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Bo Li
Mitchell Luskin

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Department of Mathematics
University of California, Los Angeles
Los Angeles, CA. 90024-1555

APPROXIMATION OF A MARTENSITIC LAMINATE WITH VARYING VOLUME FRACTIONS

BO LI AND MITCHELL LUSKIN

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

Martensitic crystals such as metals and alloys are characterized by their capability of undergoing diffusionless, structural, and reversible phase transformations. The austenitic phase is most stable above the transformation temperature, and the martensitic phase is most stable below the transformation temperature. With a fixed orthonormal basis for $\mathbb{R}^3$, these martensitic lattice structures are represented by several symmetry-related matrices, $U_1, \cdots, U_N$, for $N > 1$, called martensitic variants. They represent the linear transformations that can transform the austenitic lattice into the martensitic lattices.

In nonlinear elasticity, martensitic crystals are described by deformations which are mappings from a reference configuration to $\mathbb{R}^3$. Usually, the undistorted austenitic state at the transformation temperature is chosen to be the

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reference configuration of the crystal. We model the martensitic crystal by a rotationally invariant energy density, so the martensitic phase is characterized by a deformation with deformation gradient taking values in the set $SO(3)U_1 \cup \cdots \cup SO(3)U_N$ where $SO(3)$ is the set of all 3×3 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 below the transformation temperature can be lowered as much as possible only by the fine-scale mixing of coherent martensitic variants. 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].

Based on the hypothesis that the crystal structure is determined by the principle of energy minimization, the recently developed geometrically nonlinear theory of thermoelasticity describes the martensitic microstructure as the limiting configuration of energy minimizing sequences of deformations, see [2, 3, 10, 14, 15, 18, 20, 23] and the references therein. A central object in this theory is the elastic energy density of the crystal. Below the transformation temperature, such an energy density is minimized on multiple energy wells $SO(3)U_1, \cdots, SO(3)U_N$. The elastic energy functional is therefore non-convex and cannot attain its *infimum* for certain boundary conditions. Nevertheless, as stable configurations, martensitic microstructures can be described by energy minimizing sequences via the notion of Young measure which gives the volume fraction for the mixing of the deformation gradients of the energy minimizing microstructure and defines the macroscopic thermodynamic variables of the crystal [2, 3, 19, 32, 33].

We now focus on martensitic crystals that can undergo either an orthorhombic to monoclinic or a cubic to tetragonal transformation [3, 23]. 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 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 possibly varying volume fractions of these martensitic crystals. 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 weak L^2 approximation of the limiting macroscopic deformation gradient, 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 in [24] for the numerical analysis of simple laminates with constant volume fractions for a two-well problem which applies to the orthorhombic to monoclinic transformation. The generalization to the cubic to tetragonal problem was made possible by a reduction to a two-well problem based on the crystallography of the cubic to tetragonal transformation [3]. For constant volume fractions, an analysis for both of conforming and nonconforming finite element approximations was given in [22] and [21], respectively.

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, 25] Analyses of the approximation of relaxed variational problems have been given in [6, 16, 26, 27, 28, 30, 31]. We refer to the recent article [23] for a survey of models, computation, and numerical analysis for martensitic microstructure.

In Section 2, we describe the multi-well energy minimization problems. In Section 3, we construct energy minimizing sequences of deformations which satisfy the corresponding nonhomogeneous boundary condition. In Section 4 and Section 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 Section 6, we give error estimates for the approximation by the 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, 23].

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

$$U_1 = (I + \eta e_1 \otimes e_2)D, \qquad U_2 = (I - \eta e_1 \otimes e_2)D,$$

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

$$U_1 = \eta_1 I + (\eta_2 - \eta_1) e_1 \otimes e_1, \qquad U_2 = \eta_1 I + (\eta_2 - \eta_1) e_2 \otimes e_2,$$
$$U_3 = \eta_1 I + (\eta_2 - \eta_1) e_3 \otimes e_3,$$

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

$$\mathcal{U}_i = \mathrm{SO}(3)U_i, \quad i \in K, \qquad \text{and} \qquad \mathcal{U} = \cup\{\mathcal{U}_i : i \in K\}.$$

It is easy to see that

$$\det F = d_1 d_2 d_3 > 0, \qquad \forall F \in \mathcal{U}, \tag{2.1}$$

for the orthorhombic to monoclinic transformation, and that

$$\det F = \eta_1^2 \eta_2 > 0, \qquad \forall F \in \mathcal{U}, \tag{2.2}$$

for the cubic to tetragonal transformation.

We now denote by $\mathbb{R}^{3\times3}$ the set of all 3×3 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 $F_0, F_1 \in \mathbb{R}^{3\times3}$, there exists a continuous deformation $y : \mathbb{R}^3 \to \mathbb{R}^3$ such that ∇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, 23] 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_1U_i and R_2U_i with $R_1, R_2 \in SO(3)$ 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 $Q \in SO(3)$ 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.

