APPROXIMATION OF A MARTENSITIC LAMINATE WITH VARYING VOLUME FRACTIONS

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APPROXIMATION OF A MARTENSITIC LAMINATE WITH VARYING VOLUME FRACTIONS

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ABSTRACT. We consider multi-well energy minimization problems modeling martensitic crystals that can undergo either an orthorhombic to monoclinic or a cubic to tetragonal transformation. We give results for the approximation of a laminate with varying volume fractions. We construct energy minimizing sequences of deformations which satisfy the corresponding boundary condition, and we establish a series of error bounds in terms of the elastic energy for the approximation of the limiting macroscopic deformation and the simply laminated microstructure. Finally, we give results for the corresponding finite element approximation of the laminate with varying volume fractions.

1. Introduction

The recently developed geometrically nonlinear theory of martensite predicts the martensitic microstructure to be the limiting configuration of energy minimizing sequences of deformations for a nonconvex energy [2, 3, 10, 14, 15, 18, 19, 21, 24]. In this theory, the energy density is minimized on multiple energy wells $\text{SO}(3)U_1 \cup \cdots \cup \text{SO}(3)U_N$ where $U_1, \cdots, U_N$ for $N > 1$ are symmetry-related strains and $\text{SO}(3)$ is the set of all $3 \times 3$ real orthogonal matrices with determinant equal to one. Although the effect of surface energy makes a homogeneous deformation most stable, for certain boundary constraints or loading conditions the elastic energy of a martensitic crystal can be lowered as much as possible only by the fine-scale mixing of deformation gradients from distinct energy wells. A common example of such a microstructure is a simple laminate in which the deformation gradient oscillates in parallel layers of fine-scale between two compatible, stress-free, homogeneous states [4, 5]. More complex microstructures have been described using the notion of Young measure which gives the volume fraction for the mixing of the deformation gradients of the energy minimizing sequences of deformations [2, 3, 20, 32, 33].

We focus on martensitic crystals that can undergo either an orthorhombic to monoclinic or a cubic to tetragonal transformation [3, 24]. A martensitic crystal which can undergo an orthorhombic to monoclinic transformation has two symmetry-related martensitic variants ($N = 2$), and hence the elastic energy density has two wells. The more commonly observed cubic to tetragonal transformation has three symmetry-related martensitic variants ($N = 3$), so the elastic energy density has three wells. For both transformations, Ball and

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James have shown for boundary data which are consistent with a first-order laminate with constant volume fractions that the unique energy minimizing microstructure is the first-order laminate [3].

In this paper, we present an approximation theory for first-order laminates with varying volume fractions. We establish a series of error bounds in terms of the elastic energy of deformations for the $L^2$ approximation of the directional derivative of the limiting macroscopic deformation in any direction tangential to the parallel layers of the laminate, for the $L^2$ approximation of the limiting macroscopic deformation, for the approximation of volume fractions of the participating martensitic variants, and for the approximation of nonlinear integrals of deformation gradients.

We also give corresponding error estimates for conforming finite element approximations of the laminate with varying volume fractions. For simplicity of exposition, we restrict our analysis to continuous, piecewise linear, tetrahedral finite elements; but our analysis can be directly extended to higher order finite elements. We construct quasi-optimal finite element deformations, and we give corresponding error estimates for quasi-optimal finite element deformations.

The main framework of our analysis was given by the approximation theory developed for simple laminates with constant volume fractions for a two-well problem which applies to the orthorhombic to monoclinic transformation [25]. This analysis was extended to the cubic to tetragonal transformation in [23]. For constant volume fractions, an analysis for a nonconforming finite element approximation was given in [22].

A theory of numerical analysis for the microstructure in non-convex variational problems was developed in [12, 13], and extended in [7, 8, 9, 17, 26]. Analyses of the approximation of relaxed variational problems have been given in [6, 16, 27, 28, 29, 31]. We refer to the recent article [24] for a survey of models, computation, and numerical analysis for martensitic microstructure.

In §2, we describe the multi-well energy minimization problems. In §3, we construct energy minimizing sequences of deformations which satisfy the corresponding nonhomogeneous boundary condition. In §4 and §5, we establish a series of error bounds in terms of the elastic energy of deformations for the approximation of the limiting macroscopic deformation and the approximation of the microstructure. Finally, in §6, we give error estimates for the approximation by quasi-optimal finite element deformations.

### 2. Energy Minimization Problems

We first briefly review some basic definitions and properties of orthorhombic to monoclinic and cubic to tetragonal martensitic transformations. For more details, we refer to [2, 3, 24].

An orthorhombic to monoclinic transformation for a martensitic crystal is determined by its martensitic variants

\[ U_1 = (I + \eta e_1 \otimes e_2)D, \quad U_2 = (I - \eta e_1 \otimes e_2)D, \]

where $I$ is the identity transformation from $\mathbb{R}^3$ to $\mathbb{R}^3$, $\eta > 0$ is a material parameter, \{e_1, e_2, e_3\} is an orthonormal basis for $\mathbb{R}^3$, and $D$ is a symmetric, positive definite, linear transformation from $\mathbb{R}^3$ to $\mathbb{R}^3$, given by

\[ D = d_1 e_1 \otimes e_1 + d_2 e_2 \otimes e_2 + d_3 e_3 \otimes e_3 \]
for some \( d_1, d_2, d_3 > 0 \). A cubic to tetragonal transformation for a martensitic crystal is determined by its martensitic variants
\[
U_1 = \eta_1 I + (\eta_2 - \eta_1) e_1 \otimes e_1, \quad U_2 = \eta_1 I + (\eta_2 - \eta_1) e_2 \otimes e_2, \\
U_3 = \eta_1 I + (\eta_2 - \eta_1) e_3 \otimes e_3,
\]
where \( \eta_1 > 0 \) and \( \eta_2 > 0 \) are material parameters such that \( \eta_1 \neq \eta_2 \), and \( \{e_1, e_2, e_3\} \) is again an orthonormal basis for \( \mathbb{R}^3 \).

For convenience, we define the set of indices \( K = \{1, 2\} \) for the orthorhombic to monoclinic transformation and \( K = \{1, 2, 3\} \) for the cubic to tetragonal transformation. We also denote
\[
\mathcal{U}_i = \text{SO}(3)U_i, \quad i \in K, \quad \text{and} \quad \mathcal{U} = \cup \{\mathcal{U}_i : i \in K\}.
\]
It is easy to see that
\[
\det F = d_1 d_2 d_3 > 0, \quad \forall F \in \mathcal{U}, \tag{2.1}
\]
for the orthorhombic to monoclinic transformation, and that
\[
\det F = \eta_1^2 \eta_2 > 0, \quad \forall F \in \mathcal{U}, \tag{2.2}
\]
for the cubic to tetragonal transformation.

We now denote by \( \mathbb{R}^{3 \times 3} \) the set of all \( 3 \times 3 \) real matrices. We call two matrices rank-one connected if their difference is a rank-one matrix. The classical Hadamard compatibility condition states that, given a plane with unit normal \( n \) and two distinct constant matrices \( F_0, F_1 \in \mathbb{R}^{3 \times 3} \), there exists a continuous deformation \( y : \mathbb{R}^3 \to \mathbb{R}^3 \) such that \( \nabla y \) takes the value \( F_0 \) on one side of the plane and \( F_1 \) on the other side if and only if \( F_0 \) and \( F_1 \) are rank-one connected as
\[
F_1 - F_0 = a \otimes n \tag{2.3}
\]
for some non-zero vector \( a \in \mathbb{R}^3 \). The following lemma which is proved in [2, 3, 24] classifies all possible simple laminates formed by pairs of variants up to multiplication of rotations for the martensitic crystals in discussion and serves as a key crystallographical basis for our analysis.

**Lemma 2.1.** (1) For each \( i \in K \), there is no rank-one connection between \( \mathcal{U}_i \) and itself, that is, any two matrices \( R_1 U_i \) and \( R_2 U_i \) with \( R_1, R_2 \in \text{SO}(3) \) and \( R_1 \neq R_2 \) are not rank-one connected.

(2) For any \( i, j \in K, i \neq j \), there are exactly two rank-one connections between \( \mathcal{U}_i \) and \( \mathcal{U}_j \), that is, there are exactly two different \( Q \in \text{SO}(3) \) such that
\[
QU_i - U_j = a \otimes n
\]
for some \( a, n \in \mathbb{R}^3, |n| = 1 \), respectively. In this case, we also have for any \( \lambda \in (0, 1) \) that
\[
\lambda QU_i + (1 - \lambda) U_j \notin \mathcal{U}.
\]
Moreover, we have that
\[
n \in \{ \pm e_1, \pm e_2 \}
\]
for the orthorhombic to monoclinic transformation, and that
\[
n \in \left\{ \pm \frac{1}{\sqrt{2}} (e_i + e_j), \pm \frac{1}{\sqrt{2}} (e_i - e_j) \right\}
\]
for the cubic to tetragonal transformation.

