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STABILITY OF MICROSTRUCTURE FOR TETRAGONAL TO MONOCLINIC MARTENSITIC TRANSFORMATIONS *

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Abstract. We give an analysis of the stability and uniqueness of the simply laminated microstructure for all three tetragonal to monoclinic martensitic transformations. The energy density for tetragonal to monoclinic transformations has four rotationally invariant wells since the transformation has four variants. One of these tetragonal to monoclinic martensitic transformations corresponds to the shearing of the rectangular side, one corresponds to the shearing of the square base, and one corresponds to the shearing of the plane orthogonal to a diagonal in the square base. We show that the simply laminated microstructure is stable except for a class of special material parameters. In each case that the microstructure is stable, we derive error estimates for the finite element approximation.

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1. Introduction

We use the geometrically nonlinear theory of martensite [2, 3, 13, 28] to model tetragonal to monoclinic martensitic transformations. In this theory, the energy density is minimized on multiple energy wells $\mathrm{SO}(3)U_1 \cup \ldots \cup \mathrm{SO}(3)U_N$ where $U_1, \ldots, U_N$ for $N > 1$ are symmetry-related transformation strains (variants) and SO(3) is the set of all 3×3 real orthogonal matrices with determinant equal to one. For tetragonal to monoclinic transformations, there are four symmetry-related transformation strains ($N = 4$) [34, 35]. There are three tetragonal to monoclinic martensitic transformations — one corresponds to shearing of a rectangular face, one corresponds to shearing of the square base, and one corresponds to shearing of the plane orthogonal to the diagonal of the square base. For certain boundary constraints or loading conditions, the elastic energy of a martensitic crystal is minimized only by the fine-scale mixing of deformation gradients from distinct energy wells. The simplest example of such a microstructure is the laminate in which two compatible deformation gradients oscillate in parallel layers of fine scale. Much recent work has been done to describe more complex microstructures by using the concept of the Young measure [2, 3, 21, 36, 37].

The stability theory that we use was first used to study the orthorhombic to monoclinic transformation ($N = 2$) [27]. It was then extended to obtain results for the cubic to tetragonal transformation ($N = 3$) [23]. Most recently, the stability theory has been used to analyze a cubic to orthorhombic transformation ($N = 6$) [6].

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In general, the analysis of stability is more difficult for transformations with $N = 4$ (such as the tetragonal to monoclinic transformations studied in this paper) and $N = 6$ since the additional wells give the crystal more freedom to deform without the cost of additional energy. In fact, we show here that there are special lattice constants for which the simply laminated microstructure for the tetragonal to monoclinic transformation is not stable.

The stability theory can also be used to analyze laminates with varying volume fraction [24] and conforming and nonconforming finite element approximations [25, 27]. We also note that the stability theory was used to analyze the microstructure in ferromagnetic crystals [29]. Related results on the numerical analysis of nonconvex variational problems can be found, for example, in [7–12, 14–16, 18, 19, 22, 26, 30–33].

In this paper, we give an analysis of the stability of a laminated microstructure with infinitesimal length scale that oscillates between two compatible variants. We show that for any other deformation satisfying the same boundary conditions as the laminate, we can bound the pertubation of the volume fractions of the variants by the pertubation of the bulk energy. This implies that the volume fractions of the variants for a deformation are close to the volume fractions of the laminate if the bulk energy of the deformation is close to the bulk energy of the laminate. This concept of stability can be applied directly to obtain results on the convergence of finite element approximations and guarantees that any finite element solution with sufficiently small bulk energy gives reliable approximations of the stable quantities such as volume fraction.

In Section 2, we describe the geometrically nonlinear theory of martensite. We refer the reader to [2, 3] and to the introductory article [28] for a more detailed discussion of the geometrically nonlinear theory of martensite. We review the results given in [34, 35] on the transformation strains and possible interfaces for tetragonal to monoclinic transformations corresponding to the shearing of the square and rectangular faces, and we then give the transformation strain and possible interfaces corresponding to the shearing of the plane orthogonal to a diagonal in the square base.

In Section 3, we give the main results of this paper which give bounds on the volume fraction of the crystal in which the deformation gradient is in energy wells that are not used in the laminate. These estimates are used in Section 4 to establish a series of error bounds in terms of the elastic energy of deformations for the L^2 approximation of the directional derivative of the limiting macroscopic deformation in any direction tangential to the parallel layers of the laminate, for the L^2 approximation of the limiting macroscopic deformation, for the approximation of volume fractions of the participating martensitic variants, and for the approximation of nonlinear integrals of deformation gradients. Finally, in Section 5 we give an application of the stability theory to the finite element approximation of the simply laminated microstructure.

2. The geometrically nonlinear model

We use the austenitic tetragonal phase of the crystal at the transformation temperature as the reference configuration $\Omega \subset \mathbb{R}^3$, and we assume that Ω is a bounded domain with a Lipschitz continuous boundary $\partial\Omega$. We denote deformations by functions $y : \Omega \to \mathbb{R}^3$ and corresponding deformation gradients by $\nabla y : \Omega \to \mathbb{R}^{3\times 3}$ where $\mathbb{R}^{3\times 3}$ denotes the set of all 3×3 real matrices.

We shall minimize the total energy

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

over an admissible class $\mathcal{A}$ of deformations, where $\phi : \mathbb{R}^{3\times 3} \to \mathbb{R}$ is the free energy density per unit volume of the reference configuration of the crystal at a fixed temperature below the transformation temperature.

We shall assume that the free energy density is frame-indifferent, that is,

$$\phi(RF) = \phi(F) \qquad \text{for all } F \in \mathbb{R}^{3\times 3} \text{ and } R \in \mathrm{SO}(3). \tag{2.1}$$

We also assume that it inherits the symmetry of the austenitic phase of the crystal, so that

$$\phi(R_i^T F R_i) = \phi(F) \qquad \text{for all } F \in \mathbb{R}^{3\times 3} \text{ and } R_i \in \mathcal{G}, \tag{2.2}$$

where $\mathcal{G} = \{R_1, \ldots, R_8\} \subset \mathrm{SO}(3)$ is the symmetry group of the tetragonal phase given by

$$\begin{gathered} R_1 = R(\pi, e_1), \quad R_2 = R(\pi, e_2), \quad R_3 = R(\pi, e_3), \\ R_4 = R(\pi, e_1 + e_2), \quad R_5 = R(\pi, e_1 - e_2), \\ R_6 = R(\pi/2, e_3), \quad R_7 = R(3\pi/2, e_3), \quad R_8 = I. \end{gathered} \tag{2.3}$$

In the above, $\{e_i\}$ is a right-handed, orthonormal basis for $\mathbb{R}^3$ given by normalized lattice vectors for the tetragonal phase, and $R(\alpha, v)$ denotes the rotation of α radians about $v \in \mathbb{R}^3$, $v \neq 0$.

We assume that the free energy density is minimized at a transformation (Bain) strain U_1 for the tetragonal to monoclinic transformation. We shall see that there then exist three other distinct symmetry-related transformation strains (variants) U_2, U_3, U_4 such that

$$\{R_i^T U_1 R_i : R_i \in \mathcal{G}\} = \{U_1, \ldots, U_4\}.$$

It also follows by the frame-indifference (2.1) and the symmetry (2.2) of the energy density that the energy density is minimized on the union $\mathcal{U}$ of the four energy wells

$$\mathcal{U}_i = \mathrm{SO}(3)U_i = \{RU_i : R \in \mathrm{SO}(3)\} \qquad \text{for } i = 1, \ldots, 4.$$

By adding a constant, we may assume that the minimum value of ϕ is 0. Finally, we shall assume that ϕ is continuous and satisfies the growth condition

$$\phi(F) \geq \kappa \,\|F - \pi(F)\|^2 \qquad \text{for all } F \in \mathbb{R}^{3\times 3}, \tag{2.4}$$

where $\kappa > 0$ is a constant and $\pi : \mathbb{R}^{3\times 3} \to \mathcal{U}$ is a projection defined by

$$\|F - \pi(F)\| = \min_{G\in\mathcal{U}} \|F - G\| \qquad \text{for all } F \in \mathbb{R}^{3\times 3}. \tag{2.5}$$

This projection exists for any $F \in \mathbb{R}^{3\times 3}$, since the set $\mathcal{U}$ is compact.

We now derive the transformation strains for the three tetragonal to monoclinic transformations. The reader should note that this derivation itself is not used in the stability analysis given below; only the resulting transformation strains described in (2.6), (2.7), and (2.8) will be used.

Each of the two-fold rotations R_l for $l = 1, \ldots, 5$ in the tetragonal symmetry group determines a family of transformation strains that corresponds to shearing in the plane orthogonal to the axis of the rotation. For each two-fold rotation R_l for $l = 1, \ldots, 5$, the transformation strains $U_1^{(l)}$ in the corresponding family satisfy [3,34,35]

$$\{R_i \in \mathcal{G} : R_i^T U_1^{(l)} R_i = U_1^{(l)}\} = \{I, R_l\}.$$

The corresponding symmetry-related variants $U_2^{(l)}$, $U_3^{(l)}$, $U_4^{(l)}$ are then given by

$$\{R_i^T U_1^{(l)} R_i : R_i \in \mathcal{G}\} = \{U_1^{(l)}, \ldots, U_4^{(l)}\}.$$

The two-fold rotations R_1 and R_2 correspond to shearing of the rectangular faces and can be analyzed identically by symmetry. The two-fold rotation R_3 corresponds to shearing of the square base and must be treated as a separate case. The two-fold rotations R_4 and R_5 correspond to shearing the plane orthogonal to a diagonal of the square base and can also be analyzed identically by symmetry. Therefore, we need analyze only the following three cases corresponding to R_2, R_3, and R_4.

