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On the Stability of Microstructure for General Martensitic Transformations

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Abstract. We describe a general theory for the stability of the laminated microstructure for martensitic crystals. Our theory has been applied to the orthorhombic to monoclinic transformation, the cubic to tetragonal transformation, the tetragonal to monoclinic transformation, and the cubic to orthorhombic transformation.

1 Introduction

We describe recent results for the stability of laminated microstructure for crystals that undergo a symmetry reducing solid-solid phase transformation. In the geometrically nonlinear theory of martensite [2,3,11,25], the energy density is minimized on multiple energy wells $\mathrm{SO}(3)U_1 \cup \ldots \cup \mathrm{SO}(3)U_N$ where $U_1, \ldots, U_N \in \mathbb{R}^{3\times 3}$ 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.

An early version of the stability theory for crystal microstructure was first developed for some one-dimensional models in [13,14]. Results allowing the theory to be extended to the multi-dimensional geometrically nonlinear theory of crystals were first given for a rotationally invariant double well energy density ($N = 2$) in [24]. These results apply directly to the orthorhombic to monoclinic transformation. The theory has since been applied to the cubic to tetragonal transformation ($N = 3$) [20], the tetragonal to monoclinic transformation ($N = 4$) [5], and the cubic to orthorhombic transformation ($N = 6$) [4]. In general, the analysis of stability becomes more difficult for larger N since the additional wells give the crystal more freedom to deform without the cost of additional energy. In fact, for the tetragonal to monoclinic transformation ($N = 4$) and the cubic to orthorhombic transformation ($N = 6$) we have shown that there are special lattice constants for which the laminated microstructure is not stable.

The stability theory can also be used to analyze laminates with varying volume fraction [21] and conforming and nonconforming finite element

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approximations [22,24]. We also note that the stability theory was used to analyze the microstructure in ferromagnetic crystals [26]. Related results on the numerical analysis of nonconvex variational problems can be found, for example, in [6–10,12,16–19,23,27–29].

In Sect. 2, we describe the geometrically nonlinear theory of martensite. We refer the reader to [2,3] and to the introductory article by [25] for a more detailed discussion of the geometrically nonlinear theory of martensite. In Sect. 3, we prove a condition that allows a reduction to an approximate mixture of two strains. In Sect. 4, we show how this condition can be verified for the cubic to tetragonal transformation. In Sect. 5, give results for the stability and uniqueness of the microstructure that follows from the estimate for the reduction to an approximate mixture to two strains. Finally, in Sect., we give convergence results for finite element methods that following directly from an approximation result and the results in Sect. 5.

2 The Continuum Model

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 Ω is a bounded domain with a Lipschitz continuous boundary $\partial\Omega$. We consider the minimization of the total energy

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

over an admissible class $\mathcal{A}$ of deformations where $\phi(F) : \mathbb{R}^{3\times 3} \to \mathbb{R}$ is the energy density at a fixed temperature. Following the geometrically nonlinear theory of elasticity, we assume that the free energy density is frame-indifferent

$$\phi(RF) = \phi(F) \qquad \text{for all } F \in \mathbb{R}^{3\times 3} \text{ and } R \in \mathrm{SO}(3)\ . \tag{1}$$

We specialize the general geometrically nonlinear theory to martensitic crystals by taking the reference configuration Ω to be the high-symmetry phase (austenite) of the crystal at the transformation temperature. Following the geometrically nonlinear theory of martensite [2,3,25], we then have that

$$\phi(R_i^T F R_i) = \phi(F) \qquad \text{for all } F \in \mathbb{R}^{3\times 3} \text{ and } R_i \in \mathcal{G} \tag{2}$$

where $\mathcal{G}$ is the symmetry group of the high-symmetry phase.

