

Approximation of Martensitic Microstructure with General Homogeneous Boundary Data¹

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We consider the approximation of martensitic microstructure for a class of martensitic transformations. We model such microstructures by multi-well energy minimization problems with general homogeneous boundary data. Under our assumptions on such boundary data, the underlying microstructure can be nonunique. We first show that any energy-minimizing sequence converges strongly to a unique macroscopic deformation that is precisely the homogeneous deformation in the boundary condition. We then prove a series of estimates for the approximation of admissible deformations to the unique macroscopic deformation of the microstructure and for the closeness of the gradients of admissible deformations to the energy wells. © 2002 Elsevier Science (USA)

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1. INTRODUCTION

Martensitic microstructure is fine-scale mixture of coherent phases or phase variants of a martensitic crystal such as a shape-memory alloy. The geometrically nonlinear theory of martensite predicts such microstructure by minimizing sequences of an elastic energy functional with a rotationally invariant, multi-well energy density of the underlying crystal [4, 5]. Such energy-minimizing sequences have been extensively studied via the

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notion of Young measures. However, it is practically interesting to understand how well individual deformations with low energy can approximate a microstructure, and to seek general statements valid for all approximate energy minimizers. Along this line of thinking, a theory of approximation of a simply laminated microstructure was first developed in [18] for a two-well energy density, and then extended in [9, 10, 16, 17] for other multi-well energy densities. As realized in [9], such a theory of approximation results from the uniqueness of the underlying microstructure.

In this work, we generalize the theory of approximation of a simply laminated microstructure to that of a more general class of martensitic microstructures. Specifically, we consider multi-well energy minimization problems in the framework of the geometrically nonlinear theory of martensite. We assume that the transformation matrices—those symmetric positive definite parts of the energy wells—satisfy certain conditions of variant reduction. To study stationary properties of the underlying crystal, we impose the Dirichlet boundary condition with a general homogeneous deformation whose gradient is in the quasiconvex hull of the energy wells. Nonhomogeneous boundary data can be possibly treated as in [5] using covering techniques.

Our main contributions are as follows.

1. The identification of conditions on the Dirichlet boundary data that are sufficient for the corresponding homogeneous deformation to be the unique macroscopic deformation of all microstructures and for the possible reduction of martensitic variants in these microstructures; cf. the conditions $F1$ – $F3$ in Section 2 and Theorem 3.1 in Section 3.

2. The derivation of a series of estimates for the approximation of admissible deformations to the unique macroscopic deformation of the microstructure and for the closeness of the gradients of admissible deformations to the energy wells; cf. Theorems 4.1–4.4 in Section 4.

3. The justification of the fact that a widely used projection from the gradient space to the union of energy wells is well defined and Borel measurable; cf. the Appendix.

Our idea of identifying unified conditions on the boundary data stems from [12]. See the maximality condition in [6, 7, 13]. Independently, we formulate such conditions, slightly more general, based on our work [9] on the simply laminated microstructure modeled by a six-well problem. Examples of microstructures that satisfy our conditions can be found in [5–7, 9, 10]. For energy-minimizing sequences, our estimates in Section 4 lead to the reduction of martensitic variants in any of the limiting microstructures, the strong convergence of certain directional derivatives of deformations, the strong convergence of deformations, and the weak convergence of

deformation gradients. Notice that our results can be applied to the study of the finite element analysis of microstructure [9, 14–17, 19].

In Section 2, we describe the multi-well energy minimization problem and state our assumptions on the energy density and the boundary data. In Section 3, we show some properties of the Young measure solutions of our energy minimization problems. In Section 4, we derive a series of estimates for all the admissible deformations for the approximation of the microstructure. Finally, in the Appendix, we prove that the projection from the gradient space to the energy wells is Borel measurable.

2. MULTI-WELL ENERGY MINIMIZATION PROBLEMS AND CONSTITUTIVE ASSUMPTIONS

We denote by $\Omega \subset \mathbb{R}^3$ the reference configuration of an underlying martensitic crystal which is taken to be the homogeneous austenite around the transformation temperature. We assume that Ω is a bounded domain with a Lipschitz continuous boundary $\partial\Omega$. We denote by $y: \Omega \rightarrow \mathbb{R}^3$ a deformation of the crystal and by $\nabla y: \Omega \rightarrow \mathbb{R}^{3 \times 3}$ the deformation gradient, where $\mathbb{R}^{3 \times 3}$ denotes the set of all 3×3 real matrices. We also denote by $\phi: \mathbb{R}^{3 \times 3} \rightarrow \mathbb{R}$ the free energy density per unit volume of the reference configuration of the crystal at a fixed temperature below the transformation temperature. We consider the variational problem of infimizing the total free energy functional

$$\mathcal{E}(y) := \int_{\Omega} \phi(\nabla y(x)) \, dx \tag{2.1}$$

over a set of admissible deformations \mathcal{A} . Throughout the paper, we use the notation $A := B$ to indicate that A is defined to be B .

We assume that the free energy density $\phi: \mathbb{R}^{3 \times 3} \rightarrow \mathbb{R}$ is continuous and satisfies the following properties $\phi 1$ – $\phi 3$ [5, 9, 18].

$\phi 1$. *Frame indifference:*

$$\phi(RF) = \phi(F) \quad \forall F \in \mathbb{R}^{3 \times 3} \quad \forall R \in \text{SO}(3),$$

where $\text{SO}(3)$ is the set of all real 3×3 rotation matrices.

$\phi 2$. *Absolute minimizers:*

$$\begin{aligned} \phi(F) &\geq 0 \quad \forall F \in \mathbb{R}^{3 \times 3}, \\ \phi(F) = 0 &\text{ if and only if } F \in \mathcal{U} := \mathcal{U}_1 \cup \dots \cup \mathcal{U}_N, \end{aligned} \tag{2.2}$$

where $N \geq 1$ is an integer,

$$\mathcal{U}_i := \text{SO}(3)U_i := \{RU_i: R \in \text{SO}(3)\}, \quad 1 \leq i \leq N,$$

and $U_1, \dots, U_N \in \mathbb{R}^{3 \times 3}$ are the distinct transformation matrices, always assumed to be symmetric positive definite, for the underlying martensitic crystal.