In Case 1, corresponding to R_2 and shearing in the plane orthogonal to e_2, the transformation strain $U_1^{(2)}$ and the symmetry-related transformation strains $U_2^{(2)}$, $U_3^{(2)}$, $U_4^{(2)}$ are given by

$$\begin{aligned} U_1^{(2)} &= \begin{pmatrix} \theta_1 & 0 & \theta_4 \\ 0 & \theta_2 & 0 \\ \theta_4 & 0 & \theta_3 \end{pmatrix}, \qquad U_2^{(2)} = \begin{pmatrix} \theta_1 & 0 & -\theta_4 \\ 0 & \theta_2 & 0 \\ -\theta_4 & 0 & \theta_3 \end{pmatrix}, \\ U_3^{(2)} &= \begin{pmatrix} \theta_2 & 0 & 0 \\ 0 & \theta_1 & \theta_4 \\ 0 & \theta_4 & \theta_3 \end{pmatrix}, \qquad U_4^{(2)} = \begin{pmatrix} \theta_2 & 0 & 0 \\ 0 & \theta_1 & -\theta_4 \\ 0 & -\theta_4 & \theta_3 \end{pmatrix}, \end{aligned} \tag{2.6}$$

where $\theta_i > 0$ for $i = 1, 2, 3,\ \theta_4 \neq 0$, and $\theta_1\theta_3 - \theta_4^2 > 0$. We shall assume without loss of generality that $\theta_4 > 0$.

For Case 2, corresponding to R_3 and shearing in the plane orthogonal to e_3, the transformation strain $U_1^{(3)}$ and the symmetry-related transformation strains $U_2^{(3)}$, $U_3^{(3)}$, $U_4^{(3)}$ are given by

$$\begin{aligned} U_1^{(3)} &= \begin{pmatrix} \delta_1 & \delta_4 & 0 \\ \delta_4 & \delta_2 & 0 \\ 0 & 0 & \delta_3 \end{pmatrix}, \qquad U_2^{(3)} = \begin{pmatrix} \delta_1 & -\delta_4 & 0 \\ -\delta_4 & \delta_2 & 0 \\ 0 & 0 & \delta_3 \end{pmatrix}, \\ U_3^{(3)} &= \begin{pmatrix} \delta_2 & \delta_4 & 0 \\ \delta_4 & \delta_1 & 0 \\ 0 & 0 & \delta_3 \end{pmatrix}, \qquad U_4^{(3)} = \begin{pmatrix} \delta_2 & -\delta_4 & 0 \\ -\delta_4 & \delta_1 & 0 \\ 0 & 0 & \delta_3 \end{pmatrix}, \end{aligned} \tag{2.7}$$

where $\delta_i > 0$ for $i = 1, 2, 3,\ \delta_4 \neq 0$ and $\delta_1\delta_2 - \delta_4^2 > 0$. We shall assume without loss of generality that $\delta_1 > \delta_2$ and $\delta_4 > 0$.

In Case 3, corresponding to R_4 and shearing in the plane orthogonal to $e_1 + e_2$, the transformation strain $U_1^{(4)}$ and the symmetry-related transformation strains $U_2^{(4)}$, $U_3^{(4)}$, $U_4^{(4)}$ are given by

$$\begin{aligned} U_1^{(4)} &= \begin{pmatrix} \eta_1 & \eta_3 & \eta_4 \\ \eta_3 & \eta_1 & -\eta_4 \\ \eta_4 & -\eta_4 & \eta_2 \end{pmatrix}, \qquad U_2^{(4)} = \begin{pmatrix} \eta_1 & -\eta_3 & \eta_4 \\ -\eta_3 & \eta_1 & \eta_4 \\ \eta_4 & \eta_4 & \eta_2 \end{pmatrix}, \\ U_3^{(4)} &= \begin{pmatrix} \eta_1 & \eta_3 & -\eta_4 \\ \eta_3 & \eta_1 & \eta_4 \\ -\eta_4 & \eta_4 & \eta_2 \end{pmatrix}, \qquad U_4^{(4)} = \begin{pmatrix} \eta_1 & -\eta_3 & -\eta_4 \\ -\eta_3 & \eta_1 & -\eta_4 \\ -\eta_4 & -\eta_4 & \eta_2 \end{pmatrix}, \end{aligned} \tag{2.8}$$

where $\eta_1 > 0,\ \eta_2 > 0,\ \eta_4 \neq 0,\ \eta_1 + \eta_3 > 0$, and $\eta_2(\eta_1 - \eta_3) - 2\eta_4^2 > 0$. We shall assume without loss of generality that $\eta_4 > 0$ (Note that it follows from the preceding inequality that $\eta_1 + \eta_2 - \eta_3 > 0$ and $\eta_1\eta_2 - \eta_4^2 > 0$; we will use these inequalities in the proof of Theorem 3.1).

In what follows, we will omit the superscript in the notation for the transformation strain $U_i^{(l)}$ since the case being considered will always be explicitly given.

There exists a continuous deformation $y(x) \in \mathrm{C}^0(\mathbb{R}^3; \mathbb{R}^3)$ such that [2, 28]

$$\nabla y(x) = \begin{cases} QU_i & \text{for all } x \text{ such that } x \cdot n < s, \\ U_j & \text{for all } x \text{ such that } x \cdot n > s, \end{cases}$$

where $Q \in \mathrm{SO}(3)$, $i, j \in \{1, \ldots, 4\}$, $n \in \mathbb{R}^3$, $n \neq 0$, and $s \in \mathbb{R}$, if and only if there exists $a \in \mathbb{R}^3$ such that

$$QU_i = U_j + a \otimes n. \tag{2.9}$$

Thus, if (2.9) holds for $a \neq 0$, then $x \cdot n = s$ is an interface plane; and we say that the two wells $\mathcal{U}_i = \mathrm{SO}(3)U_i$ and $\mathcal{U}_j = \mathrm{SO}(3)U_j$ are *rank-one* connected.

The following lemma (which is a special case of Proposition 2.2 in [4]) will be used to construct rank-one connections for the tetragonal to monoclinic transformation that result from the two-fold rotations in the symmetry group. This lemma can be verified by direct substitution into (2.9).

Lemma 2.1. *Assume that U_i, $U_j \in \mathbb{R}^{3\times 3}$ are positive definite and symmetric, that there exists a unit vector $m \in \mathbb{R}^3$, and a rotation $R(\pi, m) \in \mathcal{G}$ such that*

$$U_i = R(\pi, m)^T U_j R(\pi, m). \tag{2.10}$$

Then there exist exactly two solutions to (2.9)*, up to the scaling of a and n by any nonzero constant $\rho \in \mathbb{R}$, given by*

$$a = \frac{2}{\rho}\left(\frac{U_j^{-1}m}{|U_j^{-1}m|^2} - U_j m\right), \qquad n = \rho\, m, \qquad Q = R(\pi, U_j^{-1}n)R(\pi, m),$$

and

$$a = \rho\, U_j m, \qquad n = \frac{2}{\rho}\left(m - \frac{U_j^2 m}{|U_j m|^2}\right), \qquad Q = R(\pi, a)R(\pi, m).$$

The first solution given in Lemma 2.1 determines a *type I twin* and the other solution determines a *type II twin* [2,38]. For either type of twin, we call the planes $x \cdot n = s$ *twin planes.* If a twin is both a type I twin and a type II twin, then it is said to be a *compound twin.* The following easily proven identities give type I twins and type II twins by the above lemma.

Lemma 2.2. *The two-fold rotations defined in* (2.3) *act on $U_1, \ldots, U_4$ in the following manner:*

Case 1:
$$\begin{aligned}
&R_1^T U_1 R_1 = R_3^T U_1 R_3 = U_2, && R_5^T U_2 R_5 = U_4,\\
&R_2^T U_1 R_2 = U_1, && R_4^T U_2 R_4 = U_3,\\
&R_4^T U_1 R_4 = U_4, && R_1^T U_3 R_1 = U_3,\\
&R_5^T U_1 R_5 = U_3, && R_2^T U_3 R_2 = R_3^T U_3 R_3 = U_4,\\
&R_2^T U_2 R_2 = U_2, && R_1^T U_4 R_1 = U_4.
\end{aligned}$$

Case 2:
$$\begin{aligned}
&R_1^T U_1 R_1 = R_2^T U_1 R_2 = U_2, && R_4^T U_2 R_4 = R_5^T U_2 R_5 = U_4,\\
&R_3^T U_1 R_3 = U_1, && R_1^T U_3 R_1 = R_2^T U_3 R_2 = U_4,\\
&R_4^T U_1 R_4 = R_5^T U_1 R_5 = U_3, && R_3^T U_3 R_3 = U_3,\\
&R_3^T U_2 R_3 = U_2, && R_3^T U_4 R_3 = U_4.
\end{aligned}$$

Case 3:
$$\begin{aligned}
&R_1^T U_1 R_1 = U_4, && R_3^T U_2 R_3 = R_4^T U_2 R_4 = U_4,\\
&R_2^T U_1 R_2 = U_2, && R_5^T U_2 R_5 = U_2,\\
&R_3^T U_1 R_3 = R_5^T U_1 R_5 = U_3, && R_2^T U_3 R_2 = U_4,\\
&R_4^T U_1 R_4 = U_1, && R_4^T U_3 R_4 = U_3,\\
&R_1^T U_2 R_1 = U_3, && R_5^T U_4 R_5 = U_4.
\end{aligned}$$

We next use the above lemma to give the following result classifying all possible rank-one connections for the tetragonal to monoclinic transformations. We note that for Case 2 there exist rank-one connections that are neither type I nor type II. The interfaces separating such rank-one connections are sometimes called *domain interfaces* rather than twin interfaces [20], and we shall maintain this distinction below.