We consider the deformation of the martensitic crystal at a temperature below the transformation temperature. The free energy density is then minimized at a transformation (Bain) strain U_1, so it follows by the frame-indifference (1) and the symmetry (2) of the energy density that the energy density is minimized on the union $\mathcal{U} = \mathcal{U}_1 \bigcup \cdots \bigcup U_N$ of the N energy wells

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

where the symmetry-related transformation strains (variants) $U_2, \ldots U_N$ satisfy

$$\{R_i^T U_1 R_i : R_i \in \mathcal{G}\} = \{U_1, \ldots, U_N\} \ . \tag{3}$$

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

$$\phi(F) \geq \kappa \|F - \pi(F)\|^2 \qquad \text{for all } F \in \mathrm{I\!R}^{3\times 3} \ , \tag{4}$$

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

$$\|F - \pi(F)\| = \min_{G\in\mathcal{U}} \|F - G\| \qquad \text{for all } F \in \mathrm{I\!R}^{3\times 3} \ . \tag{5}$$

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

There exists a continuous deformation $y(x) \in C(\mathrm{I\!R}^3; \mathrm{I\!R}^3)$ such that [2,25]

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

where $n \in \mathrm{I\!R}^3$, $n \neq 0$, and $s \in \mathrm{I\!R}$, if and only if there exists $a \in \mathrm{I\!R}^3$ such that

$$P_1 = F_0 + a \otimes n \ . \tag{6}$$

Thus, if (6) holds for $a \neq 0$, then $x \cdot n = s$ is an interface plane with normal n.

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

$$QU_i = U_j + a \otimes n \tag{7}$$

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

$$F_\lambda = \lambda QU_i + (1-\lambda)U_j = U_j + \lambda a \otimes n \ . \tag{8}$$

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

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

where C_0 and C_1 are positive constants independent of $F \in \mathrm{I\!R}^{3\times 3}$ 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

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

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

$$\mathcal{A} = \{y \in W^{\phi} : y(x) = y_0(x) \text{ for all } x \in \partial\Omega\} \tag{9}$$

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 [10,25].

Lemma 1. *Let* $\mathcal{A}$ *be defined as in* (9)*. 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 (5) and (9) of π and $\mathcal{A}$, respectively. For each $k \in \{1, \ldots, N\}$ 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

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

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

$$\sum_{k=1}^{N} \tau_k(y) = 1 \qquad \text{for all } y \in \mathcal{A} \ . \tag{10}$$

By the rank-one connection (7) and the definition of F_λ (8) we have

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

so

$$|F_\lambda w| = |U_i w| = |U_j w| \text{ for all } w \in \mathbb{R}^3 \text{ such that } \ w \cdot n = 0. \tag{11}$$

Since $\det(QU_i) = \det U_i = \det U_j > 0$ by (3), we have that $U_j^{-1} a \cdot n = 0$. Hence, we have that

$$\text{Cof}\, F_\lambda = (\text{Cof}\, U_j)\,(I - \lambda n \otimes U_j^{-1} a) \tag{12}$$

where the cofactor of a nonsingular matrix $A \in \mathbb{R}^{3\times 3}$ is defined by $\mathrm{Cof}\, A = (\det A) A^{-T}$. We then obtain from (12) that

$$|(\mathrm{Cof}\, F_\lambda) w| = |(\mathrm{Cof}\, U_i) w| = |(\mathrm{Cof}\, U_j) w| \quad \text{for all } w \in \mathbb{R}^3,\ w \cdot U_j^{-1} a = 0 \ . \tag{13}$$

We next recall that since the subdeterminant of the gradient is a null-Lagrangian [15], we have for $y \in \mathcal{A}$ that

$$\begin{aligned} \int_\Omega \nabla y(x)\, dx &= \int_\Omega F_\lambda\, dx, \\ \int_\Omega \mathrm{Cof}\, \nabla y(x)\, dx &= \int_\Omega \mathrm{Cof}\, F_\lambda\, dx \ . \end{aligned} \tag{14}$$

We note that it follows from (4) that

$$\int_\Omega \|\nabla y(x) - \pi(\nabla y(x))\|^2\, dx \le \kappa^{-1} \mathcal{E}(y) \qquad \text{for all } y \in \mathcal{A} \ . \tag{15}$$

Next, for $y \in \mathcal{A}$, we set $F(x) = \nabla y(x)$ for $x \in \Omega$, so it follows from (14) that $F(x) = (F_{kl}(x)) \in L^2(\Omega; \mathbb{R}^{3\times 3})$. 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 $L^\infty(\Omega; \mathbb{R}^{3\times 3})$ for all $y \in \mathcal{A}$. We have