$\phi 3$. *Growth condition:*

$$\phi(F) \geq \kappa[\text{dist}(F, \mathcal{U})]^2 \quad \forall F \in \mathbb{R}^{3 \times 3}, \tag{2.3}$$

where $\kappa > 0$ is a constant and

$$\text{dist}(F, \mathcal{U}) := \inf_{G \in \mathcal{U}} \|F - G\|,$$

where $\|F\| := \sqrt{\sum_{i,j=1}^3 F_{ij}^2}$ is the Frobenius norm of a matrix $F = (F_{ij}) \in \mathbb{R}^{3 \times 3}$.

We define the set of admissible deformations to be

$$\mathcal{A} = \{y \in W^{1, \infty}(\Omega; \mathbb{R}^3) : y(x) = y_0(x), x \in \partial\Omega\}, \tag{2.4}$$

where the boundary value is understood in the sense of trace and $y_0 : \Omega \rightarrow \mathbb{R}^3$ is a homogeneous deformation defined for a given $F_0 \in \mathbb{R}^{3 \times 3}$ by

$$y_0(x) = F_0 x \quad \forall x \in \Omega. \tag{2.5}$$

Except as otherwise stated, we always assume that the boundary data $F_0 \in \mathbb{R}^{3 \times 3}$ satisfies the following conditions F1–F3.

F1. *Energy-minimizing microstructure:* $F_0 \in \mathcal{U}^{qc}$, the quasiconvex hull of \mathcal{U} , i.e.,

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

F2. *Uniqueness of macroscopic deformation:* there exist a permutation $(i_1 \dots i_N)$ of $(1 \dots N)$, an integer s with $1 \leq s \leq N$, and a unit vector $e_0 \in \mathbb{R}^3$ such that

$$|F_0 e_0| = |U_{i_1} e_0| = \dots = |U_{i_s} e_0|. \tag{2.6}$$

F3. *Variant reduction:* if $s < N$, then, for each $j \in \{s + 1, \dots, N\}$, either there exists a unit vector $a_j \in \mathbb{R}^3$ such that

$$\begin{aligned} |F_0 a_j| &= |U_{i_1} a_j| = \dots = |U_{i_s} a_j| \geq \max_{s+1 \leq k \leq N} |U_{i_k} a_j|, \\ |F_0 a_j| &\neq |U_{i_j} a_j|, \end{aligned} \tag{2.7}$$

or there exists a unit vector $b_j \in \mathbb{R}^3$ such that

$$\begin{aligned} |(\text{Cof } F_0) b_j| &= |(\text{Cof } U_{i_1}) b_j| = \dots = |(\text{Cof } U_{i_s}) b_j| \\ &\geq \max_{s+1 \leq k \leq N} |(\text{Cof } U_{i_k}) b_j|, \end{aligned} \tag{2.8}$$

$$|(\text{Cof } F_0) b_j| \neq |(\text{Cof } U_{i_j}) b_j|,$$

where $\text{Cof } F \in \mathbb{R}^{3 \times 3}$ is the cofactor matrix of $F \in \mathbb{R}^{3 \times 3}$.

If all the transformation matrices U_1, \dots, U_N have the same determinant and a same pair of eigenvalue and eigenvector, then one has the explicit formula for the quasiconvex hull \mathcal{U}^{qc} [5, 7]. In this case, any $F_0 \in \mathcal{U}^{qc}$ satisfies F1–F3 with $s = N$ [5, 7]. Examples of such martensitic transformations include the tetragonal to orthorhombic or orthorhombic to monoclinic transformation modeled by a two-well problem and the tetragonal to monoclinic transformation modeled by a four-well problem. If the boundary data $F_0 \in \mathcal{U}^{qc}$ satisfy certain conditions that can lead to the reduction of variants, then they also satisfy our conditions. Examples of such reduction include that from a three-well, four-well, or six-well to a two-well problem and that from a twelve-well to a four-well problem [5, 6, 9, 10].

3. PROPERTIES OF YOUNG MEASURE SOLUTIONS

The following theorem summarizes the main properties of the Young measure solutions of our energy minimization problem.

THEOREM 3.1. *Let the continuous energy density $\phi: \mathbb{R}^{3 \times 3} \rightarrow \mathbb{R}$ and the boundary data $F_0 \in \mathbb{R}^{3 \times 3}$ satisfy the conditions $\phi 1$ – $\phi 3$ and F1–F3, respectively. Let $\{y_k\}$ be a $W^{1, \infty}(\Omega; \mathbb{R}^3)$ -bounded, energy-minimizing sequence in \mathcal{A} such that the corresponding sequence of gradients $\{\nabla y_k\}$ generates a family of Young measures $\{\nu_x: x \in \Omega\}$. Then, we have the reduction of variants*

$$\text{supp } \nu_x \subseteq \mathcal{S} := \mathcal{U}_{i_1} \cup \dots \cup \mathcal{U}_{i_s} \quad \text{a.e. } x \in \Omega, \tag{3.1}$$

where (i_1, \dots, i_s) is defined in the condition F2. We also have the strong convergence

$$\nabla y_k e_0 \rightarrow \nabla y_0 e_0 \quad \text{and} \quad y_k \rightarrow y_0 \quad \text{in } L^p(\Omega; \mathbb{R}^3) \tag{3.2}$$

for any $p \in [1, \infty)$, where y_0 is the homogeneous deformation in the boundary condition, and $e_0 \in \mathbb{R}^3$ is the unit vector satisfying (2.6), and the weak-* convergence

$$y_k \overset{*}{\rightharpoonup} y_0 \quad \text{in } W^{1, \infty}(\Omega; \mathbb{R}^3). \tag{3.3}$$

