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STABILITY OF MICROSTRUCTURES FOR SOME MARTENSITIC TRANSFORMATIONS

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Abstract. We analyze the stability of laminated microstructure for martensitic crystals that undergo cubic to trigonal, orthorhombic to triclinic, and trigonal to monoclinic transformations. We show that the microstructure is unique and stable for all laminates except when the lattice parameters satisfy certain identities.

1. Introduction

Martensitic crystals form microstructures that mix multiple symmetry-related variants. In the geometrically nonlinear theory of martensite [1–5], the free energy density of the crystal is minimized on the energy wells representing the martensitic variants. It follows as a consequence of this theory that energy-minimizing deformations for a large class of boundary conditions must have a microstructure with an infinitesimal length scale [1–4].

We have developed an analysis to determine what quantities remain stable for deformations of low energy that satisfy boundary conditions compatible with a simple laminate [4, 6–9]. We have used this analysis to study the orthorhombic to monoclinic transformation (two-well) [6], the cubic to tetragonal transformation (three-well) [7], the cubic to orthorhombic transformation (six-well) [8], and the tetragonal to monoclinic transformation (four-well) [9]. The analysis of the stability of microstructures becomes more difficult for transformations with a larger number of variants (or for transformations with a greater change of symmetry) because the existence of the additional energy-minimizing variants gives the crystal more freedom to deform without increasing the energy. In fact, we have shown that the simply laminated microstructure is not stable for some lattice parameters for some transformations.

In this work, we study the stability of laminated microstructures of martensitic crystals that can undergo cubic to trigonal, orthorhombic to triclinic, and trigonal to monoclinic transformations. For the cubic to trigonal and orthorhombic to triclinic transformations there are four symmetry-related transformation strains, and for the trigonal to monoclinic transformation there are three symmetry-related transformations strains.

We first used our theory to study the stability of microstructure in ferromagnetic crystals [10]. Our theory can be directly applied to the analysis of conforming finite element approximations of laminated microstructure [4, 6–9]. Our theory has also been extended to the analysis of laminates with varying volume fraction [11] and nonconforming finite element approximations [12]. Related results on the numerical analysis of nonconvex variational problems can be found, for example, in [13–21].

The paper is organized as follows. In Section 2, we describe the geometrically nonlinear theory of martensite. We refer the reader to [1, 2] and to the introductory article by [4] for a more detailed discussion of the geometrically nonlinear theory of martensite. In Section 3, we present some useful definitions and the results from [8, 22] which allow us to reduce the multi-well problem to a mixture of two strains.

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In Sections 4–6, the transformation strains and possible interfaces for cubic to trigonal, orthorhombic to triclinic transformation and for trigonal to monoclinic transformation are presented. If the lattice parameters do not satisfy certain identities, we give bounds on the volume fraction of the variants that do not participate in the laminate. If the lattice parameters do satisfy these identities, we are able in these cases to show that the microstructure is not stable. These estimates are used in Section 7 to establish a series of error bounds in terms of the elastic energy of the deformations for the 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. The calculations in Sections 4–6 are performed using Mathematica [23].

2. The continuum model

We take the reference configuration $\Omega \subset \mathbb{R}^3$ to be the austenite phase of the crystal and assume that Ω is a bounded domain with a Lipschitz continuous boundary $\partial\Omega$. We denote deformations of the austenitic phase 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 consider the variational problem to minimize the Helmholtz free energy

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

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 assume that the free energy density is frame-indifferent, that is, rigid body rotations of the reference configuration do not affect the free energy density

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

and that the free energy reflects the symmetry of the austenite phase, 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 $\mathcal{G}$ is the symmetry group of the austenite.

A transformation (Bain) strain is a positive definite matrix $U_1 \in \mathbb{R}^{3\times 3}$ which minimizes the free energy density and satisfies

$$R_i^T U_1 R_i = U_1 \tag{2.3}$$

for some of R_i belonging to the symmetry group of the austenite phase. Those R_i for which (2.3) holds form the symmetry group of the martensite group. It follows from the symmetry (2.2) of the energy density that the energy density has local minima at the set of variants U_i, $(i = 1, \ldots, n)$ defined by

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

It also follows by the frame-indifference (2.1) of the energy density that the energy density is minimized on the union $\mathcal{U} = \mathcal{U}_1 \bigcup \cdots \bigcup \mathcal{U}_n$ of the n energy wells

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

By adding a constant, we assume that the minimum value of ϕ is 0. Finally, we assume the following two conditions about the free energy ϕ :

(1) We assume that $\phi(F)$ is continuous and satisfies the growth condition for F near $\mathcal{U}$ given by

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

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

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

Such a projection exists for any $F \in \mathbb{R}^{3\times 3}$ since the set $\mathcal{U}$ is compact, although it generally will not be unique.

(2) We also assume that the free energy density $\phi(F)$ satisfies the growth condition for large F given by

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

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 [24]. We can then denote the set of deformations of finite energy by

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

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

$$\mathcal{A} = \{\, y \in W^\phi : y(x) = y_0(x) \text{ for all } x \in \partial\Omega \,\}. \tag{2.5}$$

In this work we are interested in a simple laminate. For fixed $i, j \in \{1, \dots, n\}$ with $i \neq j$, we suppose that the interface equation

$$QU_i = U_j + a \otimes n \tag{2.6}$$

is satisfied for some $Q \in SO(3)$, $a \in \mathbb{R}^3$, and $n \in \mathbb{R}^3$ with $a,\, n \neq 0$. Here the tensor product is defined by $v \otimes w = v_i w_j$. In this case, we say that the energy wells $\mathcal{U}_i$ and $\mathcal{U}_j$ are rank-one connected. Denoting

$$F_\lambda = \lambda QU_i + (1-\lambda)U_j = U_j + \lambda a \otimes n \tag{2.7}$$

for any fixed $\lambda \in (0,1)$, we define the boundary conditions in (2.5) to be

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

The following lemma can be proven 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 [4,16].