Lemma 2.3. *For Case 1, Case 2, and Case 3, we have:*

1. For each $i \in \{1, \ldots, 4\}$, the energy well $\mathcal{U}_i$ is not rank-one connected to itself.

2. For any $i, j \in \{1, \ldots, 4\}$, with $i \neq j$, there are exactly two solutions to the twinning equation (2.9). The characterization of the solutions to (2.9) is given in Table 1 where

$$\varepsilon_1 = \frac{\theta_2^2 - \theta_1^2 - \theta_4^2}{\left[2\left(\theta_2^2 - \theta_1^2 - \theta_4^2\right)^2 + 4\theta_4^2(\theta_1 + \theta_3)^2\right]^{1/2}}, \qquad \zeta = \arctan \frac{\delta_1 - \delta_2}{2\delta_4},$$

and

$$\varepsilon_2 = \frac{2\eta_1\eta_3 - \eta_4^2}{\left[\left(2\eta_1\eta_3 - \eta_4^2\right)^2 + \eta_4^2\left(\eta_1 + \eta_2 - \eta_3\right)^2\right]^{1/2}}.$$

Alternatively,

$$\cos\frac{\zeta}{2} = \left[\frac{1}{2} + \frac{\delta_4}{\sqrt{4\delta_4^2 + (\delta_1 - \delta_2)^2}}\right]^{1/2}, \qquad \sin\frac{\zeta}{2} = \left[\frac{1}{2} - \frac{\delta_4}{\sqrt{4\delta_4^2 + (\delta_1 - \delta_2)^2}}\right]^{1/2}.$$

Proof. There do not exist R_0, $R_1 \in \mathrm{SO}(3)$ with $R_0 \neq R_1$ and a, $n \in \mathbb{R}^3$, a, $n \neq 0$ such that [2, 28]

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

Hence, for each $i \in \{1, \ldots, 4\}$, the energy well $\mathcal{U}_i$ is not rank-one connected to itself.

By Lemma 2.2, all of the interfaces in Case 1 and Case 3 and all but the $(i, j) = (1, 4)$ or $(i, j) = (2, 3)$ interfaces of Case 2 satisfy (2.10). Hence, Lemma 2.1 can be applied to obtain the solutions to (2.9).

To compute the interface normals for $(i, j) = (1, 4)$ or $(i, j) = (2, 3)$ in Case 2, we recall from Lemma 5 in [28] that $n = (\mu_1, \mu_2, 0)$, $n \neq 0$, is an interface normal if and only if

$$|U_i v| = |U_j v|$$

for $v = (-\mu_2, \mu_1, 0)$. □

In the following, we will be interested in a simple laminate. We fix $i, j \in \{1, \ldots, 4\}$ with $i \neq j$, and Q, a, and n with a, $n \neq 0$ that satisfy the interface equation

$$QU_i = U_j + a \otimes n. \tag{2.11}$$

For any fixed $\lambda \neq 0, 1$, we denote

$$F_\lambda = \lambda QU_i + (1 - \lambda)U_j = U_j + \lambda a \otimes n. \tag{2.12}$$

Then we have the following lemma.

Lemma 2.4. *For any $\lambda \in (0, 1)$, we have that $F_\lambda \notin \mathcal{U}$.*

Proof. It is proved in Lemma 2.3 of [6] that $F_\lambda \notin \mathcal{U}$ if (i, j) is a type I or type II twin. This proves the theorem in Case 1 and Case 3.

We next consider Case 2. If $F_\lambda \in \mathcal{U}$, then

$$\lambda QU_i + (1 - \lambda)U_j = RU_k$$

TABLE 1. Characterization of the solutions to (2.9).

CASE	(i,j)	TYPE OF TWIN	INTERFACE NORMALS
CASE 1	$(1,2)$	compound	$n_1 = e_1$
		compound	$n_2 = e_3$
	$(3,4)$	compound	$n_1 = e_2$
		compound	$n_2 = e_3$
	$(1,3)$	I	$e_1 - e_2$
		II	$(-\varepsilon_1, -\varepsilon_1, \sqrt{1-2\varepsilon_1^2})$
	$(1,4)$	I	$e_1 + e_2$
		II	$(-\varepsilon_1, \varepsilon_1, \sqrt{1-2\varepsilon_1^2})$
	$(2,3)$	I	$e_1 + e_2$
		II	$(\varepsilon_1, -\varepsilon_1, \sqrt{1-2\varepsilon_1^2})$
	$(2,4)$	I	$e_1 - e_2$
		II	$(\varepsilon_1, \varepsilon_1, \sqrt{1-2\varepsilon_1^2})$
CASE 2	$(1,2)$	compound	$n_1 = e_2$
		compound	e_1
	$(1,3)$	compound	$n_1 = e_1 - e_2$
		compound	$e_1 + e_2$
	$(2,4)$	compound	$n_1 = e_1 + e_2$
		compound	$e_1 - e_2$
	$(3,4)$	compound	$n_1 = e_1$
		compound	e_2
	$(1,4)$	domain	$(\cos\frac{\zeta}{2}, -\sin\frac{\zeta}{2}, 0)$
		domain	$(\sin\frac{\zeta}{2}, \cos\frac{\zeta}{2}, 0)$
	$(2,3)$	domain	$(\cos\frac{\zeta}{2}, \sin\frac{\zeta}{2}, 0)$
		domain	$(\sin\frac{\zeta}{2}, -\cos\frac{\zeta}{2}, 0)$
CASE 3	$(1,2)$	I	e_2
		II	$(\varepsilon_2, 0, -\sqrt{1-\varepsilon_2^2})$
	$(1,3)$	compound	$n_1 = e_3$
		compound	$n_2 = e_1 - e_2$
	$(1,4)$	I	e_1
		II	$(0, \varepsilon_2, \sqrt{1-\varepsilon_2^2})$
	$(2,3)$	I	e_1
		II	$(0, -\varepsilon_2, \sqrt{1-\varepsilon_2^2})$
	$(2,4)$	compound	$n_1 = e_3$
		compound	$n_2 = e_1 + e_2$
	$(3,4)$	I	e_2
		II	$(\varepsilon_2, 0, \sqrt{1-\varepsilon_2^2})$

for some $i \neq j$ and $k \in \{1, \dots, 4\}$. Then by the interface equation (2.11) we have

$$\begin{aligned} QU_i + (1-\lambda)a \otimes n &= RU_k, \\ U_j + \lambda a \otimes n &= RU_k. \end{aligned} \tag{2.13}$$

If $k = i$ or $k = j$, then (2.13) implies that the energy well $\mathcal{U}_i$ or $\mathcal{U}_j$ is rank-one connected to itself. This contradicts Lemma 2.3. If $k \neq i$ and $k \neq j$, then (2.13) implies that an interface normal for (i,j) is the same as an interface normal for (i,k) and (j,k). This contradicts the table of interface normals for Case 2 given in Lemma 2.3. □

We shall assume that the energy density $\phi(F)$ satisfies the growth condition

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

where C_0 and C_1 are positive constants independent of $F \in \mathbb{R}^{3\times 3}$ and where we assume $p > 3$ to ensure that deformations with finite energy are uniformly continuous [1]. We can then denote the set of deformations of finite energy by

$$W^\phi = \{y \in \mathrm{C}^0(\bar{\Omega};\mathbb{R}^3) : \int_\Omega \phi(\nabla y(x))\,\mathrm{d}x < \infty\},$$

and we can define the set $\mathcal{A}$ of admissible deformations as

$$\mathcal{A} = \{y \in W^\phi : y(x) = y_0(x) \text{ for all } x \in \partial\Omega\} \tag{2.14}$$

where

$$y_0(x) = F_\lambda x \quad \text{ for all } x \in \Omega.$$

We can prove the following lemma by constructing laminates with length scale converging to zero whose deformation gradients oscillate with volume fraction λ at QU_i and $1-\lambda$ at U_j [12,28].

Lemma 2.5. *Let $\mathcal{A}$ be defined as in* (2.14)*. Then the total energy $\mathcal{E}(y)$ satisfies*

$$\inf_{y\in\mathcal{A}} \mathcal{E}(y) = 0.$$

3. Reduction to the approximate mixture of two strains

Recall the definitions (2.5) and (2.14) of π and $\mathcal{A}$, respectively. For each $k \in \{1,\ldots,4\}$ and each $y \in \mathcal{A}$, we define

$$\Omega_k(y) = \{x \in \Omega : \pi(\nabla y(x)) \in \mathcal{U}_k\}$$

and the volume fraction with respect to the k-th energy well $\mathcal{U}_k$ to be

$$\tau_k(y) = \frac{\operatorname{meas}\Omega_k(y)}{\operatorname{meas}\Omega}\cdot$$

Since every $x \in \Omega$ is in $\Omega_k(y)$ for some $k \in \{1,\ldots,4\}$, we have that

$$\sum_{k=1}^4 \tau_k(y) = 1 \qquad \text{for all } y \in \mathcal{A}. \tag{3.1}$$

By the rank-one connection (2.11) and the definition of F_λ

$$F_\lambda = \lambda QU_i + (1-\lambda)U_j = U_j + \lambda a \otimes n, \tag{3.2}$$

we have that

$$|F_\lambda w| = |U_i w| = |U_j w| \qquad \text{for all } w \in \mathbb{R}^3,\ w\cdot n = 0. \tag{3.3}$$

Since $\det(QU_i) = \det U_j > 0$, we have that $U_j^{-1}a \cdot n = 0$. Hence, we have that

$$\operatorname{Cof} F_\lambda = (\operatorname{Cof} U_j)\,(I - \lambda n \otimes U_j^{-1}a) \tag{3.4}$$

where the cofactor of a nonsingular $A \in \mathbb{R}^{3\times 3}$ is defined by $\operatorname{Cof} A = (\det A)A^{-T}$. We then obtain from (3.4) that

$$|(\operatorname{Cof} F_\lambda)w| = |(\operatorname{Cof} U_i)w| = |(\operatorname{Cof} U_j)w| \qquad \text{for all } w \in \mathbb{R}^3,\ w \cdot U_j^{-1}a = 0. \tag{3.5}$$

We next recall that since the subdeterminant of the gradient is a null-Lagrangian [17], we have for $y \in \mathcal{A}$ that

$$\begin{aligned} \int_\Omega \nabla y(x)\ \mathrm{d}x &= \int_\Omega F_\lambda\ \mathrm{d}x, \\ \int_\Omega \operatorname{Cof} \nabla y(x)\ \mathrm{d}x &= \int_\Omega \operatorname{Cof} F_\lambda\ \mathrm{d}x. \end{aligned} \tag{3.6}$$

Finally, we note that it follows from (2.4) that

$$\int_\Omega \|\nabla y(x) - \pi(\nabla y(x))\|^2\ \mathrm{d}x \le \kappa^{-1}\mathcal{E}(y) \qquad \text{for all } y \in \mathcal{A}. \tag{3.7}$$

The following result is proved in more detail in [6] for the cubic to orthorhombic transformation. In the estimates below, C will denote a generic positive constant that is independent of $y \in \mathcal{A}$ and is allowed to change from equation to equation.