Finally, we have

$$\int_{\mathcal{U}} G \, d\nu_x(G) = F_0 \quad \text{and} \quad \int_{\mathcal{U}} \text{Cof } G \, d\nu_x(G) = \text{Cof } F_0 \quad \text{a.e. } x \in \Omega. \tag{3.4}$$

Proof. It follows from the continuity of $\phi: \mathbb{R}^{3 \times 3} \rightarrow \mathbb{R}$, the assumptions $\phi 2$, $\phi 3$, and F1 that [5]

$$\text{supp } \nu_x \subseteq \mathcal{U} \quad \text{a.e. } x \in \Omega. \tag{3.5}$$

If $s = N$ in the condition $F2$, then (3.1) follows from (3.5). Suppose $s < N$. Define the volume fraction

$$\tau_i := \frac{1}{\text{meas } \Omega} \int_{\Omega} \nu_x(\mathcal{U}_i) dx \geq 0, \quad i = 1, \dots, N.$$

Fix $j \in \{s + 1, \dots, N\}$. If (2.7) holds true for some unit vector $a_j \in \mathbb{R}^3$, then it follows from the fact that $y_k = y_0$ on $\partial\Omega$ for all $k \geq 1$, the Divergence Theorem, and the fundamental theorem for Young measures [2] that

$$F_0 = \lim_{k \rightarrow \infty} \frac{1}{\text{meas } \Omega} \int_{\Omega} \nabla y_k(x) dx = \frac{1}{\text{meas } \Omega} \int_{\Omega} \int_{\mathcal{U}} G dv_x(G) dx. \quad (3.6)$$

Consequently,

$$|F_0 a_j| \leq \frac{1}{\text{meas } \Omega} \int_{\Omega} \int_{\mathcal{U}} |G a_j| dv_x(G) dx = \sum_{l=1}^N \tau_{i_l} |U_{i_l} a_j|,$$

leading to $\tau_{i_j} = 0$ by (2.7) and the fact that $\sum_{l=1}^N \tau_{i_l} = 1$. If, instead, (2.8) holds true for some unit vector $b_j \in \mathbb{R}^3$, then a similar argument using the cofactor of gradient leads to the same result. Thus, (3.1) is proved.

It follows from the fundamental theorem for Young measures [2], (3.6), (3.1), and (2.6) that as $k \rightarrow \infty$,

$$\begin{aligned} & \frac{1}{\text{meas } \Omega} \int_{\Omega} |[\nabla y_k(x) - F_0] e_0|^2 dx \\ & \rightarrow \frac{1}{\text{meas } \Omega} \int_{\Omega} \int_{\mathcal{U}} |(G - F_0) e_0|^2 dv_x(G) dx \\ & = \frac{1}{\text{meas } \Omega} \int_{\Omega} \int_{\mathcal{U}} (|G e_0|^2 + |F_0 e_0|^2 - 2G e_0 \cdot F_0 e_0) dv_x(G) dx \\ & = \frac{1}{\text{meas } \Omega} \int_{\Omega} \int_{\mathcal{U}} (|G e_0|^2 - |F_0 e_0|^2) dv_x(G) dx \\ & = \frac{1}{\text{meas } \Omega} \sum_{l=1}^s \int_{\Omega} \int_{\mathcal{U}_{i_l}} (|G e_0|^2 - |F_0 e_0|^2) dv_x(G) dx \\ & = \sum_{l=1}^s \tau_{i_l} (|U_{i_l} e_0|^2 - |F_0 e_0|^2) \\ & = 0. \end{aligned}$$

This, together with an application of the Poincaré inequality [9, 18],

$$\int_{\Omega} |y(x) - F_0 x|^2 dx \leq C \int_{\Omega} |[\nabla y(x) - F_0] e_0|^2 dx \quad \forall y \in \mathcal{A}, \quad (3.7)$$

where $C > 0$ is a constant, implies (3.2) for $p = 2$. It now follows that any subsequences of $\{\nabla y_k e_0\}$ and $\{y_k\}$ have further subsequences that converge

almost everywhere in Ω to $\nabla y_0 e_0$ and y_0 , respectively. By the Lebesgue Dominated Convergence Theorem, these further subsequences converge in L^p -norm to $\nabla y_0 e_0$ and y_0 , respectively, leading to (3.2) for any $p \in [1, \infty)$. Since $\{y_k\}$ is bounded in $W^{1,\infty}(\Omega; \mathbb{R}^3)$, any subsequence of $\{y_k\}$ has a further subsequence that converges weakly- $*$ in $W^{1,\infty}(\Omega; \mathbb{R}^3)$. By (3.2), the weak- $*$ limit is y_0 . This proves (3.3). Finally, (3.4) follows from (3.3) and the minors relations [5, 8]. ■

4. APPROXIMATION OF MICROSTRUCTURE

We define a projection $\pi: \mathbb{R}^{3 \times 3} \rightarrow \mathcal{U}$ by

$$\|F - \pi(F)\| = \text{dist}(F, \mathcal{U}), \quad F \in \mathbb{R}^{3 \times 3}.$$

In the Appendix, we show that, with a possible modification of its definition on a subset of $\mathbb{R}^{3 \times 3}$ of Lebesgue measure zero, this projection is well defined and Borel measurable. The following lemma is a direct consequence of the definition of the projection $\pi: \mathbb{R}^{3 \times 3} \rightarrow \mathcal{U}$ and the growth condition (2.3).

LEMMA 4.1. *We have*

$$\int_{\Omega} \|\nabla y(x) - \pi(\nabla y(x))\|^2 dx \leq \kappa^{-1} \mathcal{E}(y) \quad \forall y \in W^{1,\infty}(\Omega; \mathbb{R}^3).$$

We shall frequently use the following well-known result that a subdeterminant of the gradient is a null Lagrangian [1, 11].