Lemma 2.1. *Let $\mathcal{A}$ be defined as in* (2.5) *with boundary conditions given by* (2)*. 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

In this section, we define the volume fraction of the martensitic phase and present the main lemma used in the paper. For each phase $k \in \{1, \dots, n\}$ 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

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

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

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

It follows from the rank-one connection (2.6) and and the definition of F_λ (2.7) that

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

We thus have the identity

$$F_\lambda w = QU_i w = U_j w \qquad \text{for all } w \in \mathbb{R}^3,\ w \cdot n = 0, \tag{3.1}$$

so we have that

$$|F_\lambda w| = |U_i w| = |U_j w| \qquad \text{for all } w \in \mathbb{R}^3,\ w \cdot n = 0. \tag{3.2}$$

Identities similar to (3.1) and (3.2) hold for the cofactors of U_i, U_j and F_λ. Recall that the cofactor of a nonsingular $A \in \mathbb{R}^{3\times 3}$ is defined by $\operatorname{Cof} A = (\det A)A^{-T}$. Since $\det(QU_i) = \det U_j > 0$, we have that $U_j^{-1}a \cdot n = 0$, and hence,

$$\operatorname{Cof} F_\lambda = (\operatorname{Cof} U_j)\,(I - \lambda n \otimes U_j^{-1}a). \tag{3.3}$$

We then obtain from (3.3) that

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

so

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

We also recall that since the subdeterminant of the gradient is a null-Lagrangian [25], we have for $y \in \mathcal{A}$ that

$$\int_\Omega \nabla y(x)\,dx = \int_\Omega F_\lambda\,dx,$$
$$\int_\Omega \operatorname{Cof} \nabla y(x)\,dx = \int_\Omega \operatorname{Cof} F_\lambda\,dx.$$

Finally, it follows from (2.4) that

$$\int_\Omega \|\nabla y(x) - \pi\left(\nabla y(x)\right)\|^2\,dx \le \kappa^{-1}\mathcal{E}(y) \qquad \text{for all } y \in \mathcal{A}.$$

The following result is proved in [22]. In the estimates below, C will denote a generic positive constant that is independent of $y \in \mathcal{A}$.

Lemma 3.1. *Given $i, j \in \{1, \ldots, n\}$, $Q \in SO(3)$, and a, $n \in \mathbb{R}^3$, a, $n \neq 0$ satisfying the interface equation (2.6), there exists a constant $C > 0$ such that for any $y \in \mathcal{A}$*

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

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

Using Lemma 3.1 we will establish the following inequality for all lattice parameters not satisfying certain identities:

$$\tau_k(y) \le C\left[\mathcal{E}(y)^{1/2} + \mathcal{E}(y)\right] \qquad \text{for all } k \in \{1, \ldots, n\}\backslash\{i, j\} \text{ and all } y \in \mathcal{A}. \tag{3.4}$$

We will show in Section 7 that the stability of the microstructure for a laminate follows from the inequality (3.4). The conditions on the lattice parameters under which the inequality (3.4) cannot be established will be derived for several phase transformations in the following sections. The uniqueness or nonuniqueness of the Young measures associated with energy minimizing sequences of deformations follows from the stability or instability of the microstructure.

The following lemma (which is a special case of Proposition 2.2 in [26]) will be used to construct rank-one connections. This lemma can be verified by direct substitution into the interface equation. In what follows, we denote the rotation of θ radians about the nonzero vector m by $R(\theta, m)$.

Lemma 3.2. *Assume that U_i, $U_j \in \mathbb{R}^{3\times 3}$ are positive definite and symmetric and that there exists a unit vector $m \in \mathbb{R}^3$, and a rotation $R(\pi, m) \in \mathcal{G}$ such that*

$$U_i = R(\pi, m)^T U_j R(\pi, m). \tag{3.5}$$

Then there exist exactly two solutions to the interface equation (2.6)*, 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

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

4. The stability of the simple laminate for the cubic to trigonal phase transformation

The symmetry group of the cubic (high temperature) phase $\mathcal{G} = \{ R_1, \dots, R_{24} \}$ 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 $\{e_1, e_2, e_3\}$ is an orthonormal basis of $\mathbb{R}^3$. We assume that $\{e_1, e_2, e_3\}$ is an orthonormal basis of $\mathbb{R}^3$. The variants of the trigonal phase are described solely by the trigonal angle ψ, $0 < \psi < \frac{4\pi}{3}$, [27]:

$$U_1 = \begin{bmatrix} \eta_1 & \eta_2 & \eta_2 \\ \eta_2 & \eta_1 & \eta_2 \\ \eta_2 & \eta_2 & \eta_1 \end{bmatrix}, \; U_2 = \begin{bmatrix} \eta_1 & -\eta_2 & \eta_2 \\ -\eta_2 & \eta_1 & -\eta_2 \\ \eta_2 & -\eta_2 & \eta_1 \end{bmatrix}, \; U_3 = \begin{bmatrix} \eta_1 & \eta_2 & -\eta_2 \\ \eta_2 & \eta_1 & -\eta_2 \\ -\eta_2 & -\eta_2 & \eta_1 \end{bmatrix},$$

$$U_4 = \begin{bmatrix} \eta_1 & -\eta_2 & -\eta_2 \\ -\eta_2 & \eta_1 & \eta_2 \\ -\eta_2 & \eta_2 & \eta_1 \end{bmatrix},$$

where $\eta_1 = (\sqrt{1 + 2\cos(\psi)} + 2\sqrt{1 - \cos(\psi)})/3$ and $\eta_2 = (\sqrt{1 + 2\cos(\psi)} - \sqrt{1 - \cos(\psi)})/3$. It follows that

$$\eta_1 > 0, \; \eta_2 > 0 \quad \text{and} \quad \eta_1 > \eta_2 > -\frac{\eta_1}{2}. \tag{4.1}$$

A two-fold rotation with axis e where e is a unit vector can be expressed as $R(\pi, e) = -I + 2e \otimes e$. The following relations can be easily justified:

$$\begin{aligned} R(\pi, e_2)^T U_1 R(\pi, e_2) &= R(\pi, e_1 + e_3)^T U_1 R(\pi, e_1 + e_3) = U_2, \\ R(\pi, e_3)^T U_1 R(\pi, e_3) &= R(\pi, e_1 + e_2)^T U_1 R(\pi, e_1 + e_2) = U_3, \\ R(\pi, e_1)^T U_1 R(\pi, e_1) &= R(\pi, e_2 + e_3)^T U_1 R(\pi, e_2 + e_3) = U_4, \\ R(\pi, e_1)^T U_2 R(\pi, e_1) &= R(\pi, e_2 - e_3)^T U_2 R(\pi, e_2 - e_3) = U_3, \\ R(\pi, e_3)^T U_2 R(\pi, e_3) &= R(\pi, e_1 - e_2)^T U_2 R(\pi, e_1 - e_2) = U_4, \\ R(\pi, e_2)^T U_3 R(\pi, e_2) &= R(\pi, e_1 - e_3)^T U_3 R(\pi, e_1 - e_3) = U_4. \end{aligned} \tag{4.2}$$

Using these relations between the variants of low temperature martensite we can solve the interface equations (2.6) for each (i, j) and classify these interfaces.

Lemma 4.1. *1. For each $i \in \{1, \dots, 4\}$, the energy well $\mathcal{U}_i$ is not rank-one connected to itself.*

2. For any $i, j \in \{1, \dots, 4\}$, with $i \neq j$, there are exactly two solutions to the interface equation (2.6). The classification of the solutions to the interface equation is given in Table 1.

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 [1, 4]

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

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

Using (4.2) and lemma 3.2, we can obtain the two solutions of the interface equation (2.6). These solutions are given in Table 1. □

TABLE 1. Classification of the interfaces for the cubic to trigonal transformation.