For a given martensitic crystal, we denote by Ω 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 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 $\phi : \mathbb{R}^{3\times3} \to \mathbb{R}$. The elastic energy of a deformation $y : \Omega \to \mathbb{R}^3$ is given by

$$\mathcal{E}(y) = \int_\Omega \phi(\nabla y(x))\, dx, \tag{2.4}$$

where $\nabla y : \Omega \to \mathbb{R}^{3\times3}$ is the deformation gradient. We define the set of deformations of finite energy by

$$W^\phi = \left\{ y \in C(\bar{\Omega}; \mathbb{R}^3) : \int_\Omega \phi(\nabla y(x))\, dx < \infty \right\}. \tag{2.5}$$

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

$$\phi(F) \geq 0, \qquad \forall F \in \mathbb{R}^{3\times 3}, \tag{2.6}$$

$$\phi(F) = 0 \quad \text{if and only if} \quad F \in \mathcal{U} = \cup\{\mathcal{U}_i : i \in K\}\,. \tag{2.7}$$

We shall also assume that the energy density ϕ grows quadratically away from the energy wells, that is,

$$\phi(F) \geq \kappa \|F - \pi(F)\|^2, \qquad \forall F \in \mathbb{R}^{3\times 3}, \tag{2.8}$$

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

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

and where

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

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 [23].

To study a simple laminate, we let $F_0, F_1 \in \mathcal{U}$ be rank-one connected as in (2.3). By Lemma 2.1, we may assume without loss of generality that $F_1 \in \mathcal{U}_1$ and $F_0 \in \mathcal{U}_2$, and we may 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. The following theorem 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. We note that it follows from (2.3) that if $\hat{\lambda} \in L^\infty(\mathbb{R}^3)$ is a volume fraction so that $0 \leq \hat{\lambda}(x) \leq 1$, for almost all $x \in \mathbb{R}^3$, then

$$\left(1 - \hat{\lambda}(x)\right) F_0 + \hat{\lambda}(x) F_1 = F_0 + \hat{\lambda}(x) a \otimes n = F_1 + \left(1 - \hat{\lambda}(x)\right) a \otimes n \tag{2.9}$$

for almost all $x \in \mathbb{R}^3$.

Lemma 2.2. *Let $\hat{\lambda} \in L^\infty(\mathbb{R}^3)$ and $y \in W^{1,\infty}(\mathbb{R}^3; \mathbb{R}^3)$. We have that*

$$\nabla y(x) = F_0 + \hat{\lambda}(x) a \otimes n, \qquad \text{for almost all } x \in \mathbb{R}^3, \tag{2.10}$$

if and only if

$$\hat{\lambda}(x) = \lambda(x \cdot n), \qquad \text{for almost all } x \in \mathbb{R}^3, \tag{2.11}$$

for some $\lambda \in L^\infty(\mathbb{R})$, and

$$y(x) = F_0 x + \left[\int_0^{x \cdot n} \lambda(s) ds \right] a + y_0, \qquad \text{for almost all } x \in \mathbb{R}^3, \tag{2.12}$$

for some constant $y_0 \in \mathbb{R}^3$.

Proof. It follows from (2.10) that for almost all $x \in \Omega$

$$(\nabla y(x) - F_0) w = 0 \qquad \text{if } w \cdot n = 0.$$

Therefore, except on a subset of $\mathbb{R}^3$ of measure zero, $y(x) - F_0 x$ depends only on $x \cdot n$. Consequently, $\hat{\lambda}$ only depends on $x \cdot n$ since

$$\hat{\lambda}(x) = \frac{1}{|a|^2 \, |n|^2} \left(\nabla y(x) - F_0 \right) n \cdot a, \qquad \text{for almost all } x \in \mathbb{R}^3,$$

by (2.10). Thus, (2.11) is proved. Setting

$$z(x) = y(x) - F_0 x - \left[\int_0^{x \cdot n} \lambda(s) ds \right] a, \qquad x \in \mathbb{R}^3,$$

we get by (2.10) and (2.11) that

$$\nabla z(x) = \nabla y(x) - F_0 - \lambda(x \cdot n) a \otimes n = 0, \qquad \text{for almost all } x \in \mathbb{R}^3,$$

proving (2.12). Conversely, we can obtain (2.10) from (2.11) and (2.12) by a direct calculation. □

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 given by a deformation with a gradient that is a mixture of the two matrices F_0 and F_1. By the above theorem, the most general such deformation (up to translation by a constant $y_0 \in \mathbb{R}^3$) is given by

$$y_\lambda(x) = F_0 x + \left[\int_0^{x \cdot n} \lambda(s) ds \right] a, \qquad x \in \mathbb{R}^3, \tag{2.13}$$

where the volume fraction $\lambda \in L^\infty(\mathbb{R})$ satisfies

$$0 \le \lambda(s) \le 1, \qquad \text{for almost all } s \in \mathbb{R}.$$

We thus define the set of admissible deformations to be

$$W_\lambda^\phi = \left\{ y \in W^\phi : y = y_\lambda \text{ on } \partial\Omega \right\}.$$

Our multi-well energy minimization problem is to minimize the elastic energy (2.4) among all deformations $y \in W_\lambda^\phi$. For a constant volume fraction λ, the Ball-James result [2, 3] states that there exist no energy minimizers for such an energy minimization problem, and that any energy minimizing sequences will converge to a unique microstructure which is the simple laminate composed of the gradient F_0 with the volume fraction $1-\lambda$ and the gradient F_1 with the volume fraction λ.