LEMMA 4.2. *We have for any $y \in \mathcal{A}$ that*

$$\begin{aligned} \int_{\Omega} \nabla y(x) dx &= \int_{\Omega} F_0 dx, \\ \int_{\Omega} \text{Cof } \nabla y(x) dx &= \int_{\Omega} \text{Cof } F_0 dx. \end{aligned}$$

In what follows, we denote by C a generic positive constant which is always assumed to be independent of admissible deformations $y \in \mathcal{A}$.

LEMMA 4.3. *Let the continuous energy density $\phi: \mathbb{R}^{3 \times 3} \rightarrow \mathbb{R}$ and the boundary data $F_0 \in \mathbb{R}^{3 \times 3}$ satisfy the conditions $\phi 1$ – $\phi 3$ and $F 1$ – $F 3$, respectively. We have for any $y \in \mathcal{A}$ and any unit vector $w \in \mathbb{R}^3$ that*

$$\int_{\Omega} |[\pi(\nabla y(x)) - F_0]w|^2 dx - \int_{\Omega} [|\pi(\nabla y(x))w|^2 - |F_0 w|^2] dx \leq C \mathcal{E}(y)^{1/2} \tag{4.1}$$

and

$$\begin{aligned} & \int_{\Omega} |[\text{Cof } \pi(\nabla y(x)) - \text{Cof } F_0]w|^2 dx \\ & - \int_{\Omega} \{ |[\text{Cof } \pi(\nabla y(x))]w|^2 - |(\text{Cof } F_0)w|^2 \} dx \leq C[\mathcal{E}(y)^{1/2} + \mathcal{E}(y)]. \quad (4.2) \end{aligned}$$

Proof. Fix $y \in \mathcal{A}$ and $w \in \mathbb{R}^3$ with $|w| = 1$. We have by Lemma 4.2 that

$$\begin{aligned} & \int_{\Omega} |[\pi(\nabla y(x)) - F_0]w|^2 dx \\ & = \int_{\Omega} [|\pi(\nabla y(x))w|^2 + |F_0w|^2 - 2\pi(\nabla y(x))w \cdot F_0w] dx \\ & = \int_{\Omega} [|\pi(\nabla y(x))w|^2 + |F_0w|^2 - 2\nabla y(x)w \cdot F_0w] dx \\ & \quad + \int_{\Omega} [2\nabla y(x)w \cdot F_0w - 2\pi(\nabla y(x))w \cdot F_0w] dx \\ & = \int_{\Omega} [|\pi(\nabla y(x))w|^2 - |F_0w|^2] dx + 2 \int_{\Omega} [\nabla y(x) - \pi(\nabla y(x))]w \cdot F_0w dx. \end{aligned}$$

Consequently, we have by the Cauchy–Schwarz inequality and Lemma 4.1 that

$$\begin{aligned} & \int_{\Omega} |[\pi(\nabla y(x)) - F_0]w|^2 dx - \int_{\Omega} [|\pi(\nabla y(x))w|^2 - |F_0w|^2] dx \\ & = 2 \int_{\Omega} [\nabla y(x) - \pi(\nabla y(x))]w \cdot F_0w dx \\ & \leq 2\|F_0\| \int_{\Omega} \|\nabla y(x) - \pi(\nabla y(x))\| dx \\ & \leq 2\|F_0\|(\text{meas } \Omega)^{1/2} \left[\int_{\Omega} \|\nabla y(x) - \pi(\nabla y(x))\|^2 dx \right]^{1/2} \\ & \leq 2\|F_0\|(\text{meas } \Omega)^{1/2} \kappa^{-1/2} \mathcal{E}(y)^{1/2}, \end{aligned}$$

proving (4.1).

A similar argument leads to

$$\begin{aligned} & \int_{\Omega} |[\text{Cof } \pi(\nabla y(x)) - \text{Cof } F_0]w|^2 dx \\ & - \int_{\Omega} \{ |[\text{Cof } \pi(\nabla y(x))]w|^2 - |(\text{Cof } F_0)w|^2 \} dx \\ & = 2 \int_{\Omega} [\text{Cof } \nabla y(x) - \text{Cof } \pi(\nabla y(x))]w \cdot F_0w dx \\ & \leq 2\|F_0\| \int_{\Omega} \|\text{Cof } \nabla y(x) - \text{Cof } \pi(\nabla y(x))\| dx. \quad (4.3) \end{aligned}$$

Setting $V(x) = (V_{ij}(x)) = \nabla y(x) \in \mathbb{R}^{3 \times 3}$ and $W(x) = (W_{ij}(x)) = \pi(\nabla y(x)) \in \mathcal{U}$ for $x \in \Omega$, we have that both V and W are in $L^\infty(\Omega; \mathbb{R}^{3 \times 3})$ and that the L^∞ -norm of W is bounded uniformly for all $y \in \mathcal{A}$. Moreover,

$$V_{ij}V_{kl} - W_{ij}W_{kl} = (V_{ij} - W_{ij})W_{kl} + W_{ij}(V_{kl} - W_{kl}) + (V_{ij} - W_{ij})(V_{kl} - W_{kl})$$

for any $i, j, k, l \in \{1, 2, 3\}$. Consequently, it follows from the definition of cofactor matrix, the Cauchy–Schwarz inequality, and Lemma 4.1 that

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

This, together with (4.3), leads to (4.2). ■

The following theorem gives an estimate on the reduction of martensitic variants. See (3.1) in Theorem 3.1 for its Young measure version.