(i,j)	TYPE OF THE TWIN	INTERFACE NORMAL	
$(1,2)$	compound	$n_1 = e_2$	
	compound	$n_2 = e_1 + e_3$	
$(1,3)$	compound	$n_1 = e_3$	
	compound	$n_2 = e_1 + e_2$	
$(1,4)$	compound	$n_1 = e_1$	
	compound	$n_2 = e_2 + e_3$	
$(2,3)$	compound	$n_1 = e_1$	
	compound	$n_2 = e_2 - e_3$	
$(2,4)$	compound	$n_1 = e_3$	
	compound	$n_2 = e_1 - e_2$	
$(3,4)$	compound	$n_1 = e_2$	
	compound	$n_2 = e_1 - e_3$	

Now we formulate the main theorem of this section that states that (3.4) holds for any simple laminate for the cubic to trigonal transformation.

Theorem 4.1. *Assume that* ϕ *satisfies* (2.1), (2.2), *and* (2.4), F_λ *is defined as in* (2.7) *for any* $i, j \in \{1, \dots, 4\}$, *with* $i \neq j$, $\lambda \in (0,1)$, *and* $\mathcal{A}$ *is defined by* (2.5). *Then* (3.4) *holds for all parameters* η_i.

Proof. All laminates mixing QU_i and U_j for (i,j), $i,j = 1,2,3,4$, with $n = n_1$ can be analyzed identically by symmetry. Thus, without loss of generality we assume that $(i,j) = (1,2)$ and $n = e_2$. Let ξ and ζ be such that $w = (\xi, 0, \zeta)$ has unit length. Then $\rho_1(y;w)$ can be evaluated for our choice of w (see Lemma 3.1),

$$\rho_1(y;w) = 4\xi\zeta\eta_2(\eta_2 + 2\eta_1)(\tau_3 + \tau_4).$$

Consequently, if

$$\eta_2(\eta_2 + 2\eta_1) \neq 0,$$

then we can choose ξ and ζ such that

$$\xi\zeta\eta_2(\eta_2 + 2\eta_1) > 0.$$

Thus, it follows from Lemma 3.1 that

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

since $\eta_2(\eta_2 + 2\eta_1) \neq 0$ follows from (4.1).

All possible laminates mixing QU_i and U_j for (i,j), $i,j = 1,2,3,4$, with $n = n_2$ can also be analyzed identically by symmetry. Without loss of generality, we assume that $(i,j) = (1,2)$ and $n = e_1 + e_3$. Choosing $w = (1/\sqrt{2}, 0, -1/\sqrt{2})$, we calculate $\rho_1(y;w)$ and $\rho_2(y;w)$ (see Lemma 3.1) to obtain:

$$\rho_1(y;w) = -2\eta_2(\eta_2 + 2\eta_1)(\tau_3 + \tau_4),$$
$$\rho_2(y;w) = 2\eta_2(\eta_2 - \eta_1)^2(\eta_2 + 2\eta_1)(\tau_3 + \tau_4).$$

Thus, depending on the sign of η_2, we can use either $\rho_1(y;w)$ or $\rho_2(y;w)$ to show that

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

holds for all possible η_1 and η_2 since it follows from (4.1) that

$$\eta_2 + 2\eta_1 \neq 0,$$
$$(\eta_2 - \eta_1)^2(\eta_2 + 2\eta_1) \neq 0.$$

□

TABLE 2. Classification of the interfaces for the orthorhombic to triclinic transformation.

(i,j)	TYPE OF THE TWIN	INTERFACE NORMAL	
$(1,2)$	I II	$n_1 = e_1$ $n_2 = (0, \eta_5\eta_6 + \eta_4\eta_1 + \eta_4\eta_2, \eta_4\eta_6 + \eta_5\eta_1 + \eta_5\eta_3)$	
$(1,3)$	I II	$n_1 = e_2$ $n_2 = (\eta_5\eta_6 + \eta_4\eta_1 + \eta_4\eta_2, 0, \eta_4\eta_5 + \eta_6\eta_2 + \eta_6\eta_3)$	
$(1,4)$	I II	$n_1 = e_3$ $n_2 = (\eta_4\eta_6 + \eta_5\eta_1 + \eta_5\eta_3, \eta_4\eta_5 + \eta_6\eta_2 + \eta_6\eta_3, 0)$	
$(2,3)$	I II	$n_1 = e_3$ $n_2 = \big(-(\eta_4\eta_6 + \eta_5\eta_1 + \eta_5\eta_3), \eta_4\eta_5 + \eta_6\eta_2 + \eta_6\eta_3, 0\big)$	
$(2,4)$	I II	$n_1 = e_2$ $n_2 = \big(\eta_5\eta_6 + \eta_4\eta_1 + \eta_4\eta_2, 0, -(\eta_4\eta_5 + \eta_6\eta_2 + \eta_6\eta_3)\big)$	
$(3,4)$	I II	$n_1 = e_1$ $n_2 = \big(0, \eta_5\eta_6 + \eta_4\eta_1 + \eta_4\eta_2, -(\eta_4\eta_6 + \eta_5\eta_1 + \eta_5\eta_3)\big)$	

5. THE STABILITY OF THE LAMINATE FOR ORTHORHOMBIC TO TRICLINIC PHASE TRANSFORMATIONS

The symmetry group of the orthorhombic (high-temperature) phase is composed of the rotations of π radians about an orthogonal set of axes:

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

where $\{e_1, e_2, e_3\}$ is a right-handed orthonormal basis in $\mathbb{R}^3$. The variants of the triclinic (low-temperature) phase are defined as $\{R^T U_1 R : R \in \mathcal{G}\}$:

$$U_1 = \begin{bmatrix} \eta_1 & \eta_4 & \eta_5 \\ \eta_4 & \eta_2 & \eta_6 \\ \eta_5 & \eta_6 & \eta_3 \end{bmatrix}, \; U_2 = \begin{bmatrix} \eta_1 & -\eta_4 & -\eta_5 \\ -\eta_4 & \eta_2 & \eta_6 \\ -\eta_5 & \eta_6 & \eta_3 \end{bmatrix}, \; U_3 = \begin{bmatrix} \eta_1 & -\eta_4 & \eta_5 \\ -\eta_4 & \eta_2 & -\eta_6 \\ \eta_5 & -\eta_6 & \eta_3 \end{bmatrix},$$

$$U_4 = \begin{bmatrix} \eta_1 & \eta_4 & -\eta_5 \\ \eta_4 & \eta_2 & -\eta_6 \\ -\eta_5 & -\eta_6 & \eta_3 \end{bmatrix}.$$

The condition that the U_i are positive definite requires that $\eta_i > 0$ for $i = 1, 2, 3$, $\eta_1\eta_2 - \eta_4^2 > 0$, $\eta_1\eta_3 - \eta_5^2 > 0$, $\eta_2\eta_3 - \eta_6^2 > 0$, and $\eta_1\eta_2\eta_3 - \eta_3\eta_4^2 - \eta_2\eta_5^2 - \eta_1\eta_6^2 + 2\eta_4\eta_5\eta_6 > 0$; and the condition that the U_i are distinct requires that $\eta_i \neq 0$ for at least two of $i = 4, 5, 6$. The following relations between U_i can be readily justified:

$$\begin{aligned} R_1^T U_1 R_1 &= U_2, \quad R_2^T U_1 R_2 = U_3, \quad R_3^T U_1 R_3 = U_4, \\ R_1^T U_3 R_1 &= U_4, \quad R_2^T U_2 R_2 = U_4, \quad R_3^T U_2 R_3 = U_3, \end{aligned} \tag{5.1}$$

where $R_1 = -I + 2e_1 \otimes e_1$, $R_2 = -I + 2e_2 \otimes e_2$, and $R_3 = -I + 2e_3 \otimes e_3$.