3. Construction of Energy Minimizing Sequences

We now construct in two steps a family of deformations $\hat{u}_\gamma \in W_\lambda^\phi$, $\gamma \in (0, \gamma_0]$, 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 γ such that $\nabla u_\gamma(x) = F_0$ or F_1 for almost all $x \in \mathbb{R}^3$. Second, we construct $\hat{u}_\gamma \in W_\lambda^\phi$, $\gamma \in (0, \gamma_0]$, by modifying u_γ by interpolation on the boundary. A key objective is to construct a sequence of characteristic functions converging weakly for any finite interval of $\mathbb{R}^1$ to the volume fraction function λ.

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

$$I_\gamma^{(i)} = [(i-1)\gamma, i\gamma] \qquad \text{and} \qquad \lambda_\gamma^{(i)} = \frac{1}{\gamma} \int_{I_\gamma^{(i)}} \lambda(s)\,ds, \qquad \forall i \in \mathbb{Z}.$$

Define the piecewise constant function $\lambda_\gamma : \mathbb{R} \to \mathbb{R}$ by

$$\lambda_\gamma(s) = \lambda_\gamma^{(i)} \qquad \text{if } s \in I_\gamma^{(i)},\ i \in \mathbb{Z},$$

where the effect of a set of measure zero has been neglected. Define the characteristic function $\chi_\gamma : \mathbb{R} \to \mathbb{R}$ by

$$\chi_\gamma(s) = \begin{cases} 1 & \text{if } (i-1)\gamma < s \le \left(i - 1 + \lambda_\gamma^{(i)}\right)\gamma \text{ for some } i \in \mathbb{Z}, \\ 0 & \text{if } \left(i - 1 + \lambda_\gamma^{(i)}\right)\gamma < s \le i\gamma \text{ for some } i \in \mathbb{Z}, \end{cases}$$

Since $0 \le \lambda(s)$, $\lambda_\gamma(s)$, $\chi_\gamma(s) \le 1$ for almost all $s \in \mathbb{R}$, we have for any finite interval $I \subset \mathbb{R}^1$ that

$$\left| \int_I \left[\chi_\gamma(s) - \lambda(s) \right] ds \right| \le 2\gamma. \tag{3.1}$$

Define now

$$u_\gamma(x) = F_0 x + \left[\int_0^{x\cdot n} \chi_\gamma(s)ds\right] a, \qquad \forall x \in \mathbb{R}^3.$$

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

$$\nabla u_\gamma(x) = F_0 + \chi_\gamma(x\cdot n)a\otimes n \in \{F_0, F_1\}, \qquad \text{for almost all } x \in \mathbb{R}^3. \quad (3.2)$$

In view of (2.13) and (3.1), we also have

$$|u_\gamma(x) - y_\lambda(x)| \le 2|a|\gamma, \qquad \forall x \in \mathbb{R}^3. \quad (3.3)$$

Step 2. Construction of $\hat{u}_\gamma \in W_\lambda^\phi$, $\gamma \in (0,\gamma_0]$. Set

$$\Omega_\gamma = \{x \in \Omega : \operatorname{dist}(x,\partial\Omega) > \upsilon\gamma\}$$

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

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

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

$$\begin{array}{ll} 0 \le \psi_\gamma(x) \le 1, & \forall x \in \Omega, \\ \psi_\gamma(x) = 1, & \forall x \in \Omega_\gamma, \\ \psi_\gamma(x) = 0, & \forall x \in \partial\Omega, \\ |\nabla\psi_\gamma(x)| \le (\upsilon\gamma)^{-1}, & \text{for almost all } x \in \Omega. \end{array} \quad (3.4)$$

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

$$\hat{u}_\gamma(x) = \psi_\gamma(x)u_\gamma(x) + (1-\psi_\gamma(x))y_\lambda(x), \qquad \forall x \in \Omega.$$

It is easy to verify that

$$\begin{aligned}\nabla\hat{u}_\gamma(x) = {} & [u_\gamma(x) - y_\lambda(x)]\otimes\nabla\psi_\gamma(x) + \psi_\gamma(x)\nabla u_\gamma(x) \\ & + (1-\psi_\gamma(x))\nabla y_\lambda(x), \qquad \text{for almost all } x \in \Omega. \end{aligned} \quad (3.5)$$

By (3.2) – (3.5), we have for all $\gamma \in (0,\gamma_0]$ that

$$\|\nabla\hat{u}_\gamma(x)\| \le C \qquad \text{for almost all } x \in \Omega, \quad (3.6)$$

where C is a constant independent of γ, and that

$$\nabla\hat{u}_\gamma(x) \in \{F_0, F_1\}, \qquad \text{for almost all } x \in \Omega_\gamma. \quad (3.7)$$