Lemma 3.1. *Given $i, j \in \{1, \ldots, 4\}$, $Q \in SO(3)$, and $a, n \in \mathbb{R}$, $a, n \neq 0$ satisfying the twinning equation (2.11), there exists a constant $C > 0$ such that for any $y \in \mathcal{A}$*

$$\begin{aligned} \rho_1(y; w) &\equiv \sum_{k\neq i,j} \tau_k(y)\left(|F_\lambda w|^2 - |U_k w|^2\right) \\ &\le C\mathcal{E}(y)^{1/2} \qquad \textit{for all } w \in \mathbb{R}^3,\ |w| = 1,\ w \cdot n = 0, \end{aligned} \tag{3.8}$$

$$\begin{aligned} \rho_2(y; w) &\equiv \sum_{k\neq i,j} \tau_k(y)\left[|\operatorname{Cof}(F_\lambda)w|^2 - |(\operatorname{Cof} U_k)w|^2\right] \\ &\le C\left[\mathcal{E}(y)^{1/2} + \mathcal{E}(y)\right] \qquad \textit{for all } w \in \mathbb{R}^3,\ |w| = 1,\ w \cdot U_j^{-1}a = 0. \end{aligned} \tag{3.9}$$

Proof. We have by (3.1) and (3.6) that for any $w \in \mathbb{R}^3$ with $|w| = 1$

$$\begin{aligned} \rho_1(y; w) &= \sum_{k=1}^4 \tau_k(y)\left(|F_\lambda w|^2 - |U_k w|^2\right) \\ &= \frac{1}{\operatorname{meas}\Omega}\int_\Omega \left[|F_\lambda w|^2 - |\pi(\nabla y(x))w|^2\right]\ \mathrm{d}x \\ &= -\frac{1}{\operatorname{meas}\Omega}\int_\Omega \left|\left[F_\lambda - \pi(\nabla y(x))\right]w\right|^2\ \mathrm{d}x \\ &\quad + \frac{2}{\operatorname{meas}\Omega}\int_\Omega [\nabla y(x) - \pi(\nabla y(x))]\,w \cdot F_\lambda w\ \mathrm{d}x \\ &\le \frac{2}{\operatorname{meas}\Omega}\int_\Omega [\nabla y(x) - \pi(\nabla y(x))]\,w \cdot F_\lambda w\ \mathrm{d}x. \end{aligned} \tag{3.10}$$

We obtain from the Cauchy-Schwarz inequality and the above inequality (3.7) that

$$\left| \int_\Omega [\nabla y(x) - \pi(\nabla y(x))]\, w \cdot F_\lambda w \;\mathrm{d}x \right| \le C\mathcal{E}(y)^{1/2}.$$

So, it follows from (3.10) that for all $w \in \mathbb{R}^3$ with $|w| = 1$

$$\rho_1(y;w) = \sum_{k=1}^{4} \tau_k(y) \left(|F_\lambda w|^2 - |U_k w|^2\right) \le C\mathcal{E}(y)^{1/2}. \tag{3.11}$$

The result (3.8) then follows from the above inequality (3.11) and (3.3).

Next, we obtain similar estimates for the cofactor. We have from (3.1) and (3.6) that for any $w \in \mathbb{R}^3$, $|w| = 1$,

$$\begin{aligned}
\rho_2(y;w) &= \sum_{k=1}^{4} \tau_k(y) \left[|(\mathrm{Cof}\, F_\lambda)w|^2 - |(\mathrm{Cof}\, U_k)w|^2\right] \\
&= \frac{1}{\mathrm{meas}\,\Omega} \int_\Omega \left[|(\mathrm{Cof}\, F_\lambda)w|^2 - |(\mathrm{Cof}\, \pi(\nabla y(x)))w|^2\right] \mathrm{d}x \\
&= -\frac{1}{\mathrm{meas}\,\Omega} \int_\Omega \Big| [\mathrm{Cof}\, F_\lambda - \mathrm{Cof}\, \pi(\nabla y(x))]\, w \Big|^2 \mathrm{d}x \\
&\quad + \frac{2}{\mathrm{meas}\,\Omega} \int_\Omega [\mathrm{Cof}\, \nabla y(x) - \mathrm{Cof}\, \pi(\nabla y(x))]\, w \cdot (\mathrm{Cof}\, F_\lambda) w \;\mathrm{d}x \\
&\le \frac{2}{\mathrm{meas}\,\Omega} \int_\Omega [\mathrm{Cof}\, \nabla y(x) - \mathrm{Cof}\, \pi(\nabla y(x))]\, w \cdot (\mathrm{Cof}\, F_\lambda) w \;\mathrm{d}x.
\end{aligned} \tag{3.12}$$

Letting $F(x) = \nabla y(x)$ for $x \in \Omega$, we have that $F(x) = (F_{kl}(x)) \in \mathrm{L}^2(\Omega; \mathbb{R}^{3\times 3})$. Now $\pi(\nabla y(x)) \in \mathcal{U}$ for all $x \in \Omega$, so if we set $P(x) = \pi(\nabla y(x))$ for $x \in \Omega$ we have that $P(x) = (P_{kl}(x))$ is uniformly bounded in $\mathrm{L}^\infty(\Omega; \mathbb{R}^{3\times 3})$ for all $y \in \mathcal{A}$. We have for any k, l, p, $q \in \{1, 2, 3\}$ that

$$F_{kl}F_{pq} - P_{kl}P_{pq} = (F_{kl} - P_{kl})P_{pq} + P_{kl}(F_{pq} - P_{pq}) + (F_{kl} - P_{kl})(F_{pq} - P_{pq}).$$

Hence, we have by the Cauchy-Schwarz inequality and (3.7) that

$$\int_\Omega \Big| [\mathrm{Cof}\, \nabla y(x) - \mathrm{Cof}\, \pi(\nabla y(x))]\, w \Big| \;\mathrm{d}x \le C\left[\mathcal{E}(y)^{1/2} + \mathcal{E}(y)\right]. \tag{3.13}$$

Thus, we have from (3.12) and (3.13) that

$$\begin{aligned}
\rho_2(y;w) &= \sum_{k=1}^{4} \tau_k(y) \left[|(\mathrm{Cof}\, F_\lambda)w|^2 - |(\mathrm{Cof}\, U_k)w|^2\right] \\
&\le C\left[\mathcal{E}(y)^{1/2} + \mathcal{E}(y)\right] \qquad \text{for all } w \in \mathbb{R}^3,\ |w| = 1.
\end{aligned} \tag{3.14}$$

The result (3.9) then follows from the above inequality (3.14) and (3.5). □

We will use Lemma 3.1 to establish the following inequality for all material parameters not satisfying certain identities:

$$\tau_k(y) \le C\left[\mathcal{E}(y)^{1/2} + \mathcal{E}(y)\right] \qquad \text{for all } k \in \{1, \ldots, 4\}\backslash\{i, j\} \text{ and all } y \in \mathcal{A}. \tag{3.15}$$

We will also give conditions on the material parameters θ_i, δ_i, and η_i under which this inequality cannot be established. This, in turn, will lead to uniqueness or nonuniqueness of the Young measures associated with energy minimizing sequences of deformations, which we discuss in the next section.

Theorem 3.1. *Assume that* ϕ *satisfies* (2.1), (2.2), *and* (2.4), F_λ *is defined as in* (2.12) *with* $\lambda \in (0,1)$, *and* $\mathcal{A}$ *is defined by* (2.14).

Case 1A: *Suppose* (i,j) *in the definition of* F_λ *determines either of the compound twins with* $n = n_1$. *Then* (3.15) *holds for all the parameters* θ_i, *except those that satisfy*

$$\theta_2^2\left(\theta_3^2+\theta_4^2\right)=\left(\theta_1\theta_3-\theta_4^2\right)^2, \tag{3.16}$$

in which case (3.15) *does not hold for* $\lambda = 1/2$.

Case 1B: *Suppose* (i,j) *in the definition of* F_λ *determines either of the compound twins with* $n = n_2$. *Then* (3.15) *holds for all the parameters* θ_i, *except those that satisfy*

$$\theta_2^2=\theta_1^2+\theta_4^2, \tag{3.17}$$

in which case (3.15) *does not hold for* $\lambda = 1/2$.

Case 1C: *Suppose* (i,j) *and* n *in the definition of* F_λ *determine any of the remaining type I or type II twins. Then* (3.15) *holds for all the parameters* θ_i.

Case 2A: *Suppose* (i,j) *in the definition of* F_λ *determines any of the four compound twins with* $n = n_1$. *Then* (3.15) *holds for all the parameters* δ_i.

Case 2B: *Suppose* (i,j) *in the definition of* F_λ *determines any other twin than those in Case 2A above. Then* (3.15) *does not hold for any choice of the parameters* δ_i.

Case 3A: *Suppose* (i,j) *in the definition of* F_λ *determines either of the compound twins with* $n = n_1$. *Then* (3.15) *holds for all the parameters* η_i, *except those that satisfy*

$$2\eta_1\eta_3=\eta_4^2, \tag{3.18}$$

in which case (3.15) *does not hold for* $\lambda = 1/2$.

Case 3B: *Suppose* (i,j) *in the definition of* F_λ *determines any other twin than those in Case 3A above. Then* (3.15) *holds for any choice of the parameters* η_i.

