$

for some constant $C > 1$ independent of h. For instance, if we compute a local minimum that oscillates on a scale of $2h$, then it is reasonable from Theorem 9 to take $C = \sqrt{2}$.

The following corollaries are direct consequences of the estimate given in Theorem 9 and the bounds given in Section 5. We note that the results in this section hold for both the case of a double well energy density (5.3) and the case of an energy density for the cubic to tetragonal transformation (5.4).

We recall that these estimates hold for general finite element meshes satisfying only the conditions given at the beginning of this section. Improved estimates are possible for meshes which are aligned with the microstructure.

Corollary 3 If u_h satisfies the quasi-optimality condition (6.10) and $\omega \subset \Omega$ is a smooth domain, then there exists a positive constant C such that

$$\int_\Omega |(\nabla u_h(x) - F_\lambda)w|^2 \, \mathrm{d}x \leq Ch^{1/4}.$$

Corollary 4 If u_h satisfies the quasi-optimality condition (6.10), then there exists a positive constant C such that

$$\int_\Omega |u_h(x) - F_\lambda x|^2 \, \mathrm{d}x \leq Ch^{1/4}.$$

Corollary 5 If u_h satisfies the quasi-optimality condition (6.10) and $\omega \subset \Omega$ is a smooth domain, then there exists a positive constant C such that

$$\left\| \int_\omega (\nabla v(x) - F_\lambda) \, \mathrm{d}x \right\| \leq Ch^{1/16} \qquad \text{for all } v \in W^\phi_{F_\lambda}.$$

Corollary 6 If u_h satisfies the quasi-optimality condition (6.10) and $\omega \subset \Omega$ is a smooth domain, then there exists a positive constant C such that

$$\left| \frac{\mathrm{meas}\left(\omega^0_\rho(u_h)\right)}{\mathrm{meas}(\omega)} - (1-\lambda) \right| \leq Ch^{\frac{1}{16}}, \qquad \left| \frac{\mathrm{meas}\left(\omega^1_\rho(u_h)\right)}{\mathrm{meas}(\omega)} - \lambda \right| \leq Ch^{\frac{1}{16}}.$$

Corollary 7 If u_h satisfies the quasi-optimality condition (6.10), then there exists a positive constant C such that

$$\left| \int_\Omega f(x, \nabla u_h(x)) - [(1-\lambda) f(x, F_0) + \lambda f(x, F_1)] \, dx \right|$$
$$\leq C \left\{ \int_\Omega \left[\left\| \frac{\partial f}{\partial F}(x, \cdot) \right\|_{L^\infty}^2 + |\nabla G(x) \cdot n|^2 + G(x)^2 \right] dx \right\}^{1/2} h^{1/8}$$

for all $f(x, F) \in \mathcal{V}$ where

$$G(x) = f(x, F_1) - f(x, F_0).$$

7. Relaxation

We have seen that the deformation gradients of energy-minimizing sequences of the non-convex energy $\mathcal{E}(y)$ develop oscillations that allow the energy to converge to the lowest possible value. The minimum energy attainable by a microstructure that is constrained by the boundary condition $y(x) = Fx$ for $x \in \partial\omega$, where $\omega \subset \mathbb{R}^3$ is a bounded domain, is given by the relaxed energy density $Q\phi(F)$, which can be defined by

$$Q\phi(F) = \inf \left\{ \frac{1}{\operatorname{meas} \omega} \int_\omega \phi(\nabla v(x)) \, dx : \right.$$
$$\left. v \in W^{1,\infty}(\omega; \mathbb{R}^3) \text{ and } v(x) = Fx \text{ for } x \in \partial\omega \right\}. \tag{7.1}$$

The definition of $Q\phi(F)$ can be shown to be independent of ω (Dacorogna 1989).

An energy density $\psi(F)$ is defined to be *quasi-convex* if $Q\psi(F) = \psi(F)$ for all $F \in \mathbb{R}^{3\times 3}$. It can be shown that $Q\phi(F)$ is quasi-convex and that $Q\phi(F)$ is the quasi-convex envelope of $\phi(F)$ since

$$Q\phi = \sup \{ \psi \leq \phi : \psi \text{ quasi-convex} \}.$$

We note that in general the relaxed energy density $Q\psi(F)$ is not convex (Kohn 1991).