THEOREM 4.1. *Let the continuous energy density $\phi: \mathbb{R}^{3 \times 3} \rightarrow \mathbb{R}$ and the boundary data $F_0 \in \mathbb{R}^{3 \times 3}$ satisfy the conditions $\phi 1$ – $\phi 3$ and $F 1$ – $F 3$ with $s < N$, respectively. We have*

$$\text{meas}\{x \in \Omega: \pi(\nabla y(x)) \notin \mathcal{F}\} \leq C[\mathcal{E}(y)^{1/2} + \mathcal{E}(y)] \quad \forall y \in \mathcal{A}.$$

Proof. Fix $y \in \mathcal{A}$ and denote

$$\Omega_i(y) := \{x \in \Omega: \pi(\nabla y(x)) \in \mathcal{U}_i\}, \quad i = 1, \dots, N. \tag{4.4}$$

Notice that all $\Omega_i(y)$ ($i = 1, \dots, N$) are pairwise disjoint. Fix $j \in \{s + 1, \dots, N\}$. If (2.7) holds true for some $a_j \in \mathbb{R}^3$, then we have by (4.1) with $w = a_j$ that

$$\begin{aligned} C\mathcal{E}(y)^{1/2} & \geq \int_{\Omega} [|F_0 a_j|^2 - |\pi(\nabla y(x)) a_j|^2] \, dx \\ & = \sum_{i=1}^N \int_{\Omega_i(y)} [|F_0 a_j|^2 - |\pi(\nabla y(x)) a_j|^2] \, dx \\ & = \sum_{i=1}^N \text{meas } \Omega_i(y) [|F_0 a_j|^2 - |U_i a_j|^2] \\ & \geq \text{meas } \Omega_j(y) [|F_0 a_j|^2 - |U_j a_j|^2], \end{aligned}$$

which, together with (2.7), leads to

$$\text{meas } \Omega_{i_j}(y) \leq C \mathcal{E}(y)^{1/2}. \quad (4.5)$$

If, instead, (2.8) holds true for some $b_j \in \mathbb{R}^3$, then we have by (4.2) with $w = b_j$ that

$$\begin{aligned} C[\mathcal{E}(y)^{1/2} + \mathcal{E}(y)] &\geq \int_{\Omega} \{ |(\text{Cof } F_0)b_j|^2 - |[\text{Cof } \pi(\nabla y(x))]b_j|^2 \} dx \\ &= \sum_{i=1}^N \int_{\Omega_{i_j}(y)} \{ |(\text{Cof } F_0)b_j|^2 - |[\text{Cof } \pi(\nabla y(x))]b_j|^2 \} dx \\ &= \sum_{i=1}^N \text{meas } \Omega_{i_j}(y) [|(\text{Cof } F_0)b_j|^2 - |(\text{Cof } U_{i_j})b_j|^2] \\ &\geq \text{meas } \Omega_{i_j}(y) [|(\text{Cof } F_0)b_j|^2 - |(\text{Cof } U_{i_j})b_j|^2], \end{aligned}$$

which, together with (2.8), leads to

$$\text{meas } \Omega_{i_j}(y) \leq C[\mathcal{E}(y)^{1/2} + \mathcal{E}(y)]. \quad (4.6)$$

Now, the estimates (4.5) and (4.6), together with the fact that

$$\{x \in \Omega: \pi(\nabla y(x)) \notin \mathcal{S}\} = \bigcup_{j=s+1}^N \Omega_{i_j}(y), \quad (4.7)$$

imply the desired estimate. ■

Recall from Theorem 3.1 that $F_0 = \nabla y_0$ is the gradient of the unique macroscopic deformation y_0 which coincides with the boundary data. The following result gives an estimate for the approximation of certain directional derivatives of admissible deformations to that of the deformation y_0 . It implies immediately the strong convergence of the directional derivative for any energy-minimizing sequence; cf. (3.2) with $p = 2$ in Theorem 3.1.

THEOREM 4.2. *Let the continuous energy density $\phi: \mathbb{R}^{3 \times 3} \rightarrow \mathbb{R}$ and the boundary data $F_0 \in \mathbb{R}^{3 \times 3}$ satisfy the conditions $\phi 1$ – $\phi 3$ and $F 1$ – $F 3$, respectively. We have for the unit vector $e_0 \in \mathbb{R}^3$ satisfying (2.6) that*

$$\int_{\Omega} |[\nabla y(x) - F_0]e_0|^2 dx \leq C[\mathcal{E}(y)^{1/2} + \mathcal{E}(y)] \quad \forall y \in \mathcal{A}.$$

Proof. We have for any $y \in \mathcal{A}$ that

$$\begin{aligned} \int_{\Omega} |[\nabla y(x) - F_0]e_0|^2 dx &\leq 2 \int_{\Omega} |[\nabla y(x) - \pi(\nabla y(x))]e_0|^2 dx \\ &\quad + 2 \int_{\Omega} |[\pi(\nabla y(x)) - F_0]e_0|^2 dx. \end{aligned} \quad (4.8)$$

Since $|e_0| = 1$, we have by Lemma 4.1 that

$$\int_{\Omega} |[\nabla y(x) - \pi(\nabla y(x))]e_0|^2 dx \leq \int_{\Omega} \|\nabla y(x) - \pi(\nabla y(x))\|^2 dx \leq \kappa^{-1} \mathcal{E}(y). \tag{4.9}$$

In view of (4.1) with $w = e_0$, (2.6), (4.7), and Theorem 4.1, we have

$$\begin{aligned} & \int_{\Omega} |[\pi(\nabla y(x)) - F_0]e_0|^2 dx \\ & \leq C \mathcal{E}(y)^{1/2} + \int_{\Omega} [|\pi(\nabla y(x))e_0|^2 - |F_0 e_0|^2] dx \\ & = C \mathcal{E}(y)^{1/2} + \int_{\{x \in \Omega: \pi(\nabla y(x)) \in \mathcal{S}\}} [|\pi(\nabla y(x))e_0|^2 - |F_0 e_0|^2] dx \\ & \quad + \int_{\{x \in \Omega: \pi(\nabla y(x)) \notin \mathcal{S}\}} [|\pi(\nabla y(x))e_0|^2 - |F_0 e_0|^2] dx \\ & \leq C \mathcal{E}(y)^{1/2} + \sum_{j=1}^s \text{meas } \Omega_{i_j} [|U_{i_j} e_0|^2 - |F_0 e_0|^2] \\ & \quad + C \text{meas}\{x \in \Omega: \pi(\nabla y(x)) \notin \mathcal{S}\} \\ & \leq C[\mathcal{E}(y)^{1/2} + \mathcal{E}(y)], \end{aligned} \tag{4.10}$$

where $\Omega_i(y)$ ($1 \leq i \leq N$) is defined in (4.4). The assertion of the theorem now follows from (4.8)–(4.10). ■

The following result gives an L^2 estimate for the approximation of any admissible deformation to the unique macroscopic deformation y_0 . Applying this estimate to an energy-minimizing sequence, we can immediately obtain the strong convergence of such a sequence to the unique macroscopic deformation y_0 ; cf. (3.2) with $p = 2$ in Theorem 3.1.