Proof. **Case 1A.** Assume that $(i,j) = (1,2)$ and $n = e_1$. Since this is a compound twin, it follows from Lemma 2.1 that $U_2^{-1}a$ is parallel to e_3. Let $s,t \in \mathbb{R}$ be such that $w = (s,t,0)^T$ has unit length. Then using Lemma 3.1 we have

$$\begin{aligned}\rho_2(y;w) &= (s^2-t^2)\left(\theta_2^2\left(\theta_3^2+\theta_4^2\right)-\left(\theta_1\theta_3-\theta_4^2\right)^2\right)[\tau_3(y)+\tau_4(y)]\\ &\le C\left[\mathcal{E}(y)^{1/2}+\mathcal{E}(y)\right].\end{aligned}$$

If (3.16) does not hold, then we can choose s and t such that

$$(s^2-t^2)\left(\theta_2^2\left(\theta_3^2+\theta_4^2\right)-\left(\theta_1\theta_3-\theta_4^2\right)^2\right)>0.$$

Therefore,

$$\tau_3(y)+\tau_4(y)\le C\left[\mathcal{E}(y)^{1/2}+\mathcal{E}(y)\right] \qquad \text{for } \theta_2^2\left(\theta_3^2+\theta_4^2\right)\neq\left(\theta_1\theta_3-\theta_4^2\right)^2.$$

Let us now assume that (3.16) holds. We show that if $\lambda = 1/2$, then we can construct a sequence $\{y_n\} \subset \mathcal{A}$ of deformations whose energy converges to 0, but the volume fractions $\tau_3(y_n)$ and $\tau_4(y_n)$ converge to 1/2.

Using Lemma 2.1 and the transformation matrices (2.6), we obtain after a series of calculations that

$$a = \frac{2\hat{\sigma}}{\theta_3^2 + \theta_4^2} \begin{pmatrix} -\theta_4 \\ 0 \\ \theta_3 \end{pmatrix}$$

where

$$\hat{\sigma} = \theta_4(\theta_1 + \theta_3) > 0.$$

Using the fact that

$$F_\lambda = U_2 + \lambda a \otimes e_1,$$

we obtain

$$F_\lambda^T F_\lambda = \begin{pmatrix} \sigma(\lambda) & 0 & (2\lambda - 1)\,\hat{\sigma} \\ 0 & \theta_2^2 & 0 \\ (2\lambda - 1)\,\hat{\sigma} & 0 & \theta_3^2 + \theta_4^2 \end{pmatrix}$$

where

$$\sigma(\lambda) = \theta_1^2 + \theta_4^2 + 4\lambda(\lambda - 1)\frac{\hat{\sigma}^2}{\theta_3^2 + \theta_4^2} \quad .$$

Recall that $R_5^T U_1 R_5 = U_3$ and $R_5^T U_2 R_5 = U_4$, so that

$$QU_1 - U_2 = a \otimes e_1$$

is equivalent to

$$\tilde{Q}U_3 - U_4 = -R_5 a \otimes e_2$$

with $\tilde{Q} = R_5^T Q R_5$. Setting

$$G_\lambda = \lambda \tilde{Q} U_3 + (1 - \lambda) U_4 = R_5^T F_\lambda R_5,$$

we have

$$G_\lambda^T G_\lambda = \begin{pmatrix} \theta_2^2 & 0 & 0 \\ 0 & \sigma(\lambda) & (2\lambda - 1)\,\hat{\sigma} \\ 0 & (2\lambda - 1)\,\hat{\sigma} & \theta_3^2 + \theta_4^2 \end{pmatrix},$$

and we conclude that

$$G_\lambda^T G_\lambda = F_\lambda^T F_\lambda \quad \text{if and only if} \quad \lambda = 1/2 \;\; \text{and} \;\; \sigma(\lambda) = \theta_2^2.$$

However, it is easy to check that $\sigma(1/2) = \theta_2^2$ is equivalent to (3.16). Therefore, if (3.16) holds, then $F_{1/2} = \bar{Q} G_{1/2}$ for some $\bar{Q} \in \mathrm{SO}(3)$, and hence we can construct a sequence of deformations $\{y_n\} \subset \mathcal{A}$ with $\mathcal{E}(y_n) \to 0$ such that the volume fractions $\tau_3(y_n) \to 1/2$ and $\tau_4(y_n) \to 1/2$ [12, 28]. This proves that (3.15) cannot be proven if $\lambda = 1/2$ and (3.16) holds.

The proof for case $(i, j) = (3, 4)$ and $n = e_2$ follows by symmetry since $R_5^T U_1 R_5 = U_3$ and $R_5^T U_2 R_5 = U_4$.

Case 1B. Consider the case $(i, j) = (1, 2)$ and $n = e_3$. Let $s, t \in \mathbb{R}$ be such that $w = (s, t, 0)^T$ has unit length. Then we have

$$\begin{aligned} \rho_1(y; w) &= (s^2 - t^2)\left(\theta_1^2 + \theta_4^2 - \theta_2^2\right)[\tau_3(y) + \tau_4(y)] \\ &\leq C\mathcal{E}(y)^{1/2} \end{aligned}$$

which leads to

$$\tau_3(y) + \tau_4(y) \leq C\mathcal{E}(y)^{1/2} \quad \text{for } \theta_2^2 \neq \theta_1^2 + \theta_4^2.$$

Proceeding now as in the previous part, we can define $G_\lambda = R_5^T F_\lambda R_5$ which corresponds to the compound twin with $(i, j) = (3, 4)$ and $n = e_3$, and again we conclude that

$$G_\lambda^T G_\lambda = F_\lambda^T F_\lambda \quad \text{if and only if} \quad \lambda = 1/2 \text{ and (3.17) holds,}$$

leading again to a sequence of deformations $\{y_n\} \subset \mathcal{A}$ with $\mathcal{E}(y_n) \to 0$ and the volume fractions $\tau_3(y_n) \to 1/2$ and $\tau_4(y_n) \to 1/2$.

The proof for case $(i, j) = (3, 4)$ and $n = e_3$ again follows by symmetry since $R_5^T U_1 R_5 = U_3$ and $R_5^T U_2 R_5 = U_4$.

Case 1C. Consider first the case $(i, j) = (1, 3)$ and $n = e_1 - e_2$. Let $s, t \in \mathbb{R}$ be such that $w = (s, s, t)^T$ has unit length and $st > 0$. Then we have since $\hat{\sigma} > 0$ that

$$\begin{aligned} \rho_1(y; w) &= 4\, st\, \hat{\sigma}\, [\tau_2(y) + \tau_4(y)] \\ &\leq C\mathcal{E}(y)^{1/2}, \end{aligned}$$

leading to

$$\tau_2(y) + \tau_4(y) \leq C\mathcal{E}(y)^{1/2}.$$

Next let $(i, j) = (1, 3)$ and $n = (-\varepsilon_1, -\varepsilon_1, \sqrt{1 - 2\varepsilon_1^2})$. Since this is a type II twin, it follows from Lemma 2.1 that $U_3^{-1} a$ is parallel to $e_1 - e_2$. Let $s, t \in \mathbb{R}$ be such that $w = (s, s, t)^T$ has unit length and $st < 0$. Then we have

$$\begin{aligned} \rho_2(y; w) &= -4\, st\, \hat{\sigma}\, \theta_2^2\, [\tau_2(y) + \tau_4(y)] \\ &\leq C\left[\mathcal{E}(y)^{1/2} + \mathcal{E}(y)\right], \end{aligned}$$

leading to

$$\tau_2(y) + \tau_4(y) \leq C\left[\mathcal{E}(y)^{1/2} + \mathcal{E}(y)\right].$$

The proof for cases $(i, j) = (1, 4)$, $(i, j) = (2, 3)$, and $(i, j) = (2, 4)$ follows from symmetry since $R_2^T U_1 R_2 = U_1$ and $R_2^T U_3 R_2 = U_4$, $R_1^T U_1 R_1 = U_2$ and $R_1^T U_3 R_1 = U_3$, and $R_3^T U_1 R_3 = U_2$ and $R_3^T U_3 R_3 = U_4$.

Case 2A. Assume first that $(i, j) = (1, 2)$ and $n = e_2$. We evaluate $\rho_1(y; e_1)$ to get

$$\begin{aligned} \rho_1(y; e_1) &= [\tau_3(y) + \tau_4(y)]\left(\delta_1^2 - \delta_2^2\right) \\ &\leq C\mathcal{E}(y)^{1/2}, \end{aligned}$$

leading to

$$\tau_3(y) + \tau_4(y) \le C\mathcal{E}(y)^{1/2},$$

since we assumed $\delta_1 > \delta_2 > 0$.

The proof for case $(i, j) = (3, 4)$ and $n = e_1$ follows by symmetry since $R_4^T U_1 R_4 = U_3$ and $R_4^T U_2 R_4 = U_4$.

Assume next that $(i, j) = (1, 3)$ and $n = e_1 - e_2$. Let $w = (e_1 + e_2)/\sqrt{2}$. Then

$$\begin{aligned} \rho_1(y; w) &= [\tau_2(y) + \tau_4(y)]\, 2\delta_4 (\delta_1 + \delta_2) \\ &\le C\mathcal{E}(y)^{1/2} \end{aligned}$$

leading to

$$\tau_2(y) + \tau_4(y) \le C\mathcal{E}(y)^{1/2}.$$

The proof for case $(i, j) = (2, 4)$ and $n = e_1 + e_2$ follows by symmetry since $R_1^T U_1 R_1 = U_2$ and $R_1^T U_3 R_1 = U_4$.

Case 2B. In this case, the energy wells given by the transformation matrices in (2.7) are essentially two-dimensional, so the results given by Bhattacharya and Dolzmann in Example 7.3 in [5] give a proof of the assertion in Case 2B. For completeness, we give a modified version of their proof here.