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

for any $k,\ l,\ p,\ q \in \{1, 2, 3\}$. Hence, we have by the Cauchy-Schwarz inequality and (15) that

$$\begin{aligned} &\int_\Omega \Big| \left[\mathrm{Cof}\, \nabla y(x) - \mathrm{Cof}\, \pi(\nabla y(x))\right] w \Big|\, dx \qquad (16) \\ &\le C \left[\left(\int_\Omega \|\nabla y(x) - \pi(\nabla y(x))\|^2\, dx \right)^{1/2} + \int_\Omega \|\nabla y(x) - \pi(\nabla y(x))\|^2\, dx \right] \\ &\le C \left[\mathcal{E}(y)^{1/2} + \mathcal{E}(y) \right] \ . \end{aligned}$$

The following result was proven in [4] for the cubic to orthorhombic transformation and in [5] for the tetragonal to monoclinic 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 2. *Given* $i, j \in \{1, \ldots, N\}$, $Q \in SO(3)$, *and* $a, n \in \mathbb{R}$, $a, n \neq 0$ *satisfying the interface equation* (7), *there exists a constant* $C > 0$ *such that*

$$\rho_1(y; w) \equiv \sum_{k \neq i,j} \tau_k(y) \left(|U_i w|^2 - |U_k w|^2\right) \tag{17}$$
$$\leq C\mathcal{E}(y)^{1/2} \quad \text{for all } w \in \mathbb{R}^3,\ |w| = 1,\ w \cdot n = 0,$$

$$\rho_2(y; w) \equiv \sum_{k \neq i,j} \tau_k(y) \left[|(\mathrm{Cof}\, U_i) w|^2 - |(\mathrm{Cof}\, U_k) w|^2\right] \tag{18}$$
$$\leq C \left[\mathcal{E}(y)^{1/2} + \mathcal{E}(y)\right] \quad \text{for all } w \in \mathbb{R}^3,\ |w| = 1,\ w \cdot U_j^{-1} a = 0$$

for any $y \in \mathcal{A}$.

Proof. We have by (10), (11), (13), and (14) that for any $w \in \mathbb{R}^3$ with $|w| = 1$

$$\begin{aligned} \rho_1(y; w) &= \sum_{k=1}^{N} \tau_k(y) \left(|U_i w|^2 - |U_k w|^2\right) \\ &= \sum_{k=1}^{N} \tau_k(y) \left(|F_\lambda w|^2 - |U_k w|^2\right) \\ &= \frac{1}{\mathrm{meas}\, \Omega} \int_\Omega \left[|F_\lambda w|^2 - |\pi(\nabla y(x)) w|^2\right] dx \\ &= -\frac{1}{\mathrm{meas}\, \Omega} \int_\Omega \left| \left[F_\lambda - \pi(\nabla y(x))\right] w\right|^2 dx \\ &\quad + \frac{2}{\mathrm{meas}\, \Omega} \int_\Omega \left[\nabla y(x) - \pi(\nabla y(x))\right] w \cdot F_\lambda w \, dx \\ &\leq \frac{2}{\mathrm{meas}\, \Omega} \int_\Omega \left[\nabla y(x) - \pi(\nabla y(x))\right] w \cdot F_\lambda w \, dx \ . \end{aligned} \tag{19}$$

We obtain from the Cauchy-Schwarz inequality and the above inequality (15) that

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

So, it follows from (19) that for all $w \in \mathbb{R}^3$ with $|w| = 1$

$$\rho_1(y; w) = \sum_{k=1}^{N} \tau_k(y) \left(|U_i w|^2 - |U_k w|^2\right) \leq C\mathcal{E}(y)^{1/2} \ . \tag{20}$$

The result (18) then follows from the above inequality (20) and (11).

Next, we obtain similar estimates for the cofactor. We have from (10) and (14) that for any $w \in \mathbb{R}^3$, $|w| = 1$,

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

The result (19) then follows from the above inequality, (13), and (16). □

We can use Lemma 2 to reduce the analysis of the stability of the laminated microstructure to an analysis of the stability of a mixture of two variants [4,5] by evaluating $\rho_1(y;w)$ and $\rho_2(y;w)$ for appropriate $w \in \mathbb{R}^3$ to establish the inequality:

$$\tau_k(y) \le C \left[\mathcal{E}(y)^{1/2} + \mathcal{E}(y) \right] \qquad \text{for all } k \in \{1, \ldots, N\} \backslash \{i, j\},\ y \in \mathcal{A}\ . \tag{21}$$

In the following section, we will show how this can be done for the cubic to tetragonal transformation [20].