THEOREM 4.3. *Let the continuous energy density $\phi: \mathbb{R}^{3 \times 3} \rightarrow \mathbb{R}$ and the boundary data $F_0 \in \mathbb{R}^{3 \times 3}$ satisfy the conditions $\phi 1$ – $\phi 3$ and $F 1$ – $F 3$, respectively. We have*

$$\int_{\Omega} |y(x) - y_0(x)|^2 dx \leq C[\mathcal{E}(y)^{1/2} + \mathcal{E}(y)] \quad \forall y \in \mathcal{A}.$$

Proof. This follows the Poincaré inequality (3.7) and Theorem 4.2. ■

COROLLARY 4.1 (cf. [3]). *Let the continuous energy density $\phi: \mathbb{R}^{3 \times 3} \rightarrow \mathbb{R}$ and the boundary data $F_0 \in \mathbb{R}^{3 \times 3}$ satisfy the conditions $\phi 1$ – $\phi 3$ and $F 1$ – $F 3$, respectively. If $F_0 \notin \mathcal{U}$, then there does not exist any $y \in \mathcal{A}$ such that*

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

Proof. If $y \in \mathcal{A}$ was a minimizer, then we would have that $\mathcal{E}(y) = 0$ by the assumption $F1$. Hence, $y = y_0$ by Theorem 4.3. Thus, $\nabla y(x) = \nabla y_0(x) = F_0$ for a.e. $x \in \Omega$. But, the assumption that $F_0 \notin \mathcal{U}$ implies that $\phi(F_0) > 0$ by (2.2). Therefore,

$$0 = \mathcal{E}(y) = (\text{meas } \Omega)\phi(F_0) > 0,$$

which is a contradiction. ■

The following result leads to the weak convergence of any energy-minimizing sequence of admissible deformations in \mathcal{A} ; cf. (3.3) in Theorem 3.1.

THEOREM 4.4. *Let the continuous energy density $\phi: \mathbb{R}^{3 \times 3} \rightarrow \mathbb{R}$ and the boundary data $F_0 \in \mathbb{R}^{3 \times 3}$ satisfy the conditions $\phi 1$ – $\phi 3$ and $F1$ – $F3$, respectively. Then, for any Lipschitz domain $\omega \subseteq \Omega$, there exists a constant $C = C(\omega) > 0$ depending on ω such that*

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

Proof. Fix $y \in \mathcal{A}$. It follows from the Divergence Theorem and the Cauchy–Schwarz inequality that

$$\begin{aligned} & \left\| \int_{\omega} [\nabla y(x) - \nabla y_0(x)] dx \right\| \\ &= \left\| \int_{\partial\omega} [y(x) - y_0(x)] \otimes \nu dS \right\| \\ &\leq \int_{\partial\omega} |y(x) - y_0(x)| dS \\ &\leq (\text{meas}_2 \partial\omega)^{1/2} \left(\int_{\partial\omega} |y(x) - y_0(x)|^2 dS \right)^{1/2}, \end{aligned} \quad (4.11)$$

where ν is the unit exterior normal to $\partial\omega$ and $\text{meas}_2 \partial\omega$ is the surface area of $\partial\omega$. By the trace theorem and the Cauchy–Schwarz inequality, we obtain that

$$\begin{aligned} & \int_{\partial\omega} |y(x) - y_0(x)|^2 dS \\ &\leq C \left\{ \int_{\omega} |y(x) - y_0(x)|^2 dx + \int_{\omega} |\nabla[|y(x) - y_0(x)|^2]| dx \right\} \\ &\leq C \left[\int_{\omega} |y(x) - y_0(x)|^2 dx + \left(\int_{\omega} |y(x) - y_0(x)|^2 dx \right)^{1/2} \right. \\ &\quad \left. \times \left(\int_{\omega} \|\nabla y(x) - \nabla y_0(x)\|^2 dx \right)^{1/2} \right]. \end{aligned} \quad (4.12)$$

Further, we have by the triangle inequality and Lemma 4.1 that

$$\begin{aligned} \left(\int_{\omega} \|\nabla y(x) - \nabla y_0(x)\|^2 dx\right)^{1/2} &\leq \left(\int_{\omega} \|\nabla y(x) - \pi(\nabla y(x))\|^2 dx\right)^{1/2} \\ &\quad + \left(\int_{\omega} \|\pi(\nabla y(x)) - \nabla y_0(x)\|^2 dx\right)^{1/2} \\ &\leq C[\mathcal{E}(y)^{1/2} + 1]. \end{aligned} \tag{4.13}$$

It now follows from (4.12), (4.13), Theorem 4.3, and the fact

$$0 \leq \mathcal{E}(y)^p \leq \max(\mathcal{E}(y), \mathcal{E}(y)^{1/4}) \leq \mathcal{E}(y) + \mathcal{E}(y)^{1/4}$$

for any $p \in [1/4, 1]$ that

$$\int_{\partial\omega} |y(x) - y_0(x)|^2 dS \leq C[\mathcal{E}(y)^{1/4} + \mathcal{E}(y)].$$

This, together with (4.11), leads to the desired estimate. ■

APPENDIX THE PROJECTION $\pi: \mathbb{R}^{3 \times 3} \rightarrow \mathcal{U}$

We recall for any $F \in \mathbb{R}^{3 \times 3}$ that the projection $\pi(F) \in \mathcal{U}$ is defined by

$$\|F - \pi(F)\| = \text{dist}(F, \mathcal{U}),$$

where $\mathcal{U} = \mathcal{U}_1 \cup \dots \cup \mathcal{U}_N$, $\mathcal{U}_i = \text{SO}(3)U_i$ ($i = 1, \dots, N$), and all $U_1, \dots, U_N \in \mathbb{R}^{3 \times 3}$ are distinct and symmetric positive definite.