Therefore $\hat{u}_\gamma \in W_\lambda^\phi$ for any $\gamma \in (0,\gamma_0]$ by the continuity of the energy density ϕ. Moreover, since $\operatorname{meas}(\Omega - \Omega_\gamma) = O(\gamma)$, as $\gamma \to 0$, we have by (3.6), (3.7), and (2.7) that

$$\mathcal{E}(\hat{u}_\gamma) = O(\gamma), \qquad \text{as } \gamma \to 0.$$

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 (see (2.1) and (2.2))

$$\det F_0 = \det F_1 > 0$$

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 (2.9) and (3.2) that

$$\psi_\gamma(x) \nabla u_\gamma(x) + (1 - \psi_\gamma(x)) \nabla y_\lambda(x) = F_0 + \xi(x) a \otimes n, \qquad \text{for almost all } x \in \Omega,$$

where

$$\xi(x) = \psi_\gamma(x) \chi_\gamma(x \cdot n) + (1 - \psi_\gamma(x))\, \lambda(x \cdot n), \qquad x \in \Omega.$$

Thus,

$$\begin{aligned} &\det \left[\psi_\gamma(x) \nabla u_\gamma(x) + (1 - \psi_\gamma(x)) \nabla y_\lambda(x)\right] \\ &\qquad = \det F_0 = \det F_1 > 0, \qquad \text{for almost all } x \in \Omega. \end{aligned}$$

Choosing $\upsilon > 0$ large enough, we can therefore conclude from (3.3) – (3.5) that

$$\det \nabla \hat{u}_\gamma(x) \geq \text{constant} > 0, \qquad \text{for almost all } x \in \Omega,\ \forall \gamma \in (0, \gamma_0]. \tag{3.8}$$

We summarize our results in the following theorem.

Theorem 3.1. *There exist a family of deformations $\hat{u}_\gamma \in W_\lambda^\phi$, $\gamma \in (0, \gamma_0]$, for any fixed $\gamma_0 > 0$, such that* (3.8) *holds and such that*

$$\lim_{\gamma \to 0} \mathcal{E}(\hat{u}_\gamma) = 0.$$

4. Approximation of the Limiting Macroscopic Deformation

Our first lemma below is a direct consequence of the growth rate of the energy density around the energy wells (2.8).

Lemma 4.1. *We have*

$$\int_\Omega \|\nabla y(x) - \pi(\nabla y(x))\|^2 \, dx \leq \kappa^{-1} \mathcal{E}(y), \qquad \forall y \in W^\phi.$$

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*

$$\int_\Omega |[\pi(\nabla y(x)) - \nabla y_\lambda(x)]\, w|^2 \, dx \le C\mathcal{E}(y)^{\frac{1}{2}}, \qquad \forall y \in W^\phi_\lambda,$$

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

$$\pi(F) \in \mathrm{SO}(3)F_0 \cup \mathrm{SO}(3)F_1, \qquad \forall F \in \mathbb{R}^{3\times 3}.$$

Fix $w \in \mathbb{R}^3$ with $w \cdot n = 0$ and $|w| = 1$. By (2.3) and (2.9), we have that

$$\nabla y_\lambda(x) w = F_0 w = F_1 w, \qquad \text{for almost all } x \in \Omega, \tag{4.1}$$

leading to

$$|\pi(F)w| = |\nabla y_\lambda(x) w|, \qquad \forall F \in \mathbb{R}^{3\times 3}, \text{ for almost all } x \in \Omega. \tag{4.2}$$

Fix $y \in W^\phi_\lambda$. Since $y(x) = y_\lambda(x), \forall x \in \partial\Omega$, we have by the divergence theorem that

$$\int_\Omega \nabla y(x)\, dx = \int_\Omega \nabla y_\lambda(x)\, dx. \tag{4.3}$$

It follows from (4.1) – (4.3), the Cauchy-Schwarz inequality, and Lemma 4.1 that

$$\begin{aligned}
&\int_\Omega |[\pi(\nabla y(x)) - \nabla y_\lambda(x)]\, w|^2 \, dx \\
&\quad = 2\int_\Omega \nabla y_\lambda(x) w \cdot [\nabla y_\lambda(x) - \pi(\nabla y(x))]\, w \, dx \\
&\quad = 2F_1 w \cdot \int_\Omega [\nabla y(x) - \pi(\nabla y(x))]\, w\, dx \\
&\quad \le 2|F_1 w| (\operatorname{meas}\Omega)^{\frac{1}{2}} \left[\int_\Omega \|\nabla y(x) - \pi(\nabla y(x))\|^2 \, dx\right]^{\frac{1}{2}} \\
&\quad \le C\mathcal{E}(y)^{\frac{1}{2}}.
\end{aligned} \tag{4.4}$$

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

$$w_1 = \frac{1}{\sqrt{3}}(e_1 - e_2 + e_3) \qquad \text{and} \qquad w_2 = \frac{1}{\sqrt{3}}(e_1 - e_2 - e_3).$$

It is easy to check that

$$w_1 \cdot n = w_2 \cdot n = 0, \qquad |w_1| = |w_2| = 1,$$

and

$$|U_i w_j| = \sqrt{\frac{2\eta_1^2 + \eta_2^2}{3}}, \qquad i = 1, 2, 3, \; j = 1, 2.$$

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_λ in any direction tangential to parallel layers of the laminate. It is a direct consequence of the triangle inequality and the above two lemmas. It will play a key role in establishing other error bounds.