By Lemma 2.1, we shall assume without loss of generality that $F_1 \in \mathcal{U}_1$ and $F_0 \in \mathcal{U}_2$, and we shall also assume that

$$n = e_1$$

for the orthorhombic to monoclinic transformation and that

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

for the cubic to tetragonal transformation.

For a given martensitic crystal, we denote by $\Omega$ the reference configuration which is taken to be the homogeneous austenitic state at the transformation temperature. We assume that $\Omega \subset \mathbb{R}^3$ is a connected, bounded domain with a Lipschitz continuous boundary. We also denote the elastic energy density of the crystal at a fixed temperature below the transformation temperature by the continuous function $\phi : \mathbb{R}^{3 \times 3} \to \mathbb{R}$. The elastic energy of a deformation $y : \Omega \to \mathbb{R}^3$ is given by

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

(2.4)

where $\nabla y : \Omega \to \mathbb{R}^{3 \times 3}$ is the deformation gradient. We define the set of deformations of finite energy by

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

To model the orthorhombic to monoclinic and the cubic to tetragonal martensitic transformations, we assume that the energy density $\phi$ is minimized on the energy wells $\mathcal{U}_i = \text{SO}(3)\mathcal{U}_i$, $i \in K$. Thus, we may assume after adding a constant to the energy density that

$$\phi(F) \geq 0, \quad \forall F \in \mathbb{R}^{3 \times 3},$$

$$\phi(F) = 0 \quad \text{if and only if} \quad F \in \mathcal{U} = \bigcup \{ \mathcal{U}_i : i \in K \}. \quad (2.5)$$

We shall also assume that the energy density $\phi$ grows quadratically away from the energy wells, that is,

$$\phi(F) \geq \kappa \|F - \pi(F)\|^2, \quad \forall F \in \mathbb{R}^{3 \times 3},$$  

(2.6)

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

$$\|F - \pi(F)\| = \min_{G \in \mathcal{U}} \|F - G\|, \quad \forall F \in \mathbb{R}^{3 \times 3},$$

and where

$$\|F\| = \left( \sum_{i,j=1}^{3} F_{ij}^2 \right)^{\frac{1}{2}}, \quad \forall F = (F_{ij}) \in \mathbb{R}^{3 \times 3}.$$

The projection $\pi(F)$ exists for any $F \in \mathbb{R}^{3 \times 3}$, since $\mathcal{U}$ is compact, although the projection may not be unique. It is unique, however, if $\|F - \pi(F)\|$ is small enough [24].
We shall assume that $F_0, F_1 \in \mathcal{U}$ are rank-one connected as in (2.3), so
\[ (1 - \lambda)F_0 + \lambda F_1 = F_0 + \lambda a \otimes n, \quad \lambda \in \mathbb{R}. \] \hspace{1cm} (2.7)

The following lemma shows that any deformation with a gradient that is a mixture of the two matrices $F_0$ and $F_1$ must be a simple laminate.

**Lemma 2.2.** Let $y \in W^{1, \infty}(\Omega; \mathbb{R}^3)$ satisfy
\[ \nabla y(x) = (1 - \lambda(x))F_0 + \lambda(x)F_1, \quad \text{a.e. } x \in \Omega, \]
for the volume fraction $\lambda \in L^\infty(\Omega)$ satisfying $0 \leq \lambda(s) \leq 1$. We then have that there exist unique $l(x) \in W^{1, \infty}(\Omega)$ and $\tilde{y} \in \mathbb{R}^3$, $\tilde{y} \cdot a = 0$, such that
\[ y(x) = F_0 x + l(x)a + \tilde{y}, \quad x \in \Omega, \]
\[ \nabla l(x) = \lambda(x)n, \quad \text{a.e. } x \in \Omega. \]

If $\hat{\Omega} \subset \Omega$ is a Lipschitz subdomain with the property that \( \{ x \in \hat{\Omega} : x \cdot n = \xi \} \) is connected for each $\xi \in \mathbb{R}$, then there exist $\bar{l}(s) \in W^{1, \infty}(\mathbb{R})$ and $\bar{\lambda}(s) \in L^\infty(\mathbb{R})$ such that
\[ l(x) = \bar{l}(x \cdot n), \quad x \in \hat{\Omega}, \]
\[ \lambda(x) = \bar{\lambda}(x \cdot n), \quad \text{a.e. } x \in \hat{\Omega}, \]
\[ \bar{l}'(s) = \bar{\lambda}'(s), \quad \text{a.e. } s \in \mathbb{R}. \]

**Proof.** The proof is identical to the proof of Proposition 1 in [2] for the case when $\lambda$ is a characteristic function. It follows by noting that if $w \in \mathbb{R}^3$, $w \cdot a = 0$, then
\[ \nabla [(y(x) - F_0 x) \cdot w] = 0, \quad \text{a.e. } x \in \Omega. \]

\[ \square \]

In this paper, we consider the minimization of the elastic energy (2.4) with respect to deformations which are constrained on the boundary to take the value
\[ y_\lambda(x) = F_0 x + l(x)a, \quad x \in \Omega, \]
\[ \nabla l(x) = \lambda(x)n, \quad \text{a.e. } x \in \Omega, \] \hspace{1cm} (2.8)

where $l(x) \in W^{1, \infty}(\Omega)$ and $\lambda(x) \in L^\infty(\Omega)$ satisfies $0 \leq \lambda(x) \leq 1$. Our energy minimization problem is to minimize the energy (2.4) in the set of admissible deformations defined by
\[ W_\lambda^\phi = \left\{ y \in W^\phi : y = y_\lambda \text{ on } \partial \Omega \right\}. \]

3. CONSTRUCTION OF ENERGY MINIMIZING SEQUENCES

We first consider the special case of (2.8) where $\lambda(x) = \tilde{\lambda}(x \cdot n)$ for $\tilde{\lambda}(s) \in L^\infty(\mathbb{R})$, so
\[ y_\lambda(x) = F_0 x + \left[ \int_0^{x \cdot n} \tilde{\lambda}(s)ds + \zeta \right] a, \quad x \in \Omega, \] \hspace{1cm} (3.1)

for some $\zeta \in \mathbb{R}^3$.

We construct in two steps a family of deformations $\hat{u}_\gamma \in W^\phi_\lambda$, $\gamma \in (0, \gamma_0]$, for any fixed $\gamma_0 > 0$, satisfying
\[ \lim_{\gamma \to 0} \mathcal{E}(\hat{u}_\gamma) = 0. \]
First, we construct \( u_\gamma \in W^{1,\infty}(\mathbb{R}^3; \mathbb{R}^3), \gamma \in (0, \gamma_0] \), which are simple laminates of scale \( \gamma \) such that \( \nabla u_\gamma(x) = F_0 \) or \( F_1 \) for almost all \( x \in \mathbb{R}^3 \). Second, we construct \( \hat{u}_\gamma \in W^{1,\infty}_\lambda, \gamma \in (0, \gamma_0] \), by modifying \( u_\gamma \) by interpolation on the boundary.

**Step 1. Construction of** \( u_\gamma \in W^{1,\infty}(\mathbb{R}^3; \mathbb{R}^3), \gamma \in (0, \gamma_0] \). Set

\[
I^{(i)}_\gamma = ((i - 1)\gamma, i\gamma) \quad \text{and} \quad \lambda^{(i)}_\gamma = \frac{1}{\gamma} \int_{I^{(i)}_\gamma} \hat{\lambda}(s) \, ds, \quad \forall i \in \mathbb{Z}.
\]

Define the piecewise constant function \( \hat{\lambda}_\gamma : \mathbb{R} \to \mathbb{R} \) by

\[
\hat{\lambda}_\gamma(s) = \lambda^{(i)}_\gamma \quad \text{if} \ s \in I^{(i)}_\gamma, \quad \forall i \in \mathbb{Z},
\]

and define the characteristic function \( \chi_\gamma : \mathbb{R} \to \mathbb{R} \) by

\[
\chi_\gamma(s) = \begin{cases} 
1 & \text{if } (i - 1)\gamma < s \leq (i - 1 + \lambda^{(i)}_\gamma)\gamma \quad \text{for some } i \in \mathbb{Z}, \\
0 & \text{if } (i - 1 + \lambda^{(i)}_\gamma)\gamma < s \leq i\gamma \quad \text{for some } i \in \mathbb{Z}.
\end{cases}
\]