Using the relations between the variants of martensite (5.1) and Lemma 3.2 we can solve the interface equations (2.6) for each (i,j) and classify the interfaces.

Lemma 5.1. *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 interface equation (2.6). The classification of the solutions to the interface equation is given in the Table 2.

We now give the main theorem of this section.

Theorem 5.1. *Assume that ϕ satisfies* (2.1), (2.2), *and* (2.4), *F_λ is defined as in* (2.7) *with $\lambda \in (0,1)$, and $\mathcal{A}$ is defined by* (2.5).

Case 1A: *Suppose (i,j) in the definition of F_λ determines twin type I with $n = e_1$. Then* (3.4) *holds for all the parameters η_i, except those that satisfy*

$$\eta_4\eta_5 + \eta_2\eta_6 + \eta_6\eta_3 \neq 0, \tag{5.2}$$

in which case (3.4) *does not hold for* $\lambda = 1/2$.

Case 1B: *Suppose* (i, j) *in the definition of* F_λ *determines twin type I with* $n = e_2$. *Then* (3.4) *holds for all the parameters* η_i, *except those that satisfy*

$$\eta_4\eta_6 + \eta_5\eta_1 + \eta_5\eta_3 \neq 0,$$

in which case (3.4) *does not hold for* $\lambda = 1/2$.

Case 1C: *Suppose* (i, j) *in the definition of* F_λ *determine twin type I with* $n = e_3$. *Then* (3.4) *holds for all the parameters* η_i, *except those that satisfy*

$$\eta_5\eta_6 + \eta_4\eta_1 + \eta_4\eta_2 \neq 0,$$

in which case (3.4) *does not hold for* $\lambda = 1/2$.

Case 2A: *Suppose* (i, j) *in the definition of* F_λ *determines twin type II with either*

$$n = (0, \eta_5\eta_6 + \eta_4\eta_1 + \eta_4\eta_2, \eta_4\eta_6 + \eta_5\eta_1 + \eta_5\eta_3)$$

or

$$n = \big(0, \eta_5\eta_6 + \eta_4\eta_1 + \eta_4\eta_2, -(\eta_4\eta_6 + \eta_5\eta_1 + \eta_5\eta_3)\big).$$

Then (3.4) *holds for all the parameters* η_i, *except those that satisfy*

$$\eta_4\eta_5(\eta_4^2 + \eta_5^2 - \eta_6^2 - \eta_1\eta_2 - \eta_2\eta_3 - \eta_1\eta_3) + \eta_6\left(\eta_4^2(\eta_3 - \eta_1) + \eta_5^2(\eta_2 - \eta_1) + \eta_1^2(\eta_2 + \eta_3)\right) \neq 0. \quad (5.3)$$

in which case (3.4) *does not hold for* $\lambda = 1/2$.

Case 2B: *Suppose* (i, j) *in the definition of* F_λ *determines twin type II with either*

$$n = (\eta_5\eta_6 + \eta_4\eta_1 + \eta_4\eta_2, 0, \eta_4\eta_5 + \eta_6\eta_2 + \eta_6\eta_3)$$

or

$$n = \big(\eta_5\eta_6 + \eta_4\eta_1 + \eta_4\eta_2, 0, -(\eta_4\eta_5 + \eta_6\eta_2 + \eta_6\eta_3)\big).$$

Then (3.4) *holds for all the parameters* η_i, *except those that satisfy*

$$\eta_4\eta_6(\eta_4^2 + \eta_6^2 - \eta_5^2 - \eta_1\eta_2 - \eta_2\eta_3 - \eta_1\eta_3) + \eta_5\left(\eta_4^2(\eta_3 - \eta_2) + \eta_6^2(\eta_1 - \eta_2) + \eta_2^2(\eta_1 + \eta_3)\right) \neq 0.$$

in which case (3.4) *does not hold for* $\lambda = 1/2$.

Case 2C: *Suppose* (i, j) *in the definition of* F_λ *determines twin type II with either*

$$n = (\eta_4\eta_6 + \eta_5\eta_1 + \eta_5\eta_3, \eta_4\eta_5 + \eta_6\eta_2 + \eta_6\eta_3, 0)$$

or

$$n = \big(-(\eta_4\eta_6 + \eta_5\eta_1 + \eta_5\eta_3), \eta_4\eta_5 + \eta_6\eta_2 + \eta_6\eta_3, 0\big).$$

Then (3.4) *holds for all the parameters* η_i, *except those that satisfy*

$$\eta_5\eta_6(\eta_5^2 + \eta_6^2 - \eta_4^2 - \eta_1\eta_2 - \eta_2\eta_3 - \eta_1\eta_3) + \eta_4\left(\eta_5^2(\eta_2 - \eta_3) + \eta_6^2(\eta_1 - \eta_3) + \eta_3^2(\eta_1 + \eta_2)\right) \neq 0.$$

in which case (3.4) *does not hold for* $\lambda = 1/2$.

Proof. We use Lemma 3.1 to derive the stability estimates. Since the proof of Case 1B and Case 1C is similar to Case 1A and the proof of Case 2B and Case 2C is similar to Case 2A, we need only prove the result for Case 1A with $(i, j) = (2, 1)$ and Case 2A with $(i, j) = (2, 1)$.

Case 1A. We let $(i, j) = (2, 1)$ and $n = e_1$. Choosing $w = (0, \xi, \zeta)$ with ξ, $\zeta \in \mathbb{R}$ such that w has unit length we evaluate $\rho_1(y, w)$ to obtain:

$$\rho_1(y; w) = (\tau_3 + \tau_4)\xi\zeta(\eta_4\eta_5 + \eta_2\eta_6 + \eta_6\eta_3).$$

If

$$\eta_4\eta_5 + \eta_2\eta_6 + \eta_6\eta_3 \neq 0,$$

we can choose ξ and ζ such that

$$\xi\zeta(\eta_4\eta_5 + \eta_2\eta_6 + \eta_6\eta_3) > 0.$$

Consequently, it follows from Lemma 3.1 that

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

if $\eta_4\eta_5 + \eta_2\eta_6 + \eta_6\eta_3 \neq 0$.