Theorem 4.1. *There exists a constant $C > 0$ such that*

$$\int_\Omega |[\nabla y(x) - \nabla y_\lambda(x)]\, w|^2 \, dx \le C \left[\mathcal{E}(y)^{\frac{1}{2}} + \mathcal{E}(y) \right], \qquad \forall y \in W_\lambda^\phi,$$

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_λ by the admissible deformations $y \in W_\lambda^\phi$.

Theorem 4.2. *There exists a constant $C > 0$ such that*

$$\int_\Omega |y(x) - y_\lambda(x)|^2 \, dx \le C \left[\mathcal{E}(y)^{\frac{1}{2}} + \mathcal{E}(y) \right], \qquad \forall y \in W_\lambda^\phi.$$

Proof. Let $z \in C^1(\bar{\Omega}; \mathbb{R}^3)$ and $w \in \mathbb{R}^3$ with $|w| = 1$. We can easily verify the following identity

$$\int_\Omega |z(x)|^2 \, dx$$
$$= \int_{\partial\Omega} |z(x)|^2 (w \cdot x)(w \cdot \nu) dS - \int_\Omega \left(\nabla |z(x)|^2 \cdot w \right) (w \cdot x) \, dx$$

$$= \int_{\partial\Omega} |z(x)|^2 (w \cdot x)(w \cdot \nu) dS - 2 \int_{\Omega} (\nabla z(x) w \cdot z(x)) (w \cdot x)\, dx \quad (4.5)$$

to get the Poincaré inequality [24, 34]

$$\int_{\Omega} |z(x)|^2 \, dx \leq C \left[\int_{\partial\Omega} |z(x)|^2 dS + \int_{\Omega} |\nabla z(x) w|^2 \, dx \right], \quad (4.6)$$

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 $C^1(\bar{\Omega}; \mathbb{R}^3)$ in W^{ϕ}. Setting $z = y - y_\lambda$ for any $y \in W_\lambda^{\phi}$, 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 above theorem implies that the *infimum* of the energy $\mathcal{E}(y)$ is not attained on W_λ^{ϕ}, the space of admissible deformations.

Corollary 4.1. *We have*

$$\inf_{y \in W_\lambda^{\phi}} \mathcal{E}(y) = 0. \quad (4.7)$$

However, there exists no $y \in W_\lambda^{\phi}$ *such that* $\mathcal{E}(y) = 0$ *if*

$$\operatorname{meas} \{ x \in \Omega : 0 < \lambda(x \cdot n) < 1 \} > 0. \quad (4.8)$$

Proof. The result (4.7) is a direct consequence of Theorem 3.1. Now, if we had some $y \in W_\lambda^{\phi}$ such that $\mathcal{E}(y) = 0$, then, in view of Theorem 4.2, we would have $y = y_\lambda$.

It follows from (4.8) that there is an integer $p \geq 3$ such that the set

$$\omega_p = \left\{ x \in \Omega : \frac{1}{p} \leq \lambda(x \cdot n) \leq 1 - \frac{1}{p} \right\}$$

has positive measure. On the other hand, the set

$$\Delta_p = \left\{ (1 - \lambda_0) F_0 + \lambda_0 F_1 \in \mathbb{R}^{3\times3} : \frac{1}{p} \leq \lambda_0 \leq 1 - \frac{1}{p} \right\}$$

is compact in $\mathbb{R}^{3\times3}$, and is disjoint with $\mathcal{U}$ by Lemma 2.1. Consequently, the continuous energy density ϕ reaches its minimum $m(\Delta_p) > 0$ on the set Δ_p. Therefore,

$$0 = \mathcal{E}(y) = \mathcal{E}(y_\lambda) \geq \int_{\omega_p} \phi(\nabla y_\lambda(x))\, dx \geq m(\Delta_p) \operatorname{meas} \omega_p > 0,$$

which is a contradiction. □

Now we establish an error bound for the weak L^2 approximation of the limiting macroscopic deformation gradient ∇y_λ. 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 ∇y_λ.