Since \( 0 \leq \hat{\lambda}(s), \hat{\lambda}_\gamma(s), \chi_\gamma(s) \leq 1 \) for almost all \( s \in \mathbb{R} \), we have for any bounded interval \( I \subset \mathbb{R}^1 \) that

\[
\left| \int_I \left[ \chi_\gamma(s) - \hat{\lambda}(s) \right] \, ds \right| \leq 2\gamma. \quad (3.2)
\]

Define now

\[
u_\gamma(x) = F_0 \mathbf{v} + \left[ \int_0^{||\mathbf{v}||} \chi_\gamma(s) \, ds + \zeta \right] \mathbf{a}, \quad x \in \mathbb{R}^3.
\]

Obviously, \( u_\gamma \in W^{1,\infty}(\mathbb{R}^3; \mathbb{R}^3) \). Moreover, we have by (2.3) that

\[
\nabla u_\gamma(x) = F_0 + \chi_\gamma(x \cdot \mathbf{n})\mathbf{a} \otimes \mathbf{n} \in \{ F_0, F_1 \}, \quad \text{a.e. } x \in \mathbb{R}^3. \quad (3.3)
\]

In view of (3.1) and (3.2), we also have

\[
|u_\gamma(x) - y_{\lambda}(x)| \leq 2|\alpha|\gamma, \quad x \in \mathbb{R}^3. \quad (3.4)
\]

**Step 2. Construction of** \( \hat{u}_\gamma \in W^{1,\infty}_\lambda, \gamma \in (0, \gamma_0] \). Set

\[
\Omega_\gamma = \{ x \in \Omega : \text{dist}(x, \partial \Omega) > v\gamma \}
\]

for some constant \( v > 0 \) which will be specified later. Define \( \psi_\gamma : \Omega \to \mathbb{R} \) by

\[
\psi_\gamma(x) = \begin{cases} 
1 & \text{if } x \in \Omega_\gamma, \\
(v\gamma)^{-1} \text{dist}(x, \partial \Omega) & \text{if } x \in \Omega - \Omega_\gamma.
\end{cases}
\]

It is easy to see that \( \psi_\gamma \in W^{1,\infty}(\Omega) \) and

\[
0 \leq \psi_\gamma(x) \leq 1, \quad x \in \Omega, \\
\psi_\gamma(x) = 1, \quad x \in \Omega_\gamma, \\
\psi_\gamma(x) = 0, \quad x \in \partial \Omega, \\
|\nabla \psi_\gamma(x)| \leq (v\gamma)^{-1}, \quad \text{a.e. } x \in \Omega. \quad (3.5)
\]

Now we define \( \hat{u}_\gamma : \Omega \to \mathbb{R}^3 \) for \( \gamma \in (0, \gamma_0] \) by

\[
\hat{u}_\gamma(x) = \psi_\gamma(x)u_\gamma(x) + (1 - \psi_\gamma(x))y_{\lambda}(x), \quad x \in \Omega.
\]
It is easy to verify that
\[ \nabla \hat{u}_\gamma(x) = [u_\gamma(x) - y_\lambda(x)] \otimes \nabla \psi_\gamma(x) + \psi_\gamma(x) \nabla u_\gamma(x) + (1 - \psi_\gamma(x)) \nabla y_\lambda(x) \] (3.6)
for almost all \( x \in \Omega \). By (3.3) – (3.6), we have for all \( \gamma \in (0, \gamma_0] \) that
\[ \| \nabla \hat{u}_\gamma(x) \| \leq C \quad \text{a.e. } x \in \Omega, \] (3.7)
where \( C \) here and below is a constant independent of \( \gamma \), and that
\[ \nabla \hat{u}_\gamma(x) \in \{ F_0, F_1 \}, \quad \text{a.e. } x \in \Omega_\gamma. \] (3.8)
Therefore \( \hat{u}_\gamma \in W^\phi_\lambda \) for any \( \gamma \in (0, \gamma_0] \) by the continuity of the energy density \( \phi \). Moreover, since \( \text{meas}(\Omega - \Omega_\gamma) = O(\gamma) \), as \( \gamma \to 0 \), we have by (3.7), (3.8), and (2.5) that
\[ \mathcal{E}(\hat{u}_\gamma) = O(\gamma), \quad \text{as } \gamma \to 0. \]
By the rank-one connection (2.3), we have that
\[ \det F_1 = \det(F_0 + a \otimes n) = (\det F_0)(1 + F_0^{-1}a \cdot n). \]
This together with the fact that \( \det F_0 = \det F_1 > 0 \) (see (2.1) and (2.2)) implies that
\[ F_0^{-1}a \cdot n = 0. \]
Consequently, for any \( \xi \in \mathbb{R} \), we have
\[ \det(F_0 + \xi a \otimes n) = (\det F_0)(1 + \xi F_0^{-1}a \cdot n) = \det F_0. \]
It now follows from the equations (2.7) and (3.3) that
\[ \psi_\gamma(x) \nabla u_\gamma(x) + (1 - \psi_\gamma(x)) \nabla y_\lambda(x) = F_0 + \xi(x) a \otimes n, \quad \text{a.e. } x \in \Omega, \]
where \( \xi(x) = \psi_\gamma(x) \chi_\gamma(x \cdot n) + (1 - \psi_\gamma(x)) \lambda(x), \quad \text{a.e. } x \in \Omega. \)
Thus,
\[ \det [\psi_\gamma(x) \nabla u_\gamma(x) + (1 - \psi_\gamma(x)) \nabla y_\lambda(x)] = \det F_0 = \det F_1 > 0, \quad \text{a.e. } x \in \Omega. \]
Choosing \( \nu > 0 \) large enough, we can therefore conclude from (3.4) – (3.6) that
\[ \det \nabla \hat{u}_\gamma(x) \geq C > 0, \quad \text{a.e. } x \in \Omega, \quad \forall \gamma \in (0, \gamma_0]. \] (3.9)
We summarize our results in the following theorem.

**Theorem 3.1.** If \( y_\lambda(x) \) has the form (3.1), then there exist a family of deformations \( \hat{u}_\gamma \in W^\phi_\lambda, \gamma \in (0, \gamma_0] \), for any fixed \( \gamma_0 > 0 \), such that (3.9) holds and such that
\[ \lim_{\gamma \to 0} \mathcal{E}(\hat{u}_\gamma) = 0. \]

Theorem 3.1 can be directly extended to more general deformations \( y_\lambda(x) \) such as described in the following lemma.

**Lemma 3.1.** Suppose that \( \Omega_i \subset \Omega \) for \( i = 1, \ldots, M \) are disjoint Lipschitz subdomains such that
\[ \bar{\Omega} = \bigcup_{i=1}^M \bar{\Omega}_i, \]
and we suppose that there exist \( \tilde{\lambda}_i(s) \in L^\infty(\mathbb{R}) \) for \( i = 1, \ldots, M \) such that
\[
\lambda(x) = \tilde{\lambda}_i(x \cdot n), \quad x \in \Omega_i.
\]
It then follows that there exist a family of deformations \( \hat{u}_\gamma \in W^\phi_\lambda \), \( \gamma \in (0, \gamma_0] \), for any fixed \( \gamma_0 > 0 \), such that (3.9) holds and such that
\[
\lim_{\gamma \to 0} E(\hat{u}_\gamma) = 0.
\]

**Proof.** We construct deformations \( \hat{u}_{i\gamma} \) defined on \( \tilde{\Omega}_i \) for \( i = 1, \ldots, M \) such that
\[
\hat{u}_{i\gamma}(x) = y_\lambda(x), \quad x \in \partial\Omega_i,
\]
by the technique of Theorem 3.1 applied to \( \Omega_i \), and we then construct \( \hat{u}_\gamma \in W^\phi_\lambda \) by
\[
\hat{u}_\gamma(x) = \hat{u}_{i\gamma}(x), \quad x \in \Omega_i, \quad i = 1, \ldots, M.
\]
\[\square\]

4. APPROXIMATION OF THE LIMITING MACROSCOPIC DEFORMATION

In this section and in the next section, we assume only that \( y_\lambda(x) \) is of the general form (2.8). Our first lemma below is a direct consequence of the growth rate of the energy density around the energy wells (2.6).

**Lemma 4.1.** We have
\[
\int_\Omega \| \nabla y(x) - \pi(\nabla y(x)) \|^2 \, dx \leq \kappa^{-1} E(y), \quad \forall y \in W^\phi.
\]

Notice that by the above lemma we have that \( W^\phi \subset W^{1,2}(\Omega, \mathbb{R}^3) \). In what follows we shall denote by \( C \) a generic positive constant which will be independent of all \( y \in W^\phi_\lambda \).