Next, following [8] we show that if $\eta_4\eta_5 + \eta_2\eta_6 + \eta_6\eta_3 = 0$, then for $\lambda = 1/2$ we can construct a sequence $\{y_n\} \in A$ of deformations whose energy converges to zero, but whose volume fractions $\tau_3(y_n)$ and $\tau_4(y_n)$ converge to $1/2$. For this reason, we need to evaluate F_λ,

$$F_\lambda = U_1 + \lambda a \otimes n$$

for our choice of $(i, j) = (2, 1)$ and $n = e_1$. The vector a can be calculated from the interface equation

$$QU_2 - U_1 = a \otimes n. \tag{5.4}$$

where $n = e_1$. The three components of the vector $a = (a_1, a_2, a_3)$ (assuming $\rho = 1$, see lemma 3.2) are:

$$\begin{aligned}
a_1 &= \beta\Big[\eta_4^2\big(\eta_6^2(\eta_1 - \eta_3) + (\eta_1 + \eta_2)\eta_3^2\big) + \eta_5^2\big(\eta_6^2(\eta_1 - \eta_2) + \eta_2^2(\eta_1 + \eta_3)\big) \\
&\quad + 2\eta_4\eta_5\eta_6(\eta_6^2 - \eta_2\eta_3 - \eta_3(\eta_2 + \eta_3))\Big], \\
a_2 &= \beta\Big[\eta_4^3\eta_6^2 + \eta_4^2\eta_5\eta_6\big(-2\eta_2 + \eta_3\big) + \eta_5\eta_6(\eta_6^2\eta_1 + \eta_2(\eta_5^2 - \eta_1\eta_3)) \\
&\quad + \eta_4((\eta_6^2 - \eta_2\eta_3)(\eta_6^2 - (\eta_1 + \eta_2)\eta_3) - \eta_5^2(\eta_6^2 + \eta_2(-\eta_2 + \eta_3)))\Big], \\
a_3 &= \beta\Big[\eta_4^3\eta_6\eta_3 + \eta_4\eta_6\big(\eta_6^2\eta_1 + \eta_5^2(\eta_2 - 2\eta_3) - \eta_1\eta_2\eta_3\big) - \eta_4^2\eta_5\big(\eta_6^2 + (\eta_2 - \eta_3)\eta_3\big) \\
&\quad + \eta_5\big(\eta_5^2\eta_6^2 + (\eta_6^2 - \eta_2\eta_3)(\eta_6^2 - \eta_2(\eta_1 + \eta_3))\big)\Big].
\end{aligned}$$

where

$$\beta = -\frac{2}{\eta_5^2(\eta_6^2 + \eta_2^2) - 2\eta_4\eta_5\eta_6(\eta_2 + \eta_3) + (\eta_6^2 - \eta_2\eta_3)^2 + \eta_4^2(\eta_6^2 + \eta_3^2)}.$$

Next, using the expression for F_λ we calculate $F_\lambda^T F_\lambda$ for $\lambda = 1/2$. We omit the expressions for F_λ and $F_\lambda^T F_\lambda$ because of their complexity.

Since $R_2^T U_2 R_2 = U_4$, and $R_2^T U_1 R_2 = U_3$, we have from (5.4) that

$$\tilde{Q}U_4 - U_3 = \tilde{a} \otimes \tilde{n}.$$

where $\tilde{Q} = R_2^T Q R_2$, $\tilde{a} = R_2^T a$, and $\tilde{n} = R_2^T n = R_2^T e_1 = -e_1$. So, if we set $G_\lambda = \lambda\tilde{Q}U_4 + (1-\lambda)U_3$, then G_λ can also be expressed as

$$G_\lambda = U_3 + \lambda\tilde{a} \otimes \tilde{n} = R_2^T F_\lambda R_2.$$

Thus, we can show that

$$F_{1/2}^T F_{1/2} - G_{1/2}^T G_{1/2} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \eta_4\eta_5 + \eta_6\eta_2 + \eta_6\eta_3 \\ 0 & \eta_4\eta_5 + \eta_6\eta_2 + \eta_6\eta_3 & 0 \end{bmatrix}.$$

So, if $\eta_4\eta_5 + \eta_6\eta_2 + \eta_6\eta_3 = 0$, then $F_{1/2}^T F_{1/2} = G_{1/2}^T G_{1/2}$. Therefore, if (5.2) holds, then there exists $R \in SO(3)$ such that $F_{1/2} = RG_{1/2}$. We can then conclude that there exists a sequence of deformations such that $\mathcal{E}(y_n) \to 0$ while $\tau_3(y_n) \to 1/2$ and $\tau_4(y_n) \to 1/2$.

Case 2A. We let $(i, j) = (2, 1)$ and

$$n = (0, \eta_5\eta_6 + \eta_4\eta_1 + \eta_4\eta_2, \eta_4\eta_6 + \eta_5\eta_1 + \eta_5\eta_3).$$

Since $U_1^{-1}a$ is parallel to e_1, we can choose $w = (0, \xi, \zeta)$, where ξ and ζ are arbitrary real numbers and w has unit length. For this choice of w, $\rho_2(y; w)$ to obtain can be evaluated

$$\begin{aligned}
\rho_2(y; w) = -4(\tau_3 + \tau_4)\xi\zeta\Big(&\eta_4\eta_5(\eta_4^2 + \eta_5^2 - \eta_6^2 - \eta_1\eta_2 - \eta_2\eta_3 - \eta_1\eta_3) \\
&+ \eta_6\left(\eta_4^2(\eta_3 - \eta_1) + \eta_5^2(\eta_2 - \eta_1) + \eta_1^2(\eta_2 + \eta_3)\right)\Big).
\end{aligned}$$

Consequently, if

$$\eta_4\eta_5(\eta_4^2 + \eta_5^2 - \eta_6^2 - \eta_1\eta_2 - \eta_2\eta_3 - \eta_1\eta_3) + \eta_6\left(\eta_4^2(\eta_3 - \eta_1) + \eta_5^2(\eta_2 - \eta_1) + \eta_1^2(\eta_2 + \eta_3)\right) \neq 0,$$

then choosing appropriate ξ and ζ we obtain from Lemma 3.1 that

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

Next, we show that if

$$\eta_4\eta_5(\eta_4^2 + \eta_5^2 - \eta_6^2 - \eta_1\eta_2 - \eta_2\eta_3 - \eta_1\eta_3) + \eta_6\left(\eta_4^2(\eta_3 - \eta_1) + \eta_5^2(\eta_2 - \eta_1) + \eta_1^2(\eta_2 + \eta_3)\right) = 0,$$

then there exists a sequence y_n such that $\mathcal{E}(y_n) \to 0$ while $\tau_3(y_n) \to 1/2$ and $\tau_4(y_n) \to 1/2$. The vectors a and n of the interface relation (5.4) can be calculated from Lemma 3.2 to be:

$$a = (\eta_1, \eta_4, \eta_5), \quad n = (0, \eta_5\eta_6 + \eta_4\eta_1 + \eta_4\eta_2, \eta_4\eta_6 + \eta_5\eta_1 + \eta_5\eta_3).$$