Theorem 4.3. *For any Lipschitz domain $\omega \subset \Omega$, there exists a constant $C = C(\omega) > 0$ such that*

$$\left\| \int_\omega [\nabla y(x) - \nabla y_\lambda(x)]\, dx \right\| \le C \left[\mathcal{E}(y)^{\frac{1}{8}} + \mathcal{E}(y)^{\frac{1}{2}} \right], \qquad \forall y \in W_\lambda^\phi.$$

Proof. It follows from the divergence theorem and the Cauchy-Schwarz inequality that for any $y \in W_\lambda^\phi$

$$\begin{aligned}
&\left\| \int_\omega [\nabla y(x) - \nabla y_\lambda(x)]\, dx \right\| \\
&\quad = \left\| \int_{\partial\omega} [y(x) - y_\lambda(x)] \otimes \nu \, dS \right\| \\
&\quad \le \int_{\partial\omega} |y(x) - y_\lambda(x)|\, dS \\
&\quad \le (\text{meas}_2 \partial\omega)^{\frac{1}{2}} \left(\int_{\partial\omega} |y(x) - y_\lambda(x)|^2 \, dS \right)^{\frac{1}{2}}, \qquad (4.9)
\end{aligned}$$

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 [1] we have

$$\begin{aligned}
&\int_{\partial\omega} |y(x) - y_\lambda(x)|^2 dS \\
&\quad \le C \left[\int_\omega |y(x) - y_\lambda(x)|^2 \, dx + \int_\omega \left| \nabla |y(x) - \nabla y_\lambda(x)|^2 \right| dx \right] \\
&\quad \le C \left[\int_\omega |y(x) - y_\lambda(x)|^2 \, dx + \int_\omega |y(x) - y_\lambda(x)| \|\nabla [y(x) - y_\lambda(x)]\| \, dx \right] \\
&\quad \le C \Bigg[\int_\Omega |y(x) - y_\lambda(x)|^2 \, dx \\
&\qquad + \left(\int_\Omega |y(x) - y_\lambda(x)|^2 \, dx \right)^{\frac{1}{2}} \left(\int_\Omega \|\nabla y(x) - \nabla y_\lambda(x)\|^2 \, dx \right)^{\frac{1}{2}} \Bigg]. \qquad (4.10)
\end{aligned}$$

We also have by the triangle inequality and Lemma 4.1 that

$$\begin{aligned}
&\left(\int_\Omega \|\nabla y(x) - \nabla y_\lambda(x)\|^2 \, dx\right)^{\frac{1}{2}} \\
&\quad \le \left(\int_\Omega \|\nabla y(x) - \pi\left(\nabla y(x)\right)\|^2 \, dx\right)^{\frac{1}{2}} + \left(\int_\Omega \|\pi\left(\nabla y(x)\right) - \nabla y_\lambda(x)\|^2 \, dx\right)^{\frac{1}{2}} \\
&\quad \le C\left[\mathcal{E}(y)^{\frac{1}{2}} + 1\right]. \qquad (4.11)
\end{aligned}$$

Hence, it follows by using Theorem 4.2 and (4.11) in (4.10) that

$$\int_{\partial\omega} \left|y(x) - y_\lambda(x)\right|^2 dS \le C\left[\mathcal{E}(y)^{\frac{1}{4}} + \mathcal{E}(y)\right],$$

which, together with (4.9), leads to the desired inequality. □

5. Approximation of the Simple Laminate

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

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

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

$$\pi_{12}(F) = \Theta(F)\Pi(F), \qquad \forall F \in \mathbb{R}^{3\times 3}. \qquad (5.1)$$

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*

$$\int_\Omega \|\nabla y(x) - \pi_{12}(\nabla y(x))\|^2 \, dx \le C\left[\mathcal{E}(y)^{\frac{1}{2}} + \mathcal{E}(y)\right], \qquad \forall y \in W_\lambda^\phi.$$

Proof. We have by a simple calculation that

$$\inf_{F \in \mathcal{U}_3} |[F - \nabla y_\lambda(x)]\, e_3| \ge |\eta_2 - \eta_1|, \qquad \text{for almost all } x \in \Omega.$$

Denoting

$$\Omega_3 = \{x \in \Omega : \pi(\nabla y(x)) \in \mathcal{U}_3\}$$

for a fixed $y \in W_\lambda^\phi$, we thus have by Lemma 4.2 that

$$\begin{aligned} \operatorname{meas}\Omega_3 &= \int_{\Omega_3} dx \\ &\leq |\eta_2 - \eta_1|^{-2} \int_{\Omega_3} |[\pi(\nabla y(x)) - \nabla y_\lambda(x)]\, e_3|^2 \, dx \\ &\leq C\mathcal{E}(y)^{\frac{1}{2}}, \end{aligned} \tag{5.2}$$

since $e_3 \cdot n = 0$. Consequently, we have by Lemma 4.1 that

$$\begin{aligned} &\int_\Omega \|\nabla y(x) - \pi_{12}(\nabla y(x))\|^2 \, dx \\ &\quad \leq 2\int_\Omega \|\nabla y(x) - \pi(\nabla y(x))\|^2 \, dx + 2\int_\Omega \|\pi(\nabla y(x)) - \pi_{12}(\nabla y(x))\|^2 \, dx \\ &\quad \leq 2\int_\Omega \|\nabla y(x) - \pi(\nabla y(x))\|^2 \, dx + 8(2\eta_1^2 + \eta_2^2)\operatorname{meas}\Omega_3 \\ &\quad \leq C\left[\mathcal{E}(y)^{\frac{1}{2}} + \mathcal{E}(y)\right], \end{aligned}$$

completing the proof. $\square$

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

Theorem 5.1. *There exists a constant $C > 0$ such that*

$$\int_\Omega \|\nabla y(x) - \Pi(\nabla y(x))\|^2 \, dx \leq C\left[\mathcal{E}(y)^{\frac{1}{2}} + \mathcal{E}(y)\right], \qquad \forall y \in W_\lambda^\phi.$$