To make the following discussion simple, we will assume that the energy density satisfies the growth condition that for positive constants C_0, C_1, C_2, C_3 and $p > 3$ we have

$$C_1 \|F\|^p - C_0 \leq \phi(F, \theta) \leq C_2 \|F\|^p + C_3 \qquad \text{for all } F \in \mathbb{R}^{3\times 3}. \tag{7.2}$$

Hence, we have that

$$W^\phi = W^{1,p}(\Omega; \mathbb{R}^3).$$

We shall also assume that the admissible deformations belong to the set

$$\mathcal{A} = \left\{ y \in W^\phi : y(x) = y_0(x) \text{ for } x \in \partial\Omega \right\}$$

for $y_0(x) \in W^{\phi}$.

It can then be shown under appropriate conditions on the energy density $\phi(F)$ that

$$\inf_{y \in \mathcal{A}} \int_{\Omega} Q\phi(\nabla y(x))\, dx = \inf_{y \in \mathcal{A}} \int_{\Omega} \phi(\nabla y(x))\, dx \tag{7.3}$$

and that there exists an energy-minimizing deformation $\bar{y}(x) \in \mathcal{A}$ for the relaxed energy density $Q\phi(F)$ such that

$$\int_{\Omega} Q\phi(\nabla \bar{y}(x))\, dx = \inf_{y \in \mathcal{A}} \int_{\Omega} Q\phi(\nabla y(x))\, dx. \tag{7.4}$$

Further, it can be shown that there exists an energy-minimizing sequence $\{y_k\} \subset \mathcal{A}$ for the energy density ϕ such that

$$\lim_{k \to \infty} \int_{\Omega} \phi(\nabla y_k(x))\, dx = \int_{\Omega} Q\phi(\nabla \bar{y}(x))\, dx$$

and that

$$y_k(x) \rightharpoonup \bar{y}(x) \qquad \text{weakly in } W^{1,p}(\Omega; \mathbb{R}^3)$$

as $k \to \infty$ (Dacorogna 1989).

It is natural to consider the computation of the numerical solution of (7.4) for the deformation $\bar{y}(x)$, that is, the macroscopic deformation for the energy-minimizing microstructure defined by the sequence $\{y_n\}$. We can also consider the computation of a microstructure at each $\bar{x} \in \Omega$ by computing the energy-minimizing microstructure for the problem (7.1), which defines the relaxed energy density $Q\phi(\nabla \bar{y}(\bar{x}))$. However, explicit formulae or effective algorithms to compute the relaxed energy density (7.1) for the energy densities used to model martensitic crystals have not been found. (See Kohn 1991, though, for an explicit solution to (7.1) for a double well energy density with a special 'Hooke's law'.)

We can approximate (7.1) by considering as test functions the first-order laminates $v(x) = \hat{w}_{\gamma}(x)$ defined by (3.41) with boundary values $\hat{w}_{\gamma}(x) = Fx$ for $x \in \partial\omega$. To construct the class of all first-order laminates $v(x) = \hat{w}_{\gamma}(x)$ with boundary values $\hat{w}_{\gamma}(x) = Fx$ for $x \in \partial\omega$ we consider all F_0, $F_1 \in \mathbb{R}^{3\times 3}$ and all $0 \leq \lambda \leq 1$ such that

$$F = (1 - \lambda)F_0 + \lambda F_1, \tag{7.5}$$

where

$$F_1 = F_0 + a \otimes n \tag{7.6}$$

for a, $n \in \mathbb{R}^3$, $|n| = 1$. We note that it follows from (7.5) and (7.6) that

$$F_0 = F - \lambda a \otimes n \qquad \text{and} \qquad F_1 = F + (1 - \lambda) a \otimes n.$$

The volume fraction that $\hat{w}_{\gamma}(x)$ has deformation gradient F_0 converges to

$1-\lambda$ as $\gamma \to 0$, and the volume fraction that $\hat{w}_\gamma(x)$ has deformation gradient F_1 converges to λ as $\gamma \to 0$. Thus it follows from the proof of Theorem 1 that

$$\begin{aligned}\lim_{\gamma\to 0} \frac{1}{\operatorname{meas}\omega} \int_\omega \phi(\nabla \hat{w}_\gamma(x))\,dx &= (1-\lambda)\phi(F_0) + \lambda\phi(F_1) \\ &= (1-\lambda)\phi(F - \lambda a \otimes n) + \lambda\phi(F + (1-\lambda)a \otimes n).\end{aligned}$$