Using these values of a and n we can compute

$$F_{1/2} = \frac{1}{2}QU_2 + \frac{1}{2}U_1 = U_1 + \frac{1}{2}a \otimes n.$$

The expression for $F_{1/2}$ is omitted here. Since $R_2^TU_2R_2 = U_4$, and $R_2^TU_1R_2 = U_3$, we have from (5.4) that

$$\tilde{Q}U_4 - U_3 = \tilde{a} \otimes \tilde{n}.$$

where $\tilde{Q} = R_2^TQR_2$, $\tilde{a} = R_2^Ta$, and $\tilde{n} = R_2^Tn$. So, if we set $G_{1/2} = \frac{1}{2}\tilde{Q}U_4 + \frac{1}{2}U_3$, then $G_{1/2}$ can also be expressed as

$$G_{1/2} = U_3 + \frac{1}{2}\tilde{a} \otimes \tilde{n} = R_2^TF_{1/2}R_2.$$

It can then be calculated that $F_{1/2}^TF_{1/2} - G_{1/2}^TG_{1/2}$ is equal to

$$\left[\eta_4\eta_5(\eta_4^2 + \eta_5^2 - \eta_6^2 - \eta_1\eta_2 - \eta_2\eta_3 - \eta_1\eta_3) + \eta_6\left(\eta_4^2(\eta_3 - \eta_1) + \eta_5^2(\eta_2 - \eta_1) + \eta_1^2(\eta_2 + \eta_3)\right)\right]S$$

where

$$S = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}.$$

Thus, if (5.3) holds, then $F_{1/2}^TF_{1/2} = G_{1/2}^TG_{1/2}$. As in the case 1A, it follows that the microstructure is not unique if (5.3) holds. ☐

6. THE STABILITY OF THE LAMINATED MICROSTRUCTURE FOR TRIGONAL TO MONOCLINIC PHASE TRANSFORMATIONS

The symmetry group of the trigonal (high temperature) phase $\mathcal{G} = \{R_1, R_2, R_3, R_4, R_5, R_6\}$ is composed of

$$R_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \ R_2 = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}, \ R_3 = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix},$$

$$R_4 = -\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, \ R_5 = -\begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \ R_6 = -\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

Note that R_4, R_5, and R_6 are two-fold rotations,

$$R_4 = R(\pi, e_2 - e_3), \quad R_5 = R(\pi, e_1 - e_3), \quad R_6 = R(\pi, e_1 - e_2), \tag{6.1}$$

and R_2 and R_3 are three-fold rotations with axis $\hat{e} = \frac{1}{\sqrt{3}}\{1, 1, 1\}$,

$$R_2 = R(\frac{2\pi}{3}, \hat{e}), \quad R_3 = R(\frac{4\pi}{3}, \hat{e}). \tag{6.2}$$

Note that $R_2R_3 = I$. Each of the two-fold rotations R_i $(i = 4, 5, 6)$ in the trigonal symmetry group determines a family of transformation strains that corresponds to shearing in the plane orthogonal to

TABLE 3. Classification of the interfaces for the trigonal to monoclinic transformation where

$$\mu = (\eta_3^2 - \eta_2^2) + (\eta_1^2 - \eta_3^2) + (\eta_3^2 - \eta_4^2)$$

and

$$\nu = -2\eta_4(\eta_2 - \eta_3) - 2\eta_3(\eta_3 - \eta_1) - 2\eta_2(\eta_4 - \eta_3).$$

(i,j)	TYPE OF THE TWIN	INTERFACE NORMAL	
$(1,2)$	I	$n_1 = e_1 - e_2$	
	II	$n_2 = (\,\mu,\, \mu,\, \nu\,)$	
$(1,3)$	I	$n_1 = e_1 - e_3$	
	II	$n_2 = (\,\mu,\, \nu,\, \mu\,)$	
$(2,3)$	I	$n_1 = e_2 - e_3$	
	II	$n_2 = (\,\nu,\, \mu,\, \mu\,)$	

the axis of the rotation. For each two-fold rotation R_i $(i = 4, 5, 6)$, the transformation strain U_1 in the corresponding family satisfies

$$\{\, R_j \in \mathcal{G} : R_j^T U_1 R_j \} = \{ I, R_i \,\}.$$

The stability of the microstructure for a transformation strains corresponding to the any two-fold rotations R_i $(i = 4, 5, 6)$ follows from the stability results for R_4 by symmetry. For this reason we only consider the two-fold rotation R_4.

The variants of the low temperature martensite for this case are

$$U_1 = \begin{bmatrix} \eta_1 & \eta_3 & \eta_3 \\ \eta_3 & \eta_2 & \eta_4 \\ \eta_3 & \eta_4 & \eta_2 \end{bmatrix}, \; U_2 = \begin{bmatrix} \eta_2 & \eta_3 & \eta_4 \\ \eta_3 & \eta_1 & \eta_3 \\ \eta_4 & \eta_3 & \eta_2 \end{bmatrix}, \; U_3 = \begin{bmatrix} \eta_2 & \eta_4 & \eta_3 \\ \eta_4 & \eta_2 & \eta_3 \\ \eta_3 & \eta_3 & \eta_1 \end{bmatrix},$$

where the condition that U_1 be positive definite requires that

$$\eta_1,\, \eta_2 > 0, \quad \eta_1\eta_2 - \eta_3^2 > 0, \quad \eta_2 > |\eta_4|, \quad \text{and} \quad \eta_1(\eta_2 + \eta_4) - 2\eta_3^2 > 0. \tag{6.3}$$

The condition that the U_i are distinct requires that $\eta_1 \neq \eta_2$ or $\eta_3 \neq \eta_4$.

The two-fold rotations defined in (6.1) act on U_1, U_2, U_3 in the following manner:

$$\begin{aligned} &R_6^T U_1 R_6 = U_2, \quad R_5^T U_1 R_5 = U_3, \quad R_4^T U_1 R_4 = U_1, \\ &R_6^T U_3 R_6 = U_3, \quad R_5^T U_2 R_5 = U_2, \quad R_4^T U_2 R_4 = U_3. \end{aligned} \tag{6.4}$$

The three-fold rotations defined in (6.2) act on U_1, U_2, U_3 in the following way:

$$R_2^T U_1 R_2 = U_3, \quad R_3^T U_1 R_3 = U_2, \quad R_2^T U_2 R_2 = U_1.$$

Using these relations between the variants of martensite, we can solve the interface equation (2.6) for each (i,j) and classify these twins.