Proof. For any $w \in \mathbb{R}^3$ such that $w \cdot n = 0$, we have

$$\Pi(F)w = F_0 w = F_1 w = \nabla y_\lambda(x) w, \qquad \forall F \in \mathbb{R}^{3\times 3}, \text{ for almost all } x \in \Omega.$$

Thus, it follows from (5.1) that

$$\begin{aligned} [\Theta(F) - I]\, F_0 w &= [\Theta(F) - I]\, \Pi(F) w = [\pi_{12}(F) - \nabla y_\lambda(x)]\, w \\ &= [\pi_{12}(F) - \pi(F)]\, w + [\pi(F) - \nabla y_\lambda(x)]\, w, \\ &\qquad \forall F \in \mathbb{R}^{3\times 3}, \text{ for almost all } x \in \Omega. \end{aligned}$$

We can then apply the triangle inequality to the above identity with $F = \nabla y(x)$ for any $y \in W_\lambda^\phi$ and $x \in \Omega$, and estimate the two terms by (5.2) and Lemma 4.2 to obtain

$$\int_\Omega |[\Theta(\nabla y(x)) - I]\, F_0 w|^2 \, dx$$

$$
\begin{aligned}
&\leq 2 \int_{\Omega} \left|[\pi_{12}(\nabla y(x)) - \pi\left(\nabla y(x)\right)] w\right|^2 dx \\
&\quad +2 \int_{\Omega} \left| \left[\pi\left(\nabla y(x)\right) - \nabla y_{\lambda}(x)\right] w\right|^2 dx \\
&\leq C\mathcal{E}(y)^{\frac{1}{2}}.
\end{aligned} \tag{5.3}
$$

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 $m = F_0 w_1 \times F_0 w_2$. Since

$$
Qm = QF_0w_1 \times QF_0w_2, \qquad \forall Q \in \mathrm{SO}(3),
$$

we have for all $F \in \mathbb{R}^{3\times 3}$ that

$$
\begin{aligned}
[\Theta(F) - I]\, m &= \{\Theta\left(F\right) F_0 w_1 \times \Theta\left(F\right) F_0 w_2\} - \{F_0 w_1 \times F_0 w_2\} \\
&= \{[\Theta\left(F\right) - I]\, F_0 w_1 \times \Theta\left(F\right) F_0 w_2\} - \{F_0 w_1 \times [I - \Theta\left(F\right)]\, F_0 w_2\}.
\end{aligned}
$$

This, together with (5.3), leads to

$$
\int_{\Omega} \left|[\Theta\left(\nabla y(x)\right) - I]\, m\right|^2 dx \leq C\mathcal{E}(y)^{\frac{1}{2}}. \tag{5.4}
$$

Now $\{F_0 w_1, F_0 w_2, m\}$ is a basis for $\mathbb{R}^3$, so we have from (5.3) and (5.4) that

$$
\int_{\Omega} \left\|[\Theta\left(\nabla y(x)\right) - I]\right\|^2 dx \leq C\mathcal{E}(y)^{\frac{1}{2}}. \tag{5.5}
$$

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

$$
\begin{aligned}
F - \Pi(F) &= [F - \pi_{12}(F)] + [\pi_{12}(F) - \Pi(F)] \\
&= [F - \pi_{12}(F)] + [\Theta(F) - I]\, \Pi(F), \qquad \forall F \in \mathbb{R}^{3\times 3},
\end{aligned}
$$

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

For any subset $\omega \subset \Omega$, $\rho > 0$, and $y \in W_{\lambda}^{\phi}$, we define the sets

$$
\begin{aligned}
\omega_{\rho}^{0}(y) &= \{x \in \omega : \Pi(\nabla y(x)) = F_0 \text{ and } \|F_0 - \nabla y(x)\| < \rho\}, \\
\omega_{\rho}^{1}(y) &= \{x \in \omega : \Pi(\nabla y(x)) = F_1 \text{ and } \|F_1 - \nabla y(x)\| < \rho\}
\end{aligned}
$$

and the mean value of λ on ω by

$$
\tilde{\lambda}_{\omega} = \frac{1}{\operatorname{meas}\omega} \int_{\omega} \lambda(x \cdot n)\, dx.
$$

The following theorem gives an estimate for the approximation of volume fractions. It states that for any energy minimizing sequence $\{y_k\}$ in W_{λ}^{ϕ} and for almost all $x \in \Omega$, the volume fraction that $\nabla y_k(x)$ is near F_0 converges to $1-\lambda(x\cdot n)$ and the volume fraction that $\nabla y_k(x)$ is near F_1 converges to $\lambda(x\cdot n)$.