We have also used (18) for $\rho_1(y;w)$ and (19) for $\rho_2(y;w)$ to prove the estimate (21) for the tetragonal to monoclinic transformation ($N = 4$) [5] and the cubic to orthorhombic transformation ($N = 6$) [4], except for special cases when the material parameters in the transformation strain satisfy certain identities, in which case it was shown that the inequality (21) does not hold.

4 An Example: The Cubic to Tetragonal Transformation

We consider the cubic to tetragonal transformation [20] which has three energy wells ($N = 3$) given by

$$U_1 = \nu_1 I + (\nu_2 - \nu_1) e_1 \otimes e_1, \qquad U_2 = \nu_1 I + (\nu_2 - \nu_1) e_2 \otimes e_2,$$
$$U_3 = \nu_1 I + (\nu_2 - \nu_1) e_3 \otimes e_3$$

for material parameters $0 < \nu_1$, $0 < \nu_2$, $\nu_1 \neq \nu_2$. We assume that $\{e_1, e_2, e_3\}$ is an orthonormal basis for $\mathbb{R}^3$.

The following two lemmas [2,3,25] state that for the cubic to tetragonal transformation each $F_0 \in \mathcal{U}_i$ is not rank-one connected to any $F_1 \in \mathcal{U}_i$ with $F_0 \neq F_1$, but that every $F_0 \in \mathcal{U}_i$ is rank-one connected to two distinct $F_1 \in \mathcal{U}_j$ for all $j \neq i,\, j \in \{1,\, 2,\, 3\}$.

Lemma 3. *If $F_0 \in \mathcal{U}_i$ for some $i \in \{1,\, 2,\, 3\}$, then there does not exist $F_1 \in \mathcal{U}_i$ with $F_0 \neq F_1$, such that F_0 and F_1 are rank-one connected.*

Lemma 4. *If $F_0 \in \mathcal{U}_i$ for some $i \in \{1,\, 2,\, 3\}$, then for any $j \neq i,\ j \in \{1,\, 2,\, 3\}$, there exist two distinct $F_1 \in \mathcal{U}_j$ such that F_0 and F_1 are rank-one connected. If $QU_i \in \mathcal{U}_i$ and $U_j \in \mathcal{U}_j$ are rank-one connected so that*

$$QU_i = U_j + a \otimes n \tag{22}$$

for $Q \in SO(3)$, $a \in \mathbb{R}^3$, and $n \in \mathbb{R}^3$; then (up to a scalar multiple)

$$n \in \{e_i + e_j\, e_i - e_j\} \quad . \tag{23}$$

Further, if $n = e_i \pm e_j$, then

$$U_j^{-1} a \in \mathrm{Span}(e_i \mp e_j) \quad . \tag{24}$$

By (23), we have that $e_k \cdot n = 0$ for $k \in \{1, 2, 3\}$ such that $i \neq j \neq k$, so we can take $w = e_k$ in (18) to obtain

$$\tau_k(y)(\nu_1^2 - \nu_2^2) \leq C\mathcal{E}(y)^{1/2} \quad ,$$

and we can conclude the inequality (21) if $\nu_1 > \nu_2$. Similary, by (24), we have that $e_k \cdot U_j^{-1} a = 0$ such that $k \in \{1, 2, 3\}$ and $i \neq j \neq k$, so we can take $w = e_k$ in (19) to obtain

$$\tau_k(y)(\nu_1^2\nu_2^2 - \nu_1^4) \leq C\left[\mathcal{E}(y)^{1/2} + \mathcal{E}(y)\right] \quad .$$

Hence, we can also conclude from the above inequality that the inequality (21) holds if $\nu_1 < \nu_2$.