Lemma 6.1. *1. For each $i \in \{1, \ldots, 3\}$, the energy well $\mathcal{U}_i$ is not rank-one connected to itself.*

2. For any $i, j \in \{1, \ldots, 3\}$, with $i \neq j$, there are exactly two solutions to the interface equation (2.6). The classification of the solutions to the interface equation is given in Table 3.

We now give the main theorem of this section.

Theorem 6.1. *Assume that ϕ satisfies* (2.1), (2.2), *and* (2.4), *F_λ is defined as in* (2.7) *for any $i, j \in \{1, \ldots, 3\}$, with $i \neq j$, $\lambda \in (0,1)$, and $\mathcal{A}$ is defined by* (2.5). *Then* (3.4) *holds for all parameters η_i that do not satisfy*

$$\eta_3 + \eta_1 - \eta_2 - \eta_4 = 0 \quad \textit{and} \quad \eta_2 > \eta_4 \geq \eta_3$$

for type I twins, and

$$\eta_3 + \eta_1 - \eta_2 - \eta_4 = 0 \quad \textit{and} \quad \eta_2 \geq \eta_3 \geq \eta_4$$

for type II twins.

Proof. It follows from (6.4), that the results for any pair $i, j \in \{1, \ldots, 3\}$, with $i \neq j$, follow from the results for $(i, j) = (1, 2)$ by symmetry. So, we prove the theorem for $(i, j) = (1, 2)$. We can then set $w = (\xi, \xi, \zeta)$ in $\rho_1(y; w)$ to obtain the following estimate for τ_3 if the interface is of type I

$$\begin{aligned}\rho_1(y;w) =&\tau_3\Big(\xi^2(-\eta_3^2 + 2\eta_3\eta_4 - \eta_4^2 + 2\eta_3\eta_1 + \eta_1^2 + 2\eta_3\eta_2 - 4\eta_4\eta_2 - \eta_2^2)\\ &\qquad + 2\xi\zeta(\eta_3^2 - \eta_3\eta_4 - \eta_3\eta_1 - \eta_3\eta_2 + 2\eta_4\eta_2) + \zeta^2(-\eta_3^2 + \eta_4^2 - \eta_1^2 + \eta_2^2)\Big) \le C\mathcal{E}(y)^{1/2};\end{aligned}$$

and we can set $w = (\xi, \xi, \zeta)$ in $\rho_2(y; w)$ to obtain the following estimate if the interface is of type II

$$\begin{aligned}\rho_2(y;w) =&\tau_3\Big(\xi^2(2\eta_3^4 - \eta_3^2\eta_4^2 - 2\eta_3\eta_4^3 + \eta_4^4 - 2\eta_3^2\eta_4\eta_1 - 2\eta_3\eta_4^2\eta_1 - \eta_4^2\eta_1^2 + 2\eta_3^2\eta_4\eta_2 + 2\eta_3\eta_4^2\eta_2 - 2\eta_3^2\eta_1\eta_2\\ &\quad + 4\eta_3\eta_4\eta_1\eta_2 + 4\eta_4\eta_1^2\eta_2 - \eta_3^2\eta_2^2 + 2\eta_3\eta_4\eta_2^2 - 2\eta_4^2\eta_2^2 - 2\eta_3\eta_1\eta_2^2 - \eta_1^2\eta_2^2 - 2\eta_3\eta_2^3 + \eta_2^4)\\ &+ \xi\zeta(-4\eta_3^4 + 2\eta_3^2\eta_4^2 + 2\eta_3\eta_4^3 + 4\eta_3^2\eta_4\eta_1 + 2\eta_3\eta_4^2\eta_1 - 4\eta_3^2\eta_4\eta_2 - 2\eta_3\eta_4^2\eta_2\\ &\quad + 4\eta_3^2\eta_1\eta_2 - 4\eta_3\eta_4\eta_1\eta_2 - 4\eta_4\eta_1^2\eta_2 + 2\eta_3^2\eta_2^2 - 2\eta_3\eta_4\eta_2^2 + 2\eta_3\eta_1\eta_2^2 + 2\eta_3\eta_2^3)\\ &+ \zeta^2(2\eta_3^4 - \eta_3^2\eta_4^2 - \eta_4^4 - 2\eta_3^2\eta_4\eta_1 + \eta_4^2\eta_1^2 + 2\eta_3^2\eta_4\eta_2 - 2\eta_3^2\eta_1\eta_2 - \eta_3^2\eta_2^2\\ &\quad + 2\eta_4^2\eta_2^2 + \eta_1^2\eta_2^2 - \eta_2^4)\Big) \le C\left(\mathcal{E}(y) + \mathcal{E}(y)^{1/2}\right).\end{aligned}$$

In both of these cases, the equation for τ_3 has the form

$$\tau_3(A\xi^2 + B\xi\zeta + C\zeta^2) \le C\left(\mathcal{E}(y) + \mathcal{E}(y)^{1/2}\right),$$

where the A, B, and C are polynomials in $\eta_i,\ i = 1, 2, 3$. In order to bound τ_3, we need to show that $A\xi^2 + B\xi\zeta + C\zeta^2 > 0$ for some value of ξ and ζ. So, we find all possible values of $(\eta_1, \eta_2, \eta_3, \eta_4)$ such that $A\xi^2 + B\xi\zeta + C\zeta^2 \le 0$ for all ξ and ζ. For both $\rho_1(y; w)$ and $\rho_2(y; w)$, one can show that

$$A + B + C = 0.$$

This indicates that for $\xi = \zeta$, we have $A\xi^2 + B\xi\zeta + C\zeta^2 = 0$ for both $\rho_1(y; w)$ and $\rho_2(y; w)$. Thus, in order for the quadratic form to be non-positive we need for its discriminant to be zero. The discriminants for $\rho_1(y; w)$ and $\rho_2(y; w)$ are equal to

$$B^2 - 4AC = 4(\eta_3 - \eta_4 + \eta_1 - \eta_2)^2(\eta_4 + \eta_1 + \eta_2)^2$$

and

$$B^2 - 4AC = 4(\eta_2 - \eta_4)^4(\eta_3 - \eta_4 + \eta_1 - \eta_2)^2(\eta_4 + \eta_1 + \eta_2)^2$$

respectively. Consequently, since $\eta_2 - \eta_4 > 0$ and $\eta_4 + \eta_1 + \eta_2 > 0$ by (6.3), the discriminants are zero if and only if

$$\eta_3 - \eta_4 + \eta_1 - \eta_2 = 0. \tag{6.5}$$

Since $A + B + C = 0$ and $B^2 - 4AC = 0$, it follows that

$$A = C = -\frac{B}{2}. \tag{6.6}$$

Assuming (6.5), we calculate the expression for A for $\rho_1(y; w)$ to be

$$A = 2(\eta_4 - \eta_3)(\eta_3 - \eta_2) \tag{6.7}$$

and the expression for A for $\rho_2(y; w)$ to be

$$A = 2(\eta_3 - \eta_4)(\eta_3 - \eta_2)(\eta_3 + \eta_4 + \eta_2)^2. \tag{6.8}$$