We set $\delta = \det U_i$ and consider the set $\mathcal{C}$ of symmetric positive definite matrices with determinant equal to δ^2, of the form

$$C = \begin{pmatrix} C_{11} & C_{12} & 0 \\ C_{12} & C_{22} & 0 \\ 0 & 0 & \delta_3^2 \end{pmatrix}.$$

Then there is a one-to-one correspondence between $\mathcal{C}$ and $\mathbb{R}^2$ given by

$$C \mapsto (C_{11} - C_{22}, 2C_{12}), \tag{3.19}$$

and we shall implicitly assume this correspondence in what follows. Under this map,

$$\begin{aligned} U_1^2 &\mapsto \left(\delta_1^2 - \delta_2^2, 2\delta_4(\delta_1 + \delta_2)\right), & U_2^2 &\mapsto \left(\delta_1^2 - \delta_2^2, -2\delta_4(\delta_1 + \delta_2)\right), \\ U_3^2 &\mapsto \left(\delta_2^2 - \delta_1^2, 2\delta_4(\delta_1 + \delta_2)\right), & U_4^2 &\mapsto \left(\delta_2^2 - \delta_1^2, -2\delta_4(\delta_1 + \delta_2)\right). \end{aligned}$$

Similarly as for the energy wells $\mathcal{U}_i$, we define rank-one connections between sets $\mathcal{V}_1 = \mathrm{SO}(3)V_1$ and $\mathcal{V}_2 = \mathrm{SO}(3)V_2$ where $V_1, V_2 \in \mathbb{R}^{3\times 3}$. We say that $\mathcal{V}_1$ and $\mathcal{V}_2$ are rank-one connected if there exist $Q \in \mathrm{SO}(3)$, $a \in \mathbb{R}^3$, $a \neq 0$, and $n \in \mathbb{R}^3$, $n \neq 0$, such that

$$QV_2 = V_1 + a \otimes n.$$

Note that if $\det V_1 = \det V_2$, then $V_1^{-1} a \cdot n = 0$ and $\det(\lambda Q V_2 + (1 - \lambda) V_1) = \det V_1$. Note also that if V_1 and V_2 are symmetric positive definite, we can identify $\mathcal{V}_1$ with V_1^2 and $\mathcal{V}_2$ with V_2^2 and, abusing the language slightly, talk about rank-one connections between V_1^2 and V_2^2, and in particular, between elements of $\mathcal{C}$, or, correspondingly, between points in $\mathbb{R}^2$ under the identification (3.19).

Consider now two distinct symmetric positive definite matrices A, B such that $A^2, B^2 \in \mathcal{C}$. It then follows from Lemma 5 in [28] that there exist two rank-one connections

$$QB = A + a \otimes n$$

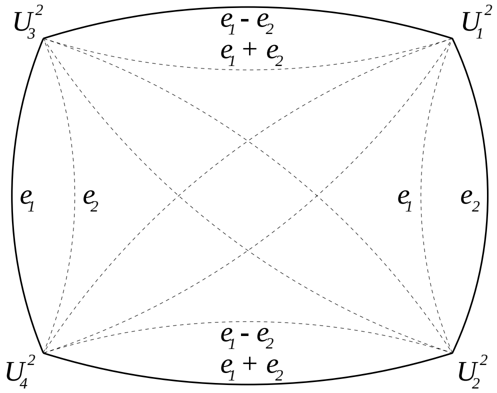

FIGURE 1. The rank-one connections in Case 2.

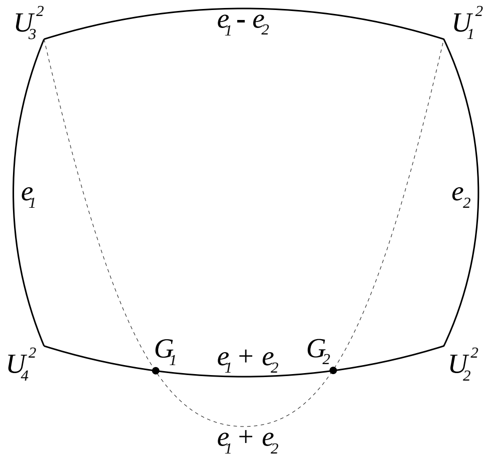

FIGURE 2. The curves of rank-one connections for compound twins with $n = n_2$ must lie in the interior of $\mathcal{D}$.

such that $n \cdot e_3 = a \cdot e_3 = 0$, and $Q = R(\alpha, e_3)$ for some $\alpha \in \mathbb{R}$. This implies that $A^{-1}a \cdot n = 0$, and we can write

$$QB = A(I + s\, n^{\perp} \otimes n)$$

for some $s \in \mathbb{R}$, where $n^{\perp} = R(\pi/2, e_3)\, n$. Thus,

$$B^2 = A^2 + s\,(A^2 n^{\perp} \otimes n + n \otimes A^2 n^{\perp}) + s^2 |An^{\perp}|^2 n \otimes n \tag{3.20}$$

and we conclude that two matrices in $\mathcal{C}$ are rank-one connected if and only if they lie on a quadratic curve parametrized by (3.20) for $s \in \mathbb{R}$.

We define the vertex of a parabola to be its point of maximum curvature. We also define its axis to be the half-line interior to the parabola that extends from the vertex to infinity. Writing $n = |n|(\cos\theta, \sin\theta, 0)$ and letting $\tilde{A} = A^2$ and $\tilde{B} = B^2$, we have

$$\tilde{B}_{11} - \tilde{B}_{22} = \tilde{A}_{11} - \tilde{A}_{22} + s|n|^2 \left(2\tilde{A}_{12} - (\tilde{A}_{11} + \tilde{A}_{22}) \sin 2\theta\right) + s^2 |n|^2 |An^{\perp}|^2 \cos 2\theta,$$

$$2\tilde{B}_{12} = 2\tilde{A}_{12} + 2s|n|^2 \left(\tilde{A}_{22} \cos^2\theta - \tilde{A}_{11} \sin^2\theta\right) + s^2 |n|^2 |An^{\perp}|^2 \sin 2\theta$$

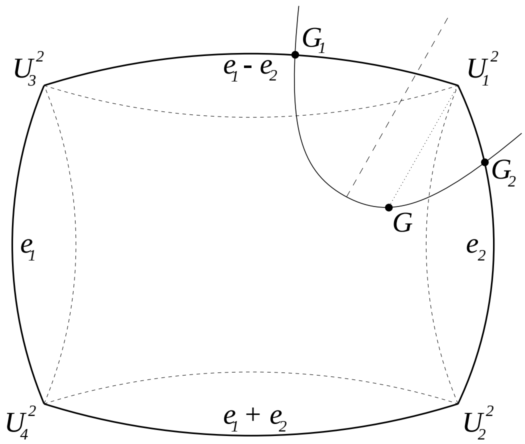

FIGURE 3. There is a curve of rank-one connections through any $G \in \mathcal{D}$ that intersects two of the parabolic curves that bound $\mathcal{D}$.

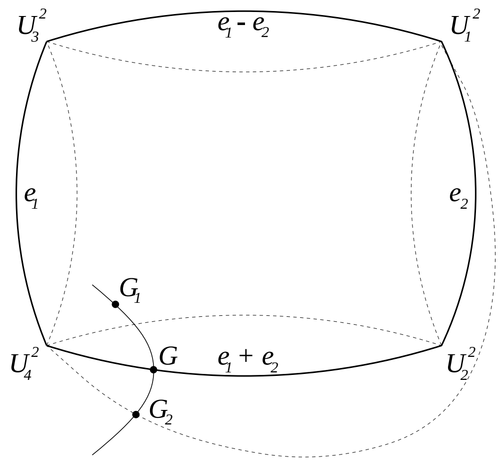

FIGURE 4. The curve of rank-one connections for domain interfaces must lie in the interior of $\mathcal{D}$.

where $|An^{\perp}|^2 > 0$. It can be seen that in the $(C_{11} - C_{22}, 2C_{12})$-plane this curve is a parabola with axis in the direction $(\cos 2\theta, \sin 2\theta)$. We note that this curve cannot cross any point $G \in \mathcal{C}$ twice since otherwise G would be rank-one connected to itself. We can also see that this curve does not degenerate since

$$\left(2\tilde{A}_{12} - (\tilde{A}_{11} + \tilde{A}_{22}) \sin 2\theta\right) \sin 2\theta \neq 2 \left(\tilde{A}_{22} \cos^2 \theta - \tilde{A}_{11} \sin^2 \theta\right) \cos 2\theta,$$

for any positive definite matrix $\tilde{A} \in \mathcal{C}$. Therefore, the four rank-one connections from Case 2A corresponding to compound twins with $n = n_1$ (see Lemma 2.3 for definition of n_1) determine a closed curve through the U_i^2, $i = 1, \ldots, 4$, in the $(C_{11} - C_{22}, 2C_{12})$-plane consisting of four parabolic segments bulging out of the domain $\mathcal{D}$ they are bounding (see Fig. 1).

The other four compound twins with $n = n_2$ determine parabolas through the corresponding U_i^2 with axes pointing in the opposite direction to the axis of the curve of rank-one connections corresponding to its compound twin system for $n = n_1$. We claim that their vertices (thus the whole segments joining U_i^2 to U_j^2 for the corresponding i and j) lie in $\mathcal{D}$. Assume this is not so, that is, assume that there exists a compound twin determined by U_i and U_j with $n = n_2$ such that the vertex of the corresponding parabola does not lie in $\mathcal{D}$. We visualize this example in Figure 2 for the parabolic curve of rank-one connections connecting U_1^2 and U_3^2 with

$n_2 = e_1 + e_2$ corresponding by Lemma 2.1 to

$$(U_3 + \lambda a_2 \otimes n_2)^T (U_3 + \lambda a_2 \otimes n_2) \in \mathcal{C}$$

where

$$n_2 = e_1 + e_2, \qquad a_2 = 2\frac{U_3^{-1} n_2}{|U_3^{-1} n_2|^2} - U_3 n_2.$$

In this case, we suppose that the parabola intersects the curve of rank-one connections connecting U_2^2 and U_4^2 with $n_1 = e_1 + e_2$ at a point

$$G_1 = (U_3 + \lambda a_2 \otimes n_2)^T (U_3 + \lambda a_2 \otimes n_2) \in \mathcal{C}$$

for $0 < \lambda < 1$. For an admissible space of deformations

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

where

$$y_0(x) = \sqrt{G_1} x \quad \text{ for all } x \in \Omega,$$

we can then construct a sequence of laminated deformations $\{y_n\} \subset \mathcal{A}$ with $\mathcal{E}(y_n) \to 0$ such that the volume fractions $\tau_1(y_n) \to \lambda \neq 0$ and $\tau_3(y_n) \to 1 - \lambda \neq 0$. This contradicts the result in Case 2A that since G_1 lies on the curve of rank-one connections connecting U_2^2 and U_4^2 with $n_1 = e_1 + e_2$ we must have that $\tau_1(y_n) \to 0$ and $\tau_3(y_n) \to 0$.