We note that the algebra for the proof of the inequality (21) for the tetragonal to monoclinic transformation ($N = 4$) [5] and the cubic to orthorhombic transformation ($N = 6$) [4] is more difficult since multiple choices of $w \in \mathbb{R}^3$ must used to obtain (21) from (18) and (19).

5 The Stability of the Microstructure

We assume in what follows that for the laminated microstructure under consideration, the inequalities (18) and (19) imply the estimate

$$\tau_k(y) \leq C\left[\mathcal{E}(y)^{1/2} + \mathcal{E}(y)\right] \quad \text{for all } k \in \{1, \ldots, N\}\backslash\{i,j\},\ y \in \mathcal{A} \quad . \tag{25}$$

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 general martensitic transformation can be deduced from the inequality (25) by the identical arguments used to deduce the results from (25) for the cubic to orthorhombic case [4] by making the obvious modifications in the argument to change $N = 6$ to general N. 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 N energy wells

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

and that ϕ is continuous and satisfies the growth condition

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

The following theorem 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 5. *We assume that the inequality* (25) *holds. Then the following results hold:*

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

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

(2) We have

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

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

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

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

Corollary 6. *If the inequality* (25) *holds, then there does not exist any* $y \in \mathcal{A}$ *such that*

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

For fixed $i, j \in \{1, \ldots, N\}$ 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

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

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

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

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

Theorem 7. *For a transformation such that* (25) *holds, we have*

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

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

$$\begin{aligned} \omega_\rho^i(y) &= \{x \in \omega : \Pi(\nabla y(x)) = QU_i \text{ and } \|\nabla y(x) - QU_i\| < \rho\}\,, \\ \omega_\rho^j(y) &= \{x \in \omega : \Pi(\nabla y(x)) = U_j \text{ and } \|\nabla y(x) - U_j\| < \rho\} \quad . \end{aligned}$$

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 [3,25] and is given by

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

Theorem 8. *We suppose that the reduction* (25) *is valid. Then for any Lipschitz domain* $\omega \subset \Omega$ *and any* $\rho > 0$, *there exists a constant* $C = C(\omega, \rho) > 0$ *such that for all* $y \in \mathcal{A}$

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

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

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

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 9. *We assume that the inequality* (25) *holds. Then we have*

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

6 The Finite Element Approximation of Microstructure

We consider the finite element approximation of the variational problem

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

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 [4,10,20–22,24,25].

Theorem 10. *For each* $h \in (0, h_0]$*, there exists* $y_h \in \mathcal{A}_h$ *such that*

$$\mathcal{E}(y_h) = \min_{z_h \in \mathcal{A}_h} \mathcal{E}(z_h) \leq C h^{1/2} \ . \tag{26}$$

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

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

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 also assume that the inequality (25) describing the reduction of low energy deformation to two energy wells holds. the following corollaries for the finite element approximation follow directly from the above estimate for the approximation of the energy (26). We assume below that $y_h \in \mathcal{A}_h$ is a finite element approximation satisfying the quasi-optimality condition

$$\mathcal{E}(y_h) \le \sigma \inf_{z_h \in \mathcal{A}_h} \mathcal{E}(z_h) \tag{27}$$

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

Corollary 11. *If the inequality* (25) *holds, then we have the following estimates:*

(1) There exists of positive constant C such that for any $y_h \in \mathcal{A}_h$ satisfying (27) *we have*

$$\int_\Omega |y_h(x) - y_0(x)|^2 \, dx \le C h^{1/4}$$

and

$$\int_\Omega \left\| \nabla y_h(x) - \Pi(\nabla y_h(x)) \right\|^2 \, dx \le C h^{1/4} \ .$$

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

$$\int_\Omega \left| [\nabla y_h(x) - \nabla y_0(x)] \, w \right|^2 \, dx \le C h^{1/4}$$

for any $y_h \in \mathcal{A}_h$ satisfying (27).

(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 (27) *we have*

$$\left\| \int_\omega [\nabla y_h(x) - \nabla y_0(x)] \, dx \right\| \le C h^{1/16} \ .$$

Corollary 12. *We assume that the inequality* (25) *holds. Then we have the following results:*

(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 (27)

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

(2) We have

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

for any $f \in \mathcal{V}$ and any $y_h \in \mathcal{A}_h$ satisfying (27).

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