**Lemma 4.2.** There exists a constant \( C > 0 \) such that
\[
\int_\Omega \| \pi(\nabla y(x)) - \nabla y_\lambda(x) \| w \|^2 \, dx \leq C E(y)^{1/2}, \quad \forall y \in W^\phi_\lambda,
\]
for all \( w \in \mathbb{R}^3 \) satisfying \( w \cdot n = 0 \) and \( |w| = 1 \).

**Proof.** We first consider the orthorhombic to monoclinic transformation. In this case, we have
\[
\pi(F) \in \text{SO}(3)F_0 \cup \text{SO}(3)F_1, \quad \forall F \in \mathbb{R}^{3 \times 3}.
\]
Fix \( w \in \mathbb{R}^3 \) with \( w \cdot n = 0 \) and \( |w| = 1 \). By (2.3) and (2.7), we have that
\[
\nabla y_\lambda(x)w = F_0w = F_1w, \quad \text{a.e. } x \in \Omega,
\]
leading to
\[
|\pi(F)w| = |\nabla y_\lambda(x)w|, \quad \forall F \in \mathbb{R}^{3 \times 3}, \quad \text{a.e. } x \in \Omega.
\]
Fix \( y \in W^\phi_\lambda \). Since \( y(x) = y_\lambda(x) \) on \( \partial\Omega \), we have by the divergence theorem that
\[
\int_\Omega \nabla y(x) \, dx = \int_\Omega \nabla y_\lambda(x) \, dx.
\]
It follows from (4.1) – (4.3), the Cauchy-Schwarz inequality, and Lemma 4.1 that
\[
\int_{\Omega} \left| \nabla y(x) - \nabla y_\lambda(x) \right|^2 dx = 2 \int_{\Omega} \nabla y_\lambda(x) w \cdot \left[ \nabla y_\lambda(x) - \pi(\nabla y(x)) \right] w dx \\
= 2 F w \cdot \int_{\Omega} \left[ \nabla y(x) - \pi(\nabla y(x)) \right] w dx \\
\leq 2 |F| \left( \text{meas } \Omega \right)^{\frac{1}{2}} \left[ \int_{\Omega} \left\| \nabla y(x) - \pi(\nabla y(x)) \right\|^2 dx \right]^{\frac{1}{2}} \\
\leq C \mathcal{E}(y)^{\frac{1}{2}} \cdot (4.4)
\]

Now let us consider the cubic to tetragonal transformation. Recall that in this case the normal \( n \) is given as \( n = (e_1 + e_2)/\sqrt{2} \). Set
\[
w_1 = \frac{1}{\sqrt{3}} (e_1 - e_2 + e_3) \quad \text{and} \quad w_2 = \frac{1}{\sqrt{3}} (e_1 - e_2 - e_3).
\]
It is easy to check that
\[
w_1 \cdot n = w_2 \cdot n = 0, \quad |w_1| = |w_2| = 1,
\]
and
\[
|U_i w_j| = \sqrt{\frac{2 \eta_1^2 + \eta_2^2}{3}}, \quad i = 1, 2, 3, \ j = 1, 2.
\]
We can thus conclude by (4.1) that (4.2), hence (4.4), also holds true for \( w = w_1 \) and \( w = w_2 \), respectively. We have in fact proved the desired inequality in this case as well, since \( \{w_1, w_2\} \) is a basis for the two-dimensional subspace \( \{w \in \mathbb{R}^3 : w \cdot n = 0\} \).

The following theorem gives an error bound for the \( L^2 \) approximation of the directional derivative of the limiting macroscopic deformation \( y_\lambda \) in any direction tangential to parallel layers of the laminate. It is a direct consequence of the triangle inequality and the above two lemmas.

**Theorem 4.1.** There exists a constant \( C > 0 \) such that
\[
\int_{\Omega} \left| \nabla y(x) - \nabla y_\lambda(x) \right|^2 dx \leq C \left[ \mathcal{E}(y)^{\frac{1}{2}} + \mathcal{E}(y) \right], \quad \forall y \in W^\phi_\lambda,
\]
for all \( w \in \mathbb{R}^3 \) satisfying \( w \cdot n = 0 \) and \( |w| = 1 \).

We now give an error bound for the \( L^2 \) approximation of the limiting macroscopic deformation \( y_\lambda \) by the admissible deformations \( y \in W^\phi_\lambda \).

**Theorem 4.2.** There exists a constant \( C > 0 \) such that
\[
\int_{\Omega} \left| y(x) - y_\lambda(x) \right|^2 dx \leq C \left[ \mathcal{E}(y)^{\frac{1}{2}} + \mathcal{E}(y) \right], \quad \forall y \in W^\phi_\lambda.
\]

**Proof.** Let \( z \in C^1(\overline{\Omega}; \mathbb{R}^3) \) and \( w \in \mathbb{R}^3 \) with \( |w| = 1 \). We can verify the identity
\[
\int_{\Omega} |z(x)|^2 dx = \int_{\partial \Omega} |z(x)|^2 (w \cdot x) (w \cdot \nu) dS - \int_{\Omega} (\nabla |z(x)|^2 \cdot w) (w \cdot x) dx \\
= \int_{\partial \Omega} |z(x)|^2 (w \cdot x) (w \cdot \nu) dS - 2 \int_{\Omega} (\nabla z(x) w \cdot z(x)) (w \cdot x) dx
\]
to get the Poincaré inequality [25, 34]
\[
\int_{\Omega} |z(x)|^2 \, dx \leq C \left[ \int_{\partial \Omega} |z(x)|^2 \, dS + \int_{\Omega} |\nabla z(x)w|^2 \, dx \right],
\]
where \( C = C(\Omega) \) is a positive constant independent of \( z \). This inequality is also true for any \( z \in W^\phi \) by the density of \( C^1(\Omega; \mathbb{R}^3) \) in \( W^\phi \). Setting \( z = y - y_\lambda \) for any \( y \in W^\phi_\lambda \), we thus obtain the desired result by Theorem 4.1 with \( w \in \mathbb{R}^3 \) so chosen that \( w \cdot n = 0 \) and \( |w| = 1 \).

The next theorem states that the infimum of the energy is not generally attained on \( W^\phi_\lambda \).

**Corollary 4.1.** There does not exist \( y \in W^\phi_\lambda \) such that \( E(y) = 0 \) if
\[
\text{meas}\{ x \in \Omega : 0 < \lambda(x) < 1 \} > 0.
\]

**Proof.** We assume that there exist \( y \in W^\phi_\lambda \) such that \( E(y) = 0 \). By Theorem 4.2, we have that \( y = y_\lambda \). It follows from (4.6) that there is an integer \( p \geq 3 \) such that the set
\[
\omega_p = \left\{ x \in \Omega : \frac{1}{p} \leq \lambda(x) \leq 1 - \frac{1}{p} \right\}
\]
has positive measure. On the other hand, the set
\[
\Delta_p = \left\{ (1 - \lambda_0)F_0 + \lambda_0 F_1 \in \mathbb{R}^{3 \times 3} : \frac{1}{p} \leq \lambda_0 \leq 1 - \frac{1}{p} \right\}
\]
is compact in \( \mathbb{R}^{3 \times 3} \) and is disjoint with \( \mathcal{U} \) by Lemma 2.1. Consequently, the continuous energy density \( \phi \) reaches its minimum \( m(\Delta_p) > 0 \) on the set \( \Delta_p \). We obtain a contradiction since
\[
0 = E(y) = E(y_\lambda) - \int_{\omega_p} \phi(\nabla y_\lambda(x)) \, dx \geq m(\Delta_p) \, \text{meas} \omega_p > 0.
\]

Now we establish an error bound for the weak \( L^2 \) approximation of the limiting macroscopic deformation gradient \( \nabla y_\lambda \). It follows from such an error bound that for any energy minimizing sequence \( \{y_k\}_{k=1}^\infty \) the corresponding sequence of gradients \( \{\nabla y_k\}_{k=1}^\infty \) converges weakly to the deformation gradient \( \nabla y_\lambda \).