PROPOSITION A.1. *There exists a closed subset $\mathcal{M} \subset \mathbb{R}^{3 \times 3}$ of zero Lebesgue measure such that there exists a unique $\pi(F) \in \mathcal{U}$ for any $F \in \mathbb{R}^{3 \times 3} \setminus \mathcal{M}$ and that $\pi: \mathbb{R}^{3 \times 3} \setminus \mathcal{M} \rightarrow \mathcal{U}$ is continuous. Moreover, with any value $\pi(F)$ assigned to any $F \in \mathcal{M}$, the projection $\pi: \mathbb{R}^{3 \times 3} \rightarrow \mathcal{U}$ is well defined and Borel measurable.*

Proof. Since $\mathcal{U} \subset \mathbb{R}^{3 \times 3}$ is compact, the distance $\text{dist}(F, \mathcal{U})$ is a continuous function of $F \in \mathbb{R}^{3 \times 3}$. A projection $\pi(F) \in \mathcal{U}$ thus exists for any $F \in \mathbb{R}^{3 \times 3}$, although it may not be unique. Let \mathcal{M} be the subset of $\mathbb{R}^{3 \times 3}$ that consists of all matrices $F \in \mathbb{R}^{3 \times 3}$ such that $\det F = 0$, or $\det F < 0$ but the smallest eigenvalue of $FU_i^2 F^T$ for some $i \in \{1, \dots, N\}$ is a repeated eigenvalue, or $\text{dist}(F, \mathcal{U}_i) = \text{dist}(F, \mathcal{U}_j)$ for some i and j with $1 \leq i, j \leq N$ and $i \neq j$. It is easy to see that \mathcal{M} is a lower dimensional smooth and closed manifold, and hence a closed subset of $\mathbb{R}^{3 \times 3}$ with zero Lebesgue measure. By Proposition A.2 below, the projection $\pi(F)$ is unique for any $F \in \mathbb{R}^{3 \times 3} \setminus \mathcal{M}$. Moreover, $\pi: \mathbb{R}^{3 \times 3} \setminus \mathcal{M} \rightarrow \mathcal{U}$ is a continuous mapping. Consequently, with a suitable modification of the definition of $\pi(F)$ for $F \in \mathcal{M}$, the projection $\pi: \mathbb{R}^{3 \times 3} \rightarrow \mathcal{U}$ is well defined and Borel measurable. ■

The following result is of its own interest.

PROPOSITION A.2. *Let $U \in \mathbb{R}^{3 \times 3}$ be a symmetric positive definite matrix. For any $F \in \mathbb{R}^{3 \times 3}$, there exists a projection $\pi_0(F) \in \text{SO}(3)U := \{RU: R \in \text{SO}(3)\}$ such that*

$$\|F - \pi_0(F)\| = \text{dist}(F, \text{SO}(3)U) := \inf_{G \in \text{SO}(3)U} \|F - G\|. \tag{A.1}$$

If $\det F > 0$, then the projection is unique and given by

$$\pi_0(F) = (FU^2F^T)^{1/2}(UF^T)^{-1}U. \tag{A.2}$$

If $\det F < 0$ and the smallest eigenvalue of the symmetric positive definite matrix $(FU^2F^T)^{1/2}$ is not a repeated eigenvalue, then the projection is unique and given by

$$\pi_0(F) = (I - 2v_1 \otimes v_1)(FU^2F^T)^{1/2}(UF^T)^{-1}U, \tag{A.3}$$

where $I \in \mathbb{R}^{3 \times 3}$ is the identity matrix and v_1 is a unit eigenvector corresponding to the smallest eigenvalue of the matrix $(FU^2F^T)^{1/2}$.

If $\det F < 0$ and the smallest eigenvalue of the matrix $(FU^2F^T)^{1/2}$ is a repeated eigenvalue, then there are infinitely many projections $\pi_0(F) \in \text{SO}(3)U$.

Proof. Fix $F \in \mathbb{R}^{3 \times 3}$. The existence of a projection $\pi_0(F) \in \text{SO}(3)U$ follows from the compactness of the set $\text{SO}(3)U$ and the continuity of the distance function defined in (A.1).

Notice that any matrix in $\text{SO}(3)U$ is of the form RU with $R \in \text{SO}(3)$. Moreover,

$$\|F - RU\|^2 = \|F\|^2 - 2\langle F, RU \rangle + \|RU\|^2 = \|F\|^2 - 2\text{tr}(RUF^T) + \|U\|^2,$$

where $\langle A, B \rangle := \text{tr}(A^T B) = \text{tr}(BA^T)$ is the matrix inner product of $A, B \in \mathbb{R}^{3 \times 3}$ and $\text{tr} A = \sum_{i=1}^3 A_{ii}$ is the trace of $A = (A_{ij}) \in \mathbb{R}^{3 \times 3}$. Hence, the infimum in (A.1) is attained by $\pi_0(F) = R_0U \in \text{SO}(3)U$ with $R_0 \in \text{SO}(3)$ such that