Next, we let $G \in \mathcal{C}$ be a point in the interior of $\mathcal{D}$, and we then construct a sequence of deformations $\{y_n\} \subset \mathcal{A}$ for

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

where

$$y_0(x) = \sqrt{G} x \quad \text{ for all } x \in \Omega,$$

such that $\mathcal{E}(y_n) \to 0$ and $\tau_k(y_n) \not\to 0$ for each $k \in \{1, \dots, 4\}$. This result then provides a proof of Case 2B for the four compound twin families with $n = n_2$. We define $F = \sqrt{G}$ and let

$$F_\lambda = F(I + \lambda\, v^\perp \otimes v)$$

for some $v \in \mathbb{R}^3$, $v \neq 0$. This determines a rank-one curve passing through G that intersects the boundary of $\mathcal{D}$ at two points G_1 and G_2. If we choose v as in Figure 3 such that the axis of the parabola is in the direction $U_i^2 - G$ for some $i = 1, \dots, 4$, then we know that the two intersections G_1 and G_2 lie on different parabolic segments of the boundary of $\mathcal{D}$. We can now construct a sequence of deformations $\{y_n\} \subset \mathcal{A}$ such that $\mathcal{E}(y_n) \to 0$ and $\tau_k(y_n) \not\to 0$ for those k for which U_k^2 participates in the rank-one connections for the parabolic segments on the boundary of $\mathcal{D}$ corresponding to G_1 and G_2. By rotating v we see that we can construct a sequence $\{y_n\} \subset \mathcal{A}$ such that $\mathcal{E}(y_n) \to 0$ and $\tau_k(y_n) \not\to 0$ for every $k \in \{1, \dots, 4\}$.

Finally, if we show that the parabolic segments of rank-one connections extending from U_1^2 to U_4^2 and from U_2^2 to U_3^2 also lie in $\mathcal{D}$, the proof will be complete. However, if this were not so, there would exist a curve of rank-one connections passing through a point G on a parabolic segment of the boundary of $\mathcal{D}$, a point G_1 in the interior of $\mathcal{D}$, and a point G_2 on one of the parabolic segments of rank-one connections extending from U_1^2

to U_4^2 or from U_2^2 to U_3^2 (see Figure 4). However, we can see as above that this violates the result in Case 2A for the boundary segment.

Case 3A. Assume that $(i,j) = (1,3)$ and $n = e_3$. Let $w = (s,t,0)^T$ for $s,t \in \mathbb{R}$ be of unit length. Then we have

$$\begin{aligned} \rho_1(y;w) &= 4\,st\left(2\eta_1\eta_3 - \eta_4^2\right)[\tau_2(y) + \tau_4(y)] \\ &\le C\mathcal{E}(y)^{1/2}. \end{aligned}$$

Choosing the sign of st to be the same as that of $2\eta_1\eta_3 - \eta_4^2$, we conclude that

$$\tau_2(y) + \tau_4(y) \le C\mathcal{E}(y)^{1/2} \quad \text{for } 2\eta_1\eta_3 \ne \eta_4^2.$$

Assume now that $2\eta_1\eta_3 = \eta_4^2$. After a series of calculations, we then find that

$$a = \frac{2\hat\sigma}{(\eta_1+\eta_3)^2}\begin{pmatrix} \eta_1 - \eta_3 \\ -(\eta_1 - \eta_3) \\ -2\eta_4 \end{pmatrix}$$

and

$$F_\lambda^T F_\lambda = \begin{pmatrix} (\eta_1+\eta_3)^2 & 0 & (2\lambda-1)\hat\sigma \\ 0 & (\eta_1+\eta_3)^2 & -(2\lambda-1)\hat\sigma \\ (2\lambda-1)\hat\sigma & -(2\lambda-1)\hat\sigma & \sigma(\lambda) \end{pmatrix}$$

where

$$\hat\sigma = \eta_4(\eta_1 + \eta_2 - \eta_3) > 0$$

and

$$\sigma(\lambda) = \eta_2^2 + 2\eta_4^2 + 8\lambda(\lambda-1)\frac{\hat\sigma^2}{(\eta_1+\eta_3)^2} \quad .$$

Recalling that $R_2^T U_1 R_2 = U_2$ and $R_2^T U_3 R_2 = U_4$, we define $G_\lambda = R_2^T F_\lambda R_2$ as in the proof for Case 1 and conclude that $G_{1/2}^T G_{1/2} = F_{1/2}^T F_{1/2}$ when (3.18) holds. Therefore we can construct a sequence of deformations $\{y_n\} \subset \mathcal{A}$ with $\mathcal{E}(y_n) \to 0$ and the volume fractions $\tau_2(y_n) \to 1/2$ and $\tau_4(y_n) \to 1/2$.
The proof for case $(i,j) = (2,4)$ and $n = e_3$ follows by symmetry since $R_2^T U_1 R_2 = U_2$ and $R_2^T U_3 R_2 = U_4$.

Case 3B. Consider first the case $(i,j) = (1,3)$ and $n = e_1 - e_2$. Since this is a compound twin, we have that $U_3^{-1}a$ is parallel to e_3. Let $s,t \in \mathbb{R}$ be such that $w = (s,t,0)^T$ has unit length and $st < 0$. We then have that

$$\begin{aligned} \rho_2(y;w) &= -4\,st\left(2(\eta_1\eta_2 - \eta_4^2)(\eta_2\eta_3 + \eta_4^2) + \eta_4^2(\eta_1+\eta_3)^2\right)[\tau_2(y) + \tau_4(y)] \\ &\le C\left[\mathcal{E}(y)^{1/2} + \mathcal{E}(y)\right]. \end{aligned}$$

Since we have $\eta_1\eta_2 - \eta_4^2 > 0$, it follows that

$$\tau_2(y) + \tau_4(y) \le C\left[\mathcal{E}(y)^{1/2} + \mathcal{E}(y)\right].$$

The proof for case $(i,j) = (2,4)$ and $n = e_1 + e_2$ follows by symmetry since $R_2^T U_1 R_2 = U_2$ and $R_2^T U_3 R_2 = U_4$.

Consider the case $(i, j) = (1, 2)$ and the type I interface $n = e_2$. Let $s, t \in \mathbb{R}$ be such that $w = (s, 0, t)^T$ has unit length and $st > 0$. We then have since $\hat{\sigma} > 0$ that

$$\begin{aligned} \rho_1(y; w) &= 4\, st\, \hat{\sigma}\, [\tau_2(y) + \tau_4(y)] \\ &\leq C\mathcal{E}(y)^{1/2}, \end{aligned}$$

leading to

$$\tau_3(y) + \tau_4(y) \leq C\mathcal{E}(y)^{1/2}.$$

Consider next the case $(i, j) = (1, 2)$ and the type II interface $n = (\varepsilon_2, 0, -\sqrt{1 - \varepsilon_2^2})$. Since this is a type II twin, we have that $U_2^{-1}a$ is parallel to e_2. Let $s, t \in \mathbb{R}$ be such that $w = (s, 0, t)^T$ has unit length and $st < 0$. We then have that

$$\begin{aligned} \rho_2(y; w) &= -4\, st\, \hat{\sigma}\, (\eta_1 + \eta_3)^2\, [\tau_3(y) + \tau_4(y)] \\ &\leq C\left[\mathcal{E}(y)^{1/2} + \mathcal{E}(y)\right], \end{aligned}$$

leading to

$$\tau_3(y) + \tau_4(y) \leq C\left[\mathcal{E}(y)^{1/2} + \mathcal{E}(y)\right].$$

The proof for the interfaces for cases $(i, j) = (1, 4)$, $(i, j) = (2, 3)$, and $(i, j) = (3, 4)$ follows by symmetry since $R_4^T U_1 R_4 = U_1$ and $R_4^T U_2 R_4 = U_4$, $R_7^T U_1 R_7 = U_2$ and $R_7^T U_2 R_7 = U_3$, and $R_3^T U_1 R_3 = U_3$ and $R_3^T U_2 R_3 = U_4$. □

4. The stability and uniqueness of the microstructure

In the previous section, we proved the estimate

$$\tau_k(y) \leq C\left[\mathcal{E}(y)^{1/2} + \mathcal{E}(y)\right] \quad \text{for } k \in \{1, \dots, 4\}\backslash\{i, j\} \text{ and all } y \in \mathcal{A}, \tag{4.1}$$

for all of the tetragonal to monoclinic transformations except when the lattice parameters satisfy the identities given in Theorem 3.1. We recall that

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

where

$$y_0(x) = [\lambda Q U_i + (1 - \lambda) U_j]x \qquad \text{for all } x \in \Omega.$$

The results in this section for the tetragonal to monoclinic transformations can be deduced from the inequality (4.1) by the identical arguments used to deduce the results from (4.1) for the cubic to orthorhombic case [6] by making the obvious modifications in the argument to change $N = 6$ to $N = 4$. For this reason, we state the results given in this section without proof.

We also recall that the energy density ϕ is minimized on the union $\mathcal{U}$ of the four energy wells

$$\mathcal{U}_i = \mathrm{SO}(3)U_i = \{RU_i : R \in \mathrm{SO}(3)\} \qquad \text{for } i = 1, \dots, 4,$$

and that ϕ is continuous and satisfies the growth condition

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

We shall also assume that the lattice parameters do not satisfy the identities given in Lemma 3.1 so that the inequality (4.1) holds.