**Theorem 4.3.** For any Lipschitz domain \( \omega \subset \Omega \), there exists a constant \( C = C(\omega) > 0 \) such that
\[
\left\| \int_{\omega} [\nabla y(x) - \nabla y_\lambda(x)] \, dx \right\| \leq C \left[ E(y)^{\frac{1}{2}} + E(y_\lambda)^{\frac{1}{2}} \right], \quad \forall y \in W^\phi_\lambda.
\]

**Proof.** It follows from the divergence theorem and the Cauchy-Schwarz inequality that
\[
\left\| \int_{\omega} [\nabla y(x) - \nabla y_\lambda(x)] \, dx \right\| = \left\| \int_{\partial \omega} [y(x) - y_\lambda(x)] \otimes \nu \, dS \right\|
\leq \int_{\partial \omega} |y(x) - y_\lambda(x)| \, dS \leq (\text{meas}_2 \partial \omega)^{\frac{1}{2}} \left( \int_{\partial \omega} |y(x) - y_\lambda(x)|^2 \, dS \right)^{\frac{1}{2}},
\]
\[
(4.7)
\]
for any \( y \in W^\phi_\nu \) where \( \nu \) 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 [1] we have

\[
\int_{\partial \omega} |y(x) - y_\lambda(x)|^2 dS \leq C \left[ \int_\omega |y(x) - y_\lambda(x)|^2 dx + \int_\omega |\nabla y(x) - \nabla y_\lambda(x)|^2 dx \right]
\leq C \left[ \int_\omega |y(x) - y_\lambda(x)|^2 dx + \int_\omega |y(x) - y_\lambda(x)||\nabla y(x) - y_\lambda(x)|| dx \right]
\leq C \left[ \int_\Omega |y(x) - y_\lambda(x)|^2 dx + \left( \int_\Omega |y(x) - y_\lambda(x)|^2 dx \right)^{\frac{1}{2}} \left( \int_\Omega \|\nabla y(x) - \nabla y_\lambda(x)\|^2 dx \right)^{\frac{1}{2}} \right].
\]  

(4.8)

We also have by the triangle inequality and Lemma 4.1 that

\[
\left( \int_\Omega \|\nabla y(x) - \nabla y_\lambda(x)\|^2 dx \right)^{\frac{1}{2}}
\leq \left( \int_\Omega \|\nabla y(x) - \pi(\nabla y(x))\|^2 dx \right)^{\frac{1}{2}} + \left( \int_\Omega \|\pi(\nabla y(x)) - \nabla y_\lambda(x)\|^2 dx \right)^{\frac{1}{2}}
\leq C \left[ \mathcal{E}(y)^{\frac{1}{2}} + 1 \right].
\]

(4.9)

Hence, it follows by using Theorem 4.2 and (4.9) in (4.8) that

\[
\int_{\partial \omega} |y(x) - y_\lambda(x)|^2 dS \leq C \left[ \mathcal{E}(y)^{\frac{1}{2}} + \mathcal{E}(y) \right],
\]

which, together with (4.7), leads to the desired inequality.

\[ \square \]

5. APPROXIMATION OF THE SIMPLE LAMINATE

We define the projection operator \( \pi_{12} : \mathbb{R}^{3 \times 3} \rightarrow \mathcal{U}_1 \cup \mathcal{U}_2 \) by

\[
\|F - \pi_{12}(F)\| = \min_{G \in \mathcal{U}_1 \cup \mathcal{U}_2} \|F - G\|, \quad \forall F \in \mathbb{R}^{3 \times 3}.
\]

For the orthorhombic to monoclinic transformation, we have \( \pi_{12} = \pi \). We also define the operators \( \Theta : \mathbb{R}^{3 \times 3} \rightarrow \text{SO}(3) \) and \( \Pi : \mathbb{R}^{3 \times 3} \rightarrow \{F_0, F_1\} \) by the relation

\[
\pi_{12}(F) = \Theta(F)\Pi(F), \quad \forall F \in \mathbb{R}^{3 \times 3}.
\]

(5.1)

The following lemma reduces the three-well problem for the cubic to tetragonal transformation to a two-well problem. Its proof indicates that the measure of the set of points at which the deformation gradient for an energy minimizing sequence is near \( \mathcal{U}_3 \) converges to zero.

Lemma 5.1. For the cubic to tetragonal transformation, there exists a constant \( C > 0 \) such that

\[
\int_\Omega \|\nabla y(x) - \pi_{12}(\nabla y(x))\|^2 dx \leq C \left[ \mathcal{E}(y)^{\frac{1}{2}} + \mathcal{E}(y) \right], \quad \forall y \in W^\phi_{\lambda}.
\]

Proof. We have by a simple calculation that

\[
\inf_{F \in \mathcal{U}_3} |(F - \nabla y_\lambda(x)) e_3| \geq |\eta_2 - \eta_1|, \quad \text{a.e. } x \in \Omega.
\]
Denoting
\[ \Omega_3 = \{ x \in \Omega : \pi(\nabla y(x)) \in \mathcal{U}_3 \} \]
for a fixed \( y \in W^\phi_\lambda \), we thus have by Lemma 4.2 that
\[ \text{meas } \Omega_3 = \int_{\Omega_3} dx \leq |\eta_2 - \eta_1|^2 \int_{\Omega_3} ||\pi(\nabla y(x)) - \nabla y_\lambda(x)||^2 \, dx \leq C\mathcal{E}(y)^{1/2}, \]
(5.2)
since \( e_3 \cdot n = 0 \). Consequently, we have by Lemma 4.1 that
\[
\int_{\Omega} \| \nabla y(x) - \pi_{12}(\nabla y(x)) \|^2 \, dx \\
\leq 2 \int_{\Omega} \| \nabla y(x) - \pi(\nabla y(x)) \|^2 \, dx + 2 \int_{\Omega} \| \pi(\nabla y(x)) - \pi_{12}(\nabla y(x)) \|^2 \, dx \\
\leq 2 \int_{\Omega} \| \nabla y(x) - \pi(\nabla y(x)) \|^2 \, dx + 8(2\eta_1^2 + \eta_3^2) \text{meas } \Omega_3 \\
\leq C \left[ \mathcal{E}(y)^{1/2} + \mathcal{E}(y) \right],
\]
completing the proof. \( \square \)

We now give an error bound for the projection operator \( \Pi : \mathbb{R}^{3 \times 3} \rightarrow \{ F_0, F_1 \} \).

**Theorem 5.1.** There exists a constant \( C > 0 \) such that
\[ \int_{\Omega} \| \nabla y(x) - \Pi(\nabla y(x)) \|^2 \, dx \leq C \left[ \mathcal{E}(y)^{1/2} + \mathcal{E}(y) \right], \quad \forall y \in W^\phi_\lambda. \]

**Proof.** For any \( w \in \mathbb{R}^3 \) such that \( w \cdot n = 0 \), we have
\[ \Pi(F)w = F_0w = F_1w = \nabla y_\lambda(x)w, \quad \forall F \in \mathbb{R}^{3 \times 3}, \text{ a.e. } x \in \Omega. \]
Thus, it follows from (5.1) that
\[ [\Theta(F) - I] F_0w = [\Theta(F) - I] \Pi(F)w = [\pi_{12}(F) - \nabla y_\lambda(x)]w = [\pi_{12}(F) - \pi(F)]w + [\pi(F) - \nabla y_\lambda(x)]w, \quad \forall F \in \mathbb{R}^{3 \times 3}, \text{ a.e. } x \in \Omega. \]
We can then apply the triangle inequality to the above identity with \( F = \nabla y(x) \) for any \( y \in W^\phi_\lambda \) and \( x \in \Omega \), and estimate the two terms by (5.2) and Lemma 4.2 to obtain
\[
\int_{\Omega} ||[\Theta(\nabla y(x)) - I] F_0w||^2 \, dx \\
\leq 2 \int_{\Omega} ||[\pi_{12}(\nabla y(x)) - \pi(\nabla y(x))]w||^2 \, dx + 2 \int_{\Omega} ||[\pi(\nabla y(x)) - \nabla y_\lambda(x)]w||^2 \, dx \\
\leq C\mathcal{E}(y)^{1/2}. \quad (5.3)
\]
Choose \( w_1 \in \mathbb{R}^3 \) and \( w_2 \in \mathbb{R}^3 \) so that \( w_1 \cdot n = w_2 \cdot n = 0 \) and that \( w_1, w_2 \) are linearly independent. Set \( m = F_0w_1 \times F_0w_2 \). Since
\[ Qm = QF_0w_1 \times QF_0w_2, \quad \forall Q \in SO(3), \]
we have for all \( F \in \mathbb{R}^{3 \times 3} \) that
\[ [\Theta(F) - I] m = [\Theta(F) F_0w_1 \times \Theta(F) F_0w_2] - \{ F_0w_1 \times F_0w_2 \} \\
= \{ [\Theta(F) - I] F_0w_1 \times \Theta(F) F_0w_2 \} - \{ F_0w_1 \times [I - \Theta(F)] F_0w_2 \}. \]
This, together with (5.3), leads to

\[ \int_{\Omega} |(\Theta(\nabla y(x)) - I) m|^2 \, dx \leq C\varepsilon(y)^{1/2}. \]  
(5.4)

Now \(\{F_0w_1, F_0w_2, m\}\) is a basis for \(\mathbb{R}^3\), so we have from (5.3) and (5.4) that

\[ \int_{\Omega} \| (\Theta(\nabla y(x)) - I) \|^2 \, dx \leq C\varepsilon(y)^{1/2}. \]  
(5.5)

We complete the proof by applying the triangle inequality to the identity

\[ F - \Pi(F) = [F - \pi_{12}(F)] + [\pi_{12}(F) - \Pi(F)] \]
\[ = [F - \pi_{12}(F)] + [\Theta(F) - I] \Pi(F), \quad \forall F \in \mathbb{R}^{3 \times 3}, \]

with \(F = \nabla y(x)\) for \(x \in \Omega\), and by estimating the two terms by Lemma 5.1 and (5.5).