$$\text{tr}(R_0UF^T) = \max_{R \in \text{SO}(3)} \text{tr}(RUF^T).$$

Suppose $\det F \neq 0$. Let $UF^T = QV$ be the unique polar decomposition of UF^T with $V = (FU^2F^T)^{1/2} \in \mathbb{R}^{3 \times 3}$ symmetric positive definite and $Q = UF^T V^{-1} = UF^T (FU^2F^T)^{-1/2} \in \mathbb{R}^{3 \times 3}$ orthogonal. Let $V = \sum_{i=1}^3 \lambda_i v_i \otimes v_i$ be the canonical decomposition of the matrix V with λ_i ($i = 1, 2, 3$) its eigenvalues such that $0 < \lambda_1 \leq \lambda_2 \leq \lambda_3$ and $v_i \in \mathbb{R}^3$ ($i = 1, 2, 3$) its corresponding orthonormal eigenvectors. We have for any $R \in \text{SO}(3)$ that

$$\text{tr}(RUF^T) = \text{tr}(RQV) = \text{tr}\left(\sum_{i=1}^3 \lambda_i RQv_i \otimes v_i\right) = \sum_{i=1}^3 \lambda_i RQv_i \cdot v_i. \tag{A.4}$$

Assume first $\det F > 0$. Then, the orthogonal matrix Q is in fact a proper rotation. Hence, $RQ \in \text{SO}(3)$. Notice for each i ($1 \leq i \leq 3$) that $RQv_i \cdot v_i \leq 1$ and $RQv_i \cdot v_i = 1$ if and only if $RQv_i = v_i$. Hence, $\text{tr}(RUF^T)$ is maximized if and only if $RQ = I$, i.e., $R = Q^{-1}$. Therefore, in this case, the projection $\pi_0(F) = Q^{-1}U \in \text{SO}(3)U$ is unique, and is given by (A.2).

Assume now $\det F < 0$. Then, $-Q \in \text{SO}(3)$ and hence $-RQ \in \text{SO}(3)$ if $R \in \text{SO}(3)$. Let $w \in \mathbb{R}^3$ with $|w| = 1$ and $\theta \in [0, \pi]$ be the axis and angle of the proper rotation $-RQ$, respectively. Denote $w_3 = w$ and choose unit vectors $w_1, w_2 \in \mathbb{R}^3$ so that w_1, w_2, w_3 form a right-handed orthonormal basis of \mathbb{R}^3 . We have by a direct calculation that

$$\begin{aligned} -RQw_1 \cdot w_1 &= -RQw_2 \cdot w_2 = \cos \theta, \\ -RQw_1 \cdot w_2 &= -(-RQw_2 \cdot w_1) = -\sin \theta, \\ -RQw_i \cdot w_3 &= -RQw_3 \cdot w_i = 0, \quad i = 1, 2, \\ -RQw_3 \cdot w_3 &= 1. \end{aligned}$$

Consequently,

$$\begin{aligned} \sum_{i=1}^3 \lambda_i RQv_i \cdot v_i &= -\sum_{i=1}^3 \lambda_i (-RQ) \left[\sum_{j=1}^3 (v_i \cdot w_j) w_j \right] \cdot \left[\sum_{k=1}^3 (v_i \cdot w_k) w_k \right] \\ &= -\sum_{i=1}^3 \lambda_i \{ [(v_i \cdot w_1)^2 + (v_i \cdot w_2)^2] \cos \theta + (v_i \cdot w_3)^2 \} \\ &\leq \sum_{i=1}^3 \lambda_i [(v_i \cdot w_1)^2 + (v_i \cdot w_2)^2 - (v_i \cdot w_3)^2] \\ &= \sum_{i=1}^3 \lambda_i [1 - 2(v_i \cdot w_3)^2] \\ &= \text{tr}(V) - 2 \sum_{i=1}^3 \lambda_i (v_i \cdot w)^2, \end{aligned} \tag{A.5}$$

where we use the fact that $a = \sum_{i=1}^3 (a \cdot w_i) w_i$ and $\sum_{i=1}^3 (a \cdot w_i)^2 = |a|^2 = 1$ for any unit vector $a \in \mathbb{R}^3$. The inequality in (A.5) becomes equality if and only if $\cos \theta = -1$, i.e., $\theta = \pi$. In this case, $-RQ$ is a 180° rotation about the axis $w = w_3$.

Now, the trace in (A.4) is maximized in this case if and only if the last sum in (A.5), $\sum_{i=1}^3 \lambda_i (v_i \cdot w)^2$, is minimized. Since $0 < \lambda_1 \leq \lambda_2 \leq \lambda_3$, we have that

$$\sum_{i=1}^3 \lambda_i (v_i \cdot w)^2 \geq \lambda_1 \sum_{i=1}^3 (v_i \cdot w)^2 = \lambda_1,$$

with the equality holding true if and only if

$$(\lambda_2 - \lambda_1)(v_2 \cdot w)^2 = (\lambda_3 - \lambda_1)(v_3 \cdot w)^2 = 0.$$

Therefore, if λ_1 is not a repeated eigenvalue, the axis of the 180° rotation $-RQ$ with $R \in \text{SO}(3)$ maximizing the trace in (A.4) is $w = \pm v_1$, and $-RQ$ is the unique 180° rotation about v_1 , i.e., $-RQ = -I + 2w \otimes w = -I + 2v_1 \otimes v_1$. Consequently, the unique projection is $\pi_0(F) = -(-I + 2v_1 \otimes v_1)Q^{-1} \in \text{SO}(3)U$ in this case, and is given by (A.3).

If, however, λ_1 is a repeated eigenvalue, then there are infinitely many rotations $-RQ$ with $R \in \text{SO}(3)$ that can maximize the trace in (A.4). The axis of such a rotation can be any unit vector $w \in \mathbb{R}^3$ such that $w \cdot v_3 = 0$ if $0 < \lambda_1 = \lambda_2 < \lambda_3$, or any unit vector in \mathbb{R}^3 if $0 < \lambda_1 = \lambda_2 = \lambda_3$. In both cases, there are infinitely many projections $\pi_0(F) \in \text{SO}(3)U$ satisfying (A.1). ■

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