Thus, it follows from (6.6), (6.7) and (6.8) that if the respective discriminants are equal to zero, then we have that

$$\begin{aligned}\rho_1(y; w) &= 2\tau_3(\xi - \zeta)^2(\eta_4 - \eta_3)(\eta_3 - \eta_2),\\ \rho_2(y; w) &= 2\tau_3(\xi - \zeta)^2(\eta_3 - \eta_4)(\eta_3 - \eta_2)(\eta_2 + \eta_3 + \eta_4)^2.\end{aligned}$$

We have that $(\eta_4-\eta_3)(\eta_3-\eta_2)\leq 0$ is possible only for $\eta_4\geq\eta_3$ and $\eta_2\geq\eta_3$, in which case $\eta_2>\eta_4\geq\eta_3$ by (6.3). If we suppose on the contrary that

$$\eta_3\geq\eta_4 \quad\text{and}\quad \eta_3\geq\eta_2, \tag{6.9}$$

then $\eta_1>\eta_3$ by the condition $\eta_1\eta_2-\eta_3^2>0$ of (6.3). However, $\eta_1>\eta_3$ implies that $\eta_2+\eta_4>2\eta_3$ by (6.5) which contradicts (6.9). Summarizing all of these conditions, we obtain that the inequality $\tau_3\leq C(\mathcal{E}(y)+\mathcal{E}(y)^{1/2})$ for $\rho_1(y;w)$ holds if the parameters η_i do not satisfy

$$\eta_3-\eta_4+\eta_1-\eta_2=0 \quad\text{and}\quad \eta_2>\eta_4\geq\eta_3.$$

Turning to expression for $\rho_2(y;w)$, we note that

$$\eta_1(\eta_2+\eta_4)-2\eta_3^2=(\eta_2+\eta_3+\eta_4)(\eta_2-2\eta_3+\eta_4).$$

Thus, it follows from (6.3) that

$$(\eta_2+\eta_3+\eta_4)^2>0.$$

We have that $(\eta_3-\eta_4)(\eta_3-\eta_2)\leq 0$ is possible only for the case $\eta_3\geq\eta_4$ and $\eta_2\geq\eta_3$ since the case $\eta_4\geq\eta_3$ and $\eta_3\geq\eta_2$ contradicts the condition $\eta_2>|\eta_4|$ in (6.3). Hence, we obtain that the inequality $\tau_3\leq C\left(\mathcal{E}(y)+\mathcal{E}(y)^{1/2}\right)$ for $\rho_2(y;w)$ holds if the parameters η_i do not satisfy

$$\eta_3-\eta_4+\eta_1-\eta_2=0 \quad\text{and}\quad \eta_2\geq\eta_3\geq\eta_4.$$

□

7. The stability of the microstructure

In the previous sections, we derived the estimate

$$\tau_k(y)\leq C\left(\mathcal{E}(y)^{1/2}+\mathcal{E}(y)\right) \qquad \text{for all } k\neq i,j,\ y\in\mathcal{A}, \tag{7.1}$$

where

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

with

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

for lattice parameters which do not satisfy certain identities. In this section we present the stability estimates which can be deduced from (7.1). The derivations of these estimates can be done by the same arguments used in [8]. For this reason we state the results without proofs.

Lemma 7.1. *(1) For any $w\in\mathbb{R}^3$ such that $w\cdot n=0$ and $|w|=1$, we have that*

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

(2) The following inequality holds:

$$\int_\Omega |y(x)-y_0(x)|^2\,dx\leq C\left(\mathcal{E}(y)+\mathcal{E}(y)^{1/2}\right) \qquad \textit{for all } y\in\mathcal{A}.$$

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

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

For fixed i,j with $i\neq j$ we define a projection operator $\pi_{ij}:\mathbb{R}^{3\times3}\to U_i\bigcup U_j$ by

$$\|F-\pi_{ij}(F)\|=\min_{G\in U_i\bigcup U_j}\|F-G\| \qquad \text{for all } F\in\mathbb{R}^{3\times3},$$

and the operators $\Theta:\mathbb{R}^{3\times3}\to SO(3)$ and $\Pi:\mathbb{R}^{3\times3}\to\{QU_i,U_j\}$ by the unique decomposition

$$\pi_{ij}(F)=\Theta(F)\Pi(F) \qquad \text{for all } F\in\mathbb{R}^{3\times3}.$$

The next lemma gives an estimate on the difference between the deformation gradient $\nabla y(x)$ and $\Pi(\nabla y(x))$. This lemma shows that the deformation gradients of energy-minimizing sequences must oscillate between QU_i and U_j.

Lemma 7.2. *The following inequality holds for all* $y \in \mathcal{A}$*:*

$$\int_\Omega \|\nabla y(x) - \Pi(\nabla y(x))\|^2 \, dx \le C \left(\mathcal{E}(y) + \mathcal{E}(y)^{1/2} \right).$$

Next we present an estimate for the volume fractions of QU_i and U_j. For this reason we define the sets

$$\omega_\rho^i(y) = \{\, x \in \omega : \Pi(\nabla y(x)) = QU_i \text{ and } \|\nabla y(x) - QU_i\| \le \rho \,\},$$
$$\omega_\rho^j(y) = \{\, x \in \omega : \Pi(\nabla y(x)) = U_j \text{ and } \|\nabla y(x) - U_j\| \le \rho \,\},$$

for any subset $\omega \in \Omega$, $\rho > 0$, and $y \in \mathcal{A}$. The next lemma demonstrates that the deformation gradients of energy-minimizing sequences must oscillate with local volume fraction λ at QU_i and local volume fraction $1 - \lambda$ at U_j.

Lemma 7.3. *For any Lipshitz domain* $\omega \subset \Omega$ *and for any* $\rho > 0$*, there exists a constant* $C = C(\omega, \rho) > 0$ *such that for all* $y \in \mathcal{A}$

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

To give an estimate for the weak convergence of nonlinear functions of deformation gradients we define by $\mathcal{V}$ the Sobolev space of all measurable functions $f : \Omega \times \mathbb{R}^{3\times 3} \to \mathbb{R}$ such that

$$\|f\|_{\mathcal{V}}^2 = \int_\Omega \left\{ (\operatorname{ess\,sup} \|\nabla_F f(x, F)\|)^2 + |\nabla z_f(x) n|^2 + z_f(x)^2 \right\} dx < \infty,$$

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

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

Then the following lemma holds.

Lemma 7.4. *We have for all* $f \in \mathcal{V}$*, and* $y \in \mathcal{A}$ *that*

$$\left| \int_\Omega \{ f(x, \nabla y(x)) - [\lambda f(x, QU_i) + (1 - \lambda) f(x, U_j)] \} \, dx \right| \le C \|f\|_{\mathcal{V}} \left[\mathcal{E}(y)^{1/4} + \mathcal{E}(y)^{1/2} \right].$$

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