For any subset \(\omega \subset \Omega\), \(\rho > 0\), and \(y \in W^\Phi_\lambda\), we define the sets

\[ \omega^0_\rho(y) = \{ x \in \omega : \Pi(\nabla y(x)) = F_0 \text{ and } \|F_0 - \nabla y(x)\| < \rho \}, \]
\[ \omega^1_\rho(y) = \{ x \in \omega : \Pi(\nabla y(x)) = F_1 \text{ and } \|F_1 - \nabla y(x)\| < \rho \} \]

and the mean value of \(\lambda\) on \(\omega\) by

\[ \hat{\lambda}_\omega = \frac{1}{\text{meas } \omega} \int_{\omega} \lambda(x) \, dx. \]

The following theorem gives an estimate for the approximation of volume fractions. It states that for any energy minimizing sequence \(\{y_k\} \in W^\Phi_\lambda\), the volume fraction that \(\nabla y_k(x)\) is near \(F_0\) converges to \(1 - \lambda(x)\) and the volume fraction that \(\nabla y_k(x)\) is near \(F_1\) converges to \(\lambda(x)\).

**Theorem 5.2.** For any Lipschitz domain \(\omega \subset \Omega\) and any \(\rho > 0\) there exists a positive constant \(C\) such that

\[ \text{meas} (\omega - \{\omega^0_\rho(y) \cup \omega^1_\rho(y)\}) \leq C \left[ \varepsilon(y)^{1/2} + \varepsilon(y) \right], \quad \forall y \in W^\Phi_\lambda, \]  
(5.6)

and

\[ \left| \frac{\text{meas } \omega^0_\rho(y)}{\text{meas } \omega} - (1 - \hat{\lambda}_\omega) \right| + \left| \frac{\text{meas } \omega^1_\rho(y)}{\text{meas } \omega} - \hat{\lambda}_\omega \right| \leq C \left[ \varepsilon(y)^{1/2} + \varepsilon(y) \right], \quad \forall y \in W^\Phi_\lambda. \]  
(5.7)

**Proof.** Fix \(y \in W^\Phi_\lambda\). We have by the definition of \(\omega^0_\rho \equiv \omega^0_\rho(y)\) and \(\omega^1_\rho \equiv \omega^1_\rho(y)\) that

\[ \text{meas} \left( \omega - \{\omega^0_\rho \cup \omega^1_\rho\} \right) \leq \frac{1}{\rho} \int_{\omega - \{\omega^0_\rho \cup \omega^1_\rho\}} \| \Pi(\nabla y(x)) - \nabla y(x) \| \, dx \]
\[ \leq \frac{\left[ \text{meas} \left( \omega - \{\omega^0_\rho \cup \omega^1_\rho\} \right) \right]^{1/2}}{\rho} \left[ \int_{\Omega} \| \Pi(\nabla y(x)) - \nabla y(x) \|^2 \, dx \right]^{1/2}. \]

Consequently, we have

\[ \text{meas} \left( \omega - \{\omega^0_\rho \cup \omega^1_\rho\} \right) \leq \frac{1}{\rho^2} \left[ \int_{\Omega} \| \Pi(\nabla y(x)) - \nabla y(x) \|^2 \, dx \right]. \]
which together with Theorem 5.1 implies (5.6).

We have by (2.7) that
\[
\left[ \text{meas } \omega_0^0 - (1 - \lambda) \text{meas } \omega \right] F_0 + \left[ \text{meas } \omega_1^1 - \lambda \text{meas } \omega \right] F_1 = \int_\omega \left[ \Pi (\nabla y(x)) - \nabla y_\lambda(x) \right] dx - \int_{\omega - \{ \omega_0^0 \cup \omega_1^1 \}} \Pi (\nabla y(x)) \, dx. \tag{5.8}
\]

By the triangle inequality, the Cauchy-Schwarz inequality, Theorem 5.1, and Theorem 4.3, we have that
\[
\left\| \int_\omega \left[ \Pi (\nabla y(x)) - \nabla y_\lambda(x) \right] dx \right\|
\leq \left\| \int_\omega \left[ \Pi (\nabla y(x)) - \nabla y(x) \right] dx \right\| + \left\| \int_\omega \left[ \nabla y(x) - \nabla y_\lambda(x) \right] dx \right\|
\leq (\text{meas } \omega)^{\frac{1}{2}} \left[ \int_\Omega \left\| \Pi (\nabla y(x)) - \nabla y(x) \right\|^2 dx \right]^{\frac{1}{2}} + \left\| \int_\omega \left[ \nabla y(x) - \nabla y_\lambda(x) \right] dx \right\|
\leq C \left[ \mathcal{E}(y)^{\frac{1}{2}} + \mathcal{E}(y)^{\frac{1}{2}} \right]. \tag{5.9}
\]

We also have by (5.6) that
\[
\left\| \int_{\omega - \{ \omega_0^0 \cup \omega_1^1 \}} \Pi (\nabla y(x)) \, dx \right\| \leq C \text{meas } (\omega - \{ \omega_0^0 \cup \omega_1^1 \}) \leq C \left[ \mathcal{E}(y)^{\frac{1}{2}} + \mathcal{E}(y) \right]. \tag{5.10}
\]

Finally, the inequality (5.7) follows from (5.8)–(5.10) and the linear independence of $F_0$ and $F_1$.

We now denote by $\mathcal{V}$ the Sobolev space of all functions $f \in L^2 (\Omega \times \mathbb{R}^{3 \times 3})$ such that
\[
\| f \|_V = \int_\Omega \left[ \text{ess sup} \left\| \nabla F f(x,F) \right\| \right]^2 dx + \| G_f \|_{W^{1,2}(\Omega)} < \infty,
\]
where
\[
G_f(x) = f(x,F_1) - f(x,F_0), \quad x \in \Omega.
\]
Functions in the space $\mathcal{V}$ represent thermodynamic variables of the underlying crystal.

**Theorem 5.3.** There exists a constant $C > 0$ such that
\[
\int_\Omega \{ f (x, \nabla y(x)) - \left[ (1 - \lambda(x)) f(x, F_0) + \lambda(x) f(x, F_1) \right] \} dx
\leq C \| f \|_V \left[ \mathcal{E}(y)^{\frac{1}{2}} + \mathcal{E}(y)^{\frac{1}{2}} \right], \quad \forall y \in W^\phi_\lambda, \forall f \in \mathcal{V}. \tag{5.11}
\]

**Proof.** We have the decomposition
\[
\int_\Omega \{ f (x, \nabla y(x)) - \left[ (1 - \lambda(x)) f(x, F_0) + \lambda(x) f(x, F_1) \right] \} dx
= \int_\Omega \{ f (x, \nabla y(x)) - f (x, \Pi (\nabla y(x))) \} dx
+ \int_\Omega \{ f (x, \Pi (\nabla y(x))) - \left[ (1 - \lambda(x)) f(x, F_0) + \lambda(x) f(x, F_1) \right] \} dx
\]
\[ J_2 = J_1 + J_2. \] (5.12)

The first term \( J_1 \) can be estimated by Theorem 5.1 as follows:

\[
|J_1| \leq \int_{\Omega} \left[ \underset{F \in \mathbb{R}^{3 \times 3}}{\text{ess sup}} \|\nabla F f(x, F)\| \right] \|\nabla y(x) - \Pi (\nabla y(x))\| \, dx \\
\leq \left\{ \int_{\Omega} \left[ \underset{F \in \mathbb{R}^{3 \times 3}}{\text{ess sup}} \|\nabla F f(x, F)\| \right]^2 \, dx \right\}^{\frac{1}{2}} \left[ \int_{\Omega} \|\nabla y(x) - \Pi (\nabla y(x))\|^2 \, dx \right]^{\frac{1}{2}} \\
\leq C \|f\|_V \left[ \mathcal{E}(y)^{\frac{1}{4}} + \mathcal{E}(y)^{\frac{1}{2}} \right]. \tag{5.13}
\]