If we optimize (7.1) by restricting $v \in W^{1,\infty}(\omega; \mathbb{R}^3)$ to the first-order laminates of the form $\hat{w}_\gamma(x)$ discussed in the preceding paragraph, then we obtain the energy density $R_1\phi(F)$ defined by

$$\begin{aligned}&R_1\phi(F) = \\ &\quad \inf\{(1-\lambda)\phi(F - \lambda a \otimes n) + \lambda\phi(F + (1-\lambda)a \otimes n) : \\ &\qquad 0 \le \lambda \le 1,\ a,\ n \in \mathbb{R}^3,\ |n| = 1\}\end{aligned}$$

for all $F \in \mathbb{R}^{3\times 3}$. We can more generally optimize (7.1) over the laminates of order k discussed in Section 3.10 and obtain the energy density $R_k\phi(F)$, which can be defined by $R_0\phi(F) = \phi(F)$ and inductively for $k = 1, \ldots$ by

$$\begin{aligned}&R_k\phi(F) = \\ &\quad \inf\{(1-\lambda)R_{k-1}\phi(F - \lambda a \otimes n) + \lambda R_{k-1}\phi(F + (1-\lambda)a \otimes n) : \\ &\qquad 0 \le \lambda \le 1,\ a,\ n \in \mathbb{R}^3,\ |n| = 1\}\end{aligned}$$

for all $F \in \mathbb{R}^{3\times 3}$ (Kohn and Strang 1986).

It can be seen that

$$Q\phi(F) \le R_k\phi(F) \le \ldots \le R_1\phi(F) \le \phi(F) \qquad \text{for all } F \in \mathbb{R}^{3\times 3},$$

so we can conclude from (7.3) that

$$\inf_{y\in\mathcal{A}} \int_\Omega Q\phi(\nabla y(x))\,dx = \inf_{y\in\mathcal{A}} \int_\Omega R_k\phi(\nabla y(x))\,dx = \inf_{y\in\mathcal{A}} \int_\Omega \phi(\nabla y(x))\,dx. \tag{7.7}$$

An energy density $\psi(F) : \mathbb{R}^{3\times 3} \to R$ is *rank-one convex* if

$$\psi((1-\lambda)F_0 + \lambda F_1) \le (1-\lambda)\psi(F_0) + \lambda\psi(F_1)$$

for all $0 \le \lambda \le 1$ and all $F_1,\ F_0 \in \mathbb{R}^{3\times 3}$ such that $\operatorname{rank}(F_1 - F_0) \le 1$. The rank-one convex envelope $R\phi(F)$ is then defined by

$$R\phi = \sup\{\, \psi \le \phi : \psi \text{ rank-one convex } \}\,.$$

We note that Kohn and Strang (1986) have shown that

$$R\phi(F) = \lim_{k\to\infty} R_k\phi(F) \qquad \text{for all } F \in \mathbb{R}^{3\times 3},$$

and that Šverák (1992) has shown that in general $Q\phi(F) \ne R\phi(F)$.

The approximation

$$\inf_{y\in\mathcal{A}_h} \int_\Omega R_k\phi(\nabla y(x))\,dx$$

for finite element spaces $\mathcal{A}_h \subset \mathcal{A}$ has been considered in Nicolaides and Walkington (1993), Roubíček (1994), Carstensen and Plecháč (1995), Roubíček (1996*a*), Pedregal (1996), Pedregal (1995), Kružík (1995).

An energy density $\psi(F) : \mathbb{R}^{3\times 3} \to R$ is *polyconvex* if it is a convex function of the minors of $F \in \mathbb{R}^{3\times 3}$ (Ball 1977, Dacorogna 1989). The polyconvex envelope $P\phi(F)$ is then defined by

$$P\phi = \sup \{ \psi \leq \phi : \psi \text{ polyconvex} \} .$$

Since a polyconvex energy density is always quasi-convex by Jensen's inequality, we have that $P\phi(F) \leq Q\phi(F)$ for all $F \in \mathbb{R}^{3\times 3}$. It can be shown that in general $P\phi(F) \neq Q\phi(F)$. Representations of the polyconvex envelope $P\phi(F)$, especially that due to Dacorogna (1989), have been used to develop numerical approximations of the lower bound for the energy given by

$$\inf_{y\in\mathcal{A}} \int_\Omega P\phi(\nabla y(x)) \, \mathrm{d}x$$

(Roubíček 1996*a*, Pedregal 1996, Pedregal 1995, Kružík 1995).

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