Our first theorem in this section gives estimates for the derivative of the limiting macroscopic deformation y in any direction tangential to the parallel layers of the laminate, for the L^2 approximation of the limiting macroscopic deformation, and for the weak convergence of the limiting macroscopic deformation.

Theorem 4.1. *(1) For any $w \in \mathbb{R}^3$ such that $w \cdot n = 0$ and $|w| = 1$, we have*

$$\int_\Omega |[\nabla y(x) - \nabla y_0(x)]\, w|^2 \ \mathrm{d}x \le C \left[\mathcal{E}(y)^{1/2} + \mathcal{E}(y)\right] \qquad \textit{for all } y \in \mathcal{A}.$$

(2) We have

$$\int_\Omega |y(x) - y_0(x)|^2 \ \mathrm{d}x \le C \left[\mathcal{E}(y)^{1/2} + \mathcal{E}(y)\right] \qquad \textit{for all } y \in \mathcal{A}.$$

(3) For any Lipschitz domain $\omega \subset \Omega$, there exists a constant $C = C(\omega) > 0$ such that

$$\left\| \int_\omega [\nabla y(x) - \nabla y_0(x)] \ \mathrm{d}x \right\| \le C \left[\mathcal{E}(y)^{1/8} + \mathcal{E}(y)^{1/2}\right] \qquad \textit{for all } y \in \mathcal{A}.$$

The following corollary shows that the deformation gradients of energy-minimizing sequences of deformations must oscillate with a length scale that converges to zero.

Corollary 4.1. *There does not exist any $y \in \mathcal{A}$ such that*

$$\mathcal{E}(y) = \min_{z \in \mathcal{A}} \mathcal{E}(z).$$

For fixed $i, j \in \{1, \ldots, 4\}$ with $i \neq j$, we can define a projection $\pi_{ij} : \mathbb{R}^{3\times 3} \to \mathcal{U}_i \cup \mathcal{U}_j$ by

$$\|F - \pi_{ij}(F)\| = \min_{G \in \mathcal{U}_i \cup \mathcal{U}_j} \|F - G\| \qquad \text{for all } F \in \mathbb{R}^{3\times 3}.$$

We also define the operators $\Theta : \mathbb{R}^{3\times 3} \to \mathrm{SO}(3)$ and $\Pi : \mathbb{R}^{3\times 3} \to \{QU_i,\, U_j\}$ by the unique decomposition

$$\pi_{ij}(F) = \Theta(F)\Pi(F) \qquad \text{for all } F \in \mathbb{R}^{3\times 3}.$$

The following theorem proves that the deformation gradients of energy-minimizing sequences of deformations must oscillate between QU_i and U_j.

Theorem 4.2. *We have*

$$\int_\Omega \|\nabla y(x) - \Pi(\nabla y(x))\|^2 \ \mathrm{d}x \le C \left[\mathcal{E}(y)^{1/2} + \mathcal{E}(y)\right] \qquad \textit{for all } y \in \mathcal{A}.$$

For any subset $\omega \subset \Omega$, $\rho > 0$, and $y \in \mathcal{A}$, we define the sets

$$\omega^i_\rho(y) = \{x \in \omega : \Pi(\nabla y(x)) = QU_i \text{ and } \|\nabla y(x) - QU_i\| < \rho\}\,,$$
$$\omega^j_\rho(y) = \{x \in \omega : \Pi(\nabla y(x)) = U_j \text{ and } \|\nabla y(x) - U_j\| < \rho\}\,.$$

The next theorem demonstrates that the deformation gradients of energy-minimizing sequences of deformations must oscillate with local volume fraction λ at QU_i and local volume fraction $1 - \lambda$ at U_j. It also demonstrates that the Young measure for this problem is unique [3, 28] and is given by

$$\nu = \lambda \delta_{QU_i} + (1 - \lambda)\delta_{U_j}.$$

Theorem 4.3. *For any Lipschitz domain $\omega \subset \Omega$ and any $\rho > 0$, there exists a constant $C = C(\omega, \rho) > 0$ such that for all $y \in \mathcal{A}$*

$$\left|\frac{\operatorname{meas}\omega_\rho^i(y)}{\operatorname{meas}\omega} - \lambda\right| + \left|\frac{\operatorname{meas}\omega_\rho^j(y)}{\operatorname{meas}\omega} - (1-\lambda)\right| \le C\left[\mathcal{E}(y)^{1/8} + \mathcal{E}(y)^{1/2}\right].$$

We now denote by $\mathcal{V}$ the Sobolev space of all measurable functions $f : \Omega \times \mathbb{R}^{3\times 3} \to \mathbb{R}$ such that

$$\|f\|_{\mathcal{V}}^2 = \int_\Omega \left\{ \left[\operatorname*{ess\,sup}_{F\in\mathbb{R}^{3\times 3}} \|\nabla_F f(x,F)\|\right]^2 + |\nabla z_f(x) n|^2 + z_f(x)^2 \right\} \, \mathrm{d}x < \infty,$$

where $z_f : \Omega \to \mathbb{R}$ is defined by

$$z_f(x) = f(x, QU_i) - f(x, U_j) \qquad \text{for all } x \in \Omega.$$

The final theorem in this section gives an estimate for the weak convergence of nonlinear functions of the deformation gradient.

Theorem 4.4. *We have*

$$\left|\int_\Omega \{f(x, \nabla y(x)) - [\lambda f(x, QU_i) + (1-\lambda) f(x, U_j)]\} \, \mathrm{d}x\right|$$
$$\le C\|f\|_{\mathcal{V}}\left[\mathcal{E}(y)^{1/4} + \mathcal{E}(y)^{1/2}\right] \qquad \textit{for all } f \in \mathcal{V} \textit{ and all } y \in \mathcal{A}.$$

5. The finite element approximation of microstructure

The simplest finite element approximation of the variational problem

$$\inf_{v\in\mathcal{A}} \mathcal{E}(v)$$

is given by

$$\inf_{v_h\in\mathcal{A}_h} \mathcal{E}(v_h)$$

where $\mathcal{A}_h$ is a finite-dimensional subspace of $\mathcal{A}$ defined for $h \in (0, h_0]$ for some $h_0 > 0$. The following approximation theorem for the energy can be proven for the most widely used P_k or Q_k type conforming finite elements on quasi-regular meshes, in particular for the P_1 linear elements defined on tetrahedra and the Q_1 trilinear elements defined on rectangular parallelepipeds [6, 12, 23–25, 27, 28].

Theorem 5.1. *For each $h \in (0, h_0]$, there exists $y_h \in \mathcal{A}_h$ such that*

$$\mathcal{E}(y_h) = \min_{z_h\in\mathcal{A}_h} \mathcal{E}(z_h) \le Ch^{1/2}. \tag{5.1}$$

For the remainder of this section, we again recall that the energy density ϕ is minimized on the union $\mathcal{U}$ of the four energy wells

$$\mathcal{U}_i = \mathrm{SO}(3)U_i = \{RU_i : R \in \mathrm{SO}(3)\} \qquad \text{for } i = 1, \ldots, 4,$$

and that ϕ is continuous and satisfies the growth condition

$$\phi(F) \ge \kappa\,\|F - \pi(F)\|^2 \qquad \text{for all } F \in \mathbb{R}^{3\times 3}.$$

We shall also assume that the lattice parameters do not satisfy the identities given in Lemma 3.1 so that the results of the previous section hold. In this case, the following corollaries for the finite element approximation follow directly from the above estimate for the approximation of the energy (5.1). We assume below that $y_h \in \mathcal{A}_h$ is a finite element approximation satisfying the quasi-optimality condition

$$\mathcal{E}(y_h) \leq \sigma \inf_{z_h \in \mathcal{A}_h} \mathcal{E}(z_h) \tag{5.2}$$

for some constant $\sigma \geq 1$ independent of h.

Corollary 5.1.
(1) There exists a positive constant C such that for any $y_h \in \mathcal{A}_h$ satisfying (5.2) *we have*

$$\int_\Omega |y_h(x) - y_0(x)|^2 \, \mathrm{d}x \leq Ch^{1/4}$$

and

$$\int_\Omega \|\nabla y_h(x) - \Pi(\nabla y_h(x))\|^2 \, \mathrm{d}x \leq Ch^{1/4}.$$

(2) For any $w \in \mathbb{R}^3$ such that $w \cdot n = 0$ and $|w| = 1$, we have

$$\int_\Omega |[\nabla y_h(x) - \nabla y_0(x)]\, w|^2 \, \mathrm{d}x \leq Ch^{1/4}$$

for any $y_h \in \mathcal{A}_h$ satisfying (5.2).
(3) If $\omega \subset \Omega$ is a Lipschitz domain, then there exists a constant $C = C(\omega) > 0$ such that for any $y_h \in \mathcal{A}_h$ satisfying (5.2) *we have*

$$\left\| \int_\omega [\nabla y_h(x) - \nabla y_0(x)] \, \mathrm{d}x \right\| \leq Ch^{1/16}.$$

Corollary 5.2. *(1) If $\omega \subset \Omega$ is a Lipschitz domain and $\rho > 0$, then there exists a constant $C = C(\omega, \rho) > 0$ such that for any $y_h \in \mathcal{A}_h$ satisfying* (5.2)

$$\left| \frac{\operatorname{meas} \omega_\rho^i(y_h)}{\operatorname{meas} \omega} - \lambda \right| + \left| \frac{\operatorname{meas} \omega_\rho^j(y_h)}{\operatorname{meas} \omega} - (1-\lambda) \right| \leq Ch^{1/16}.$$

(2) We have

$$\left| \int_\Omega \{ f(x, \nabla y_h(x)) - [\lambda f(x, QU_i) + (1-\lambda) f(x, U_j)] \} \, \mathrm{d}x \right| \leq C \|f\|_{\mathcal{V}}\, h^{1/8}$$

for any $f \in \mathcal{V}$ and any $y_h \in \mathcal{A}_h$ satisfying (5.2).

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