By (2.3) and the definition of \( \Pi : \mathbb{R}^{3 \times 3} \to \{F_0, F_1\} \), we have the identity

\[
f(x, \Pi(F)) - [(1 - \lambda(x))f(x, F_0) + \lambda(x)f(x, F_1)] = \frac{1}{|a|^2} \{a \cdot [\Pi(F) - \nabla y_\lambda(x)] n\} G_f(x),
\]

for all \( F \in \mathbb{R}^{3 \times 3} \) and for almost all \( x \in \Omega \), leading to

\[
J_2 = \int_{\Omega} \{f(x, \Pi(\nabla y(x))) - [(1 - \lambda(x))f(x, F_0) + \lambda(x)f(x, F_1)]\} \, dx \\
= \frac{1}{|a|^2} \int_{\Omega} \{a \cdot [\Pi(\nabla y(x)) - \nabla y_\lambda(x)] n\} G_f(x) \, dx \\
= \frac{1}{|a|^2} \int_{\Omega} \{a \cdot [\Pi(\nabla y(x)) - \nabla y(x)] n\} G_f(x) \, dx + \frac{1}{|a|^2} \int_{\Omega} \{a \cdot [\nabla y(x) - \nabla y_\lambda(x)] n\} G_f(x) \, dx \\
= \frac{1}{|a|^2} \int_{\Omega} \{a \cdot [\nabla y(x) - \nabla y(x)] n\} \{\nabla G_f(x) \cdot n\} \, dx,
\]

where we used the divergence theorem and the fact that \( y(x) = y_\lambda(x) \) for any \( y \in W^\phi \) and for all \( x \in \partial \Omega \). We can thus conclude from the Cauchy-Schwarz inequality, Theorem 4.2, and Theorem 5.1 that

\[
|J_2| \leq C \left\{ \int_{\Omega} [\|\nabla G_f(x) \cdot n\|^2 + G_f(x)^2] \, dx \right\}^{\frac{1}{2}} \left[ \mathcal{E}(y)^{\frac{1}{4}} + \mathcal{E}(y)^{\frac{1}{2}} \right] \\
\leq C \|f\|_V \left[ \mathcal{E}(y)^{\frac{1}{4}} + \mathcal{E}(y)^{\frac{1}{2}} \right]. \tag{5.14}
\]

We finally obtain the inequality (5.11) from (5.12) – (5.14).

\[ \square \]

6. Finite Element Approximations

For simplicity we assume in what follows that the reference configuration \( \Omega \subset \mathbb{R}^3 \) is a polyhedral domain. For a fixed positive number \( h_0 \), let \( t_h, 0 < h \leq h_0 \), be a family of tetrahedral finite element meshes of \( \Omega \), such that \( \hat{\Omega} = \cup_{T \in t_h} T \), where \( h \) is the maximum diameter of any tetrahedron \( T \) in the mesh \( t_h \). We shall assume as usual that any face of any tetrahedron in a mesh \( t_h \) has a disjoint interior with respect to any other tetrahedron in that mesh and that any face of a tetrahedron is either a subset of the boundary \( \partial \Omega \) or is the face of another tetrahedron in the mesh \( t_h \). Let \( \mathcal{A}_h, 0 < h \leq h_0, \) be the corresponding
family of piecewise linear, continuous finite element spaces with respect to the mesh \( \tau_h \) [11, 30].

We can define the interpolation operator \( I_h : C(\Omega; \mathbb{R}^3) \to A_h \) for each \( h \in (0, h_0] \) which interpolates the values at the vertices of the tetrahedral elements \( T \) of \( \tau_h \). We will assume that the family \( \tau_h \) of finite meshes is quasi-regular [11, 30], so that

\[
\text{ess sup}_{x \in \Omega} \| \nabla I_h y(x) \| \leq C \text{ ess sup}_{x \in \Omega} \| \nabla y(x) \|
\]

(6.1)

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

\[
I_h y(x)|_T = y(x)|_T \quad \text{for any } T \in \tau_h \text{ such that } y(x)|_T \in \{ P^1(T) \}^3,
\]

for \( h \in (0, h_0] \), where \( \{ P^1(T) \}^3 = P^1(T) \times P^1(T) \times P^1(T) \) and \( P^1(T) \) denotes the space of linear polynomials defined on \( T \).

To approximate the boundary data \( y_\lambda \in W^\phi \), given in (3.1), we define the finite element deformation \( y_{\lambda h} \in A_h \) by

\[
y_{\lambda h} = I_h y_\lambda(x), \quad x \in \Omega,
\]

and define the finite element space of admissible deformations

\[
A_{\lambda h} = \{ y_h \in A_h : y_h(x) = y_{\lambda h}(x) \text{ on } x \in \partial \Omega \}.
\]

Since \( \lambda \in L^\infty(\mathbb{R}) \), we have that \( \nabla y_\lambda = F_0 + \lambda a \otimes n \in L^\infty(\Omega; \mathbb{R}^3) \). Thus, it follows from well-known estimates for the interpolation error [11, 30] that

\[
\| y_\lambda - y_{\lambda h} \|_{L^\infty(\partial \Omega; \mathbb{R}^3)} \leq C h \| y_\lambda \|_{W^{1, \infty}(\partial \Omega; \mathbb{R}^3)}.
\]

In what follows we shall use the result that \( y_{\lambda h} \in A_{\lambda h}, 0 < h \leq h_0 \), satisfies the condition

\[
\| y_\lambda - y_{\lambda h} \|_{L^2(\partial \Omega; \mathbb{R}^3)} \leq C h.
\]

(6.2)

We begin our analysis of the finite element approximation of a laminate with varying volume fractions with the following result on the minimization of the energy \( E \) on the space \( A_{\lambda h} \).

**Theorem 6.1.** There exists \( y_h \in A_{\lambda h} \) for each \( h \in (0, h_0] \) such that

\[
E(y_h) = \min_{z_h \in A_{\lambda h}} E(z_h) \leq C h^{1/2}.
\]

(6.3)

**Proof.** The existence of \( y_h \in A_{\lambda h} \) can be proven by the same argument as in the proof of Theorem 6.1 in [23]. To prove the inequality in (6.3) we follow the argument given in [24] to show that \( \hat{y}_h = I_h \hat{u}_\gamma \in A_{\lambda h} \) with \( \hat{u}_\gamma(x) \) defined by Lemma 3.1 and \( \gamma = h^{1/2} \) satisfies

\[
E(\hat{y}_h) \leq C h^{1/2}.
\]

We note that since \( \Omega \) is assumed to be polyhedral in this section, \( \Omega \) is the disjoint union of tetrahedra.

We next give a series of estimates for the finite element approximation of the deformation \( y_\lambda \) by deformations \( y_h \in A_{\lambda h} \). These estimates follow those for the deformations \( y \in W^\phi_\lambda \) given in previous sections.
Theorem 6.2. We have for any \( w \in \mathbb{R}^3 \) such that \( w \cdot n = 0 \) and \( |w| = 1 \) that
\[
\int_{\Omega} |[\nabla y_h(x) - \nabla y_\lambda(x)] w|^2 \, dx \leq C \left[ \mathcal{E}(y_h)^{\frac{1}{2}} + \mathcal{E}(y_h) + \|y_\lambda - y_{\lambda h}\|_{L^2(\partial \Omega; \mathbb{R}^3)} \right], \quad \forall y_h \in A_{\lambda h}.
\]

Proof. Fix \( y_h \in A_{\lambda h} \) and \( w \in \mathbb{R}^3 \) such that \( w \cdot n = 0 \) and \( |w| = 1 \). By the decomposition
\[
y_h - y_\lambda = [y_h - \pi(y_h)] + [\pi(y_h) - y_\lambda]
\]
and Lemma 4.1, we need only to prove
\[
\int_{\Omega} |[\pi(\nabla y_h(x)) - \nabla y_\lambda(x)] w|^2 \, dx \leq C \left[ \mathcal{E}(y_h)^{\frac{1}{2}} + \|y_\lambda - y_{\lambda h}\|_{L^2(\Omega; \mathbb{R}^3)} \right]. \tag{6.4}
\]

We only consider the orthorhombic to monoclinic transformation, since the cubic to tetragonal transformation can be treated similarly (see the proofs of Lemma 4.2 and Theorem 4.1). Noting that \( y_h(x) = y_{\lambda h}(x) \) for \( x \in \partial \Omega \), we have by (4.1) and the divergence theorem that
\[
\int_{\Omega} |[\pi(\nabla y_h(x)) - \nabla y_\lambda(x)] w|^2 \, dx
\]
\[
= 2 F_0 w \cdot \int_{\Omega} [\nabla y_\lambda(x) - \pi(\nabla y_h(x))] \, w \, dx
\]
\[
= 2 F_0 w \cdot \left\{ \int_{\Omega} [\nabla y_\lambda(x) - \nabla y_h(x)] \, dx + \int_{\partial \Omega} [\nabla y_h(x) - \pi(\nabla y_h(x))] \, dS \right\} w
\]
\[
= 2 F_0 w \cdot \left\{ \int_{\partial \Omega} [y_\lambda(x) - y_{\lambda h}(x)] \otimes \nu \, dS + \int_{\Omega} [\nabla y_h(x) - \pi(\nabla y_h(x))] \, dx \right\} w
\]
This, together with Lemma 4.1 and the Cauchy-Schwarz inequality, leads to (6.4).

Theorem 6.3. We have
\[
\int_{\Omega} |y_h(x) - y_\lambda(x)|^2 \, dx \leq C \left[ \mathcal{E}(y_h)^{\frac{1}{2}} + \mathcal{E}(y_h) \right] + \left[ \|y_\lambda - y_{\lambda h}\|_{L^2(\partial \Omega; \mathbb{R}^3)}^2 + \|y_\lambda - y_{\lambda h}\|_{L^2(\partial \Omega; \mathbb{R}^3)}^2 \right], \quad \forall y_h \in A_{\lambda h}.
\]

Proof. Fix \( y_h \in A_{\lambda h} \). Setting \( z = y_h - y_\lambda \) and choosing \( w \in \mathbb{R}^3 \) so that \( w \cdot n = 1 \) and \( |w| = 1 \), we obtain the desired inequality by (4.5) and Theorem (6.2).

By an argument similar to the proof of Theorem 4.3, we can use the above theorem to obtain the following result on the weak convergence estimate for finite element deformations.

Theorem 6.4. For any Lipschitz domain \( \omega \subset \Omega \), there exists a positive constant \( C > 0 \), independent of \( h \), such that
\[
\left\| \int_{\omega} [\nabla y_h(x) - \nabla y_\lambda(x)] \, dx \right\| \leq C \left[ \mathcal{E}(y_h)^{\frac{1}{2}} + \mathcal{E}(y_h) \right] + C \left[ \|y_\lambda - y_{\lambda h}\|_{L^2(\partial \Omega; \mathbb{R}^3)}^2 + \|y_\lambda - y_{\lambda h}\|_{L^2(\partial \Omega; \mathbb{R}^3)}^2 \right], \quad \forall y_h \in A_{\lambda h}.
\]
Recall the operator $\Pi : \mathbb{R}^{3 \times 3} \to \{F_0, F_1\}$ defined by (5.1). We have the following result which is parallel to Theorem 5.1. The key estimate is (6.4).

**Theorem 6.5.** We have
\[
\int_{\Omega} \|\nabla y_h(x) - \Pi(\nabla y_h(x))\|^2 \, dx \leq C \left[ \mathcal{E}(y_h)^{\frac{1}{2}} + \mathcal{E}(y_h) + \|y_\lambda - y_{\lambda h}\|_{L^2(\partial \Omega; \mathbb{R}^3)} \right], \quad \forall y_h \in \mathcal{A}_{\lambda h}.
\]

Recall that $\lambda_\omega$ is the average of $\lambda$ on $\omega$. Using the same argument as in the proof of Theorem 5.2, we can obtain the following result from Theorem 6.4 and Theorem 6.5.

**Theorem 6.6.** For any Lipschitz domain $\omega \subset \Omega$ and any $\rho > 0$ there exists a positive constant $C = C(\omega, \rho)$, independent of $h$, such that
\[
\text{meas} \left( \omega - (\omega^0_h(\cdot) \cup \omega^1_h(\cdot)) \right) \leq C \left[ \mathcal{E}(y_h)^{\frac{1}{2}} + \mathcal{E}(y_h) + \|y_\lambda - y_{\lambda h}\|_{L^2(\partial \Omega; \mathbb{R}^3)} \right], \quad \forall y_h \in \mathcal{A}_{\lambda h},
\]
and
\[
\left| \frac{\text{meas} \omega^0_h(y_h)}{\text{meas} \omega} - (1 - \lambda_\omega) \right| + \left| \frac{\text{meas} \omega^1_h(y_h)}{\text{meas} \omega} - \lambda_\omega \right| \leq C \left[ \mathcal{E}(y_h)^{\frac{1}{2}} + \mathcal{E}(y_h) + \|y_\lambda - y_{\lambda h}\|_{L^2(\partial \Omega; \mathbb{R}^3)} + \|y_\lambda - y_{\lambda h}\|_{L^2(\partial \Omega; \mathbb{R}^3)} \right], \quad \forall y_h \in \mathcal{A}_{\lambda h}.
\]

By slightly modifying the proof of Theorem 5.3, we can obtain the following result corresponding to Theorem 5.3 for admissible finite element deformations.

**Theorem 6.7.** We have
\[
\left| \int_{\Omega} \{f(x, \nabla y_h(x)) - [(1 - \lambda(x))f(x, F_0) + \lambda(x)f(x, F_1)]\} \, dx \right| \leq C \|f\|_V \left[ \mathcal{E}(y_h)^{\frac{1}{2}} + \mathcal{E}(y_h)^{\frac{1}{2}} + \|y_\lambda - y_{\lambda h}\|_{L^2(\partial \Omega; \mathbb{R}^3)}^{\frac{1}{2}} + \|y_\lambda - y_{\lambda h}\|_{L^2(\partial \Omega; \mathbb{R}^3)}^{\frac{1}{2}} \right]
\]
for all $y_h \in \mathcal{A}_{\lambda h}$ and all $f \in V$.

The number of local minima of the problem
\[
\inf_{y_h \in \mathcal{A}_{\lambda h}} \mathcal{E}(y_h)
\]
grows arbitrarily large as the mesh size $h \to 0$. Many of these local minima are approximations on different length scales to the same optimal microstructure [24]. Thus, it is reasonable to give error estimates for finite element deformations $y_h \in \mathcal{A}_{\lambda h}$ that satisfy the following quasi-optimality condition
\[
\mathcal{E}(y_h) \leq \alpha \inf_{z_h \in \mathcal{A}_{\lambda h}} \mathcal{E}(z_h) \tag{6.5}
\]
for some constant $\alpha \geq 1$ independent of $h$.

It follows directly from the previous theorems in this section and (6.2) that we can obtain the following error estimates for quasi-optimal finite element deformations $y_h \in \mathcal{A}_{\lambda h}$.

**Corollary 6.1.** We have
\[
\int_{\Omega} |\nabla y_h(x) - \nabla y_\lambda(x)|^2 \, dx \leq C h^{\frac{1}{4}}
\]
for any $w \in \mathbb{R}^3$ such that $w \cdot n = 1$ and $|w| = 1$ and for any $y_h \in \mathcal{A}_{\lambda h}$ which satisfies the quasi-optimality condition (6.5).

**Corollary 6.2.** We have

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

for any $y_h \in \mathcal{A}_{\lambda h}$ which satisfies the quasi-optimality condition (6.5).

**Corollary 6.3.** For any Lipschitz domain $\omega \subseteq \Omega$ and any $\rho > 0$, there exists a positive constant $C = C(\omega, \rho)$, independent of $h$, such that

$$\text{meas} \left( \omega - \left( \omega^0_{\rho}(y_h) \cup \omega^1_{\rho}(y_h) \right) \right) \leq C h^{1/4}$$

and

$$\left| \frac{\text{meas} \omega^0_{\rho}(y_h)}{\text{meas} \omega} - (1 - \lambda_\omega) \right| + \left| \frac{\text{meas} \omega^1_{\rho}(y_h)}{\text{meas} \omega} - \lambda_\omega \right| \leq C h^{1/16}$$

for any $y_h \in \mathcal{A}_{\lambda h}$ which satisfies the quasi-optimality condition (6.5).

**Corollary 6.4.** We have

$$\left| \int_{\Omega} \left\{ f(x, \nabla y_h(x)) - ((1 - \lambda(x))f(x, F_0) + \lambda(x)f(x, F_1)) \right\} \, dx \right| \leq C \| f \|_{V} h^{1/8}$$

for any $f \in V$ and any $y_h \in \mathcal{A}_{\lambda h}$ which satisfies the quasi-optimality condition (6.5).

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