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

$$\operatorname{meas}\left(\omega-\{\omega_\rho^0(y)\cup\omega_\rho^1(y)\}\right)\le C\left[\mathcal{E}(y)^{\frac{1}{2}}+\mathcal{E}(y)\right] \tag{5.6}$$

and

$$\left|\frac{\operatorname{meas}\omega_\rho^0(y)}{\operatorname{meas}\omega}-(1-\tilde{\lambda}_\omega)\right|+\left|\frac{\operatorname{meas}\omega_\rho^1(y)}{\operatorname{meas}\omega}-\tilde{\lambda}_\omega\right|\le C\left[\mathcal{E}(y)^{\frac{1}{8}}+\mathcal{E}(y)\right] \tag{5.7}$$

for any $y\in W_\lambda^\phi$.

Proof. Fix $y\in W_\lambda^\phi$. We have by the definition of $\omega_\rho^0\equiv\omega_\rho^0(y)$ and $\omega_\rho^1\equiv\omega_\rho^1(y)$ that

$$\begin{aligned}
&\operatorname{meas}\left(\omega-\{\omega_\rho^0\cup\omega_\rho^1\}\right)\\
&\quad\le\frac{1}{\rho}\int_{\omega-\{\omega_\rho^0\cup\omega_\rho^1\}}\|\Pi\left(\nabla y(x)\right)-\nabla y(x)\|dx\\
&\quad\le\frac{\left[\operatorname{meas}\left(\omega-\{\omega_\rho^0\cup\omega_\rho^1\}\right)\right]^{\frac{1}{2}}}{\rho}\left[\int_\Omega\|\Pi\left(\nabla y(x)\right)-\nabla y(x)\|^2\,dx\right]^{\frac{1}{2}}.
\end{aligned}$$

Consequently, we have

$$\operatorname{meas}\left(\omega-\{\omega_\rho^0\cup\omega_\rho^1\}\right)\le\frac{1}{\rho^2}\left[\int_\Omega\|\Pi\left(\nabla y(x)\right)-\nabla y(x)\|^2\,dx\right],$$

which together with Theorem 5.1 implies (5.6).

We have by (2.9) that

$$\begin{aligned}
&\left[\operatorname{meas}\omega_\rho^0-(1-\tilde{\lambda}_\omega)\operatorname{meas}\omega\right]F_0+\left[\operatorname{meas}\omega_\rho^1-\tilde{\lambda}_\omega\operatorname{meas}\omega\right]F_1\\
&\qquad=\int_\omega\left[\Pi\left(\nabla y(x)\right)-\nabla y_\lambda(x)\right]dx-\int_{\omega-\{\omega_\rho^0\cup\omega_\rho^1\}}\Pi\left(\nabla y(x)\right)dx.
\end{aligned}\tag{5.8}$$

By the triangle inequality, the Cauchy-Schwarz inequality, Theorem 5.1, and Theorem 4.3, we have that

$$\begin{aligned}
&\left\|\int_\omega\left[\Pi\left(\nabla y(x)\right)-\nabla y_\lambda(x)\right]dx\right\|\\
&\quad\le\left\|\int_\omega\left[\Pi\left(\nabla y(x)\right)-\nabla y(x)\right]dx\right\|+\left\|\int_\omega\left[\nabla y(x)-\nabla y_\lambda(x)\right]dx\right\|
\end{aligned}$$

$$
\begin{aligned}
&\le (\operatorname{meas}\omega)^{\frac{1}{2}}\left[\int_\Omega \|\Pi(\nabla y(x)) - \nabla y(x)\|^2\, dx\right]^{\frac{1}{2}} + \left\|\int_\omega [\nabla y(x) - \nabla y_\lambda(x)]\, dx\right\| \\
&\le C\left[\mathcal{E}(y)^{\frac{1}{8}} + \mathcal{E}(y)^{\frac{1}{2}}\right]. \qquad (5.9)
\end{aligned}
$$

We also have by (5.6) that

$$
\begin{aligned}
\left\|\int_{\omega - \{\omega_\rho^0 \cup \omega_\rho^1\}} \Pi(\nabla y(x))\, dx\right\| &\le C\operatorname{meas}\left(\omega - \{\omega_\rho^0 \cup \omega_\rho^1\}\right) \\
&\le C\left[\mathcal{E}(y)^{\frac{1}{2}} + \mathcal{E}(y)\right]. \qquad (5.10)
\end{aligned}
$$

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

$$
\|f\|_{\mathcal{V}}^2 = \int_\Omega \left[\operatorname*{ess\,sup}_{F\in\mathbb{R}^{3\times 3}} \|\nabla_F f(x,F)\|\right]^2 dx + \|G_f\|_{W^{1,2}(\Omega)}^2 < \infty, \qquad (5.11)
$$

where

$$
G_f(x) = f(x, F_1) - f(x, F_0), \qquad x \in \Omega.
$$

Functions in the space $\mathcal{V}$ represent thermodynamic variables of the underlying crystal.

Theorem 5.3. *There exists a constant $C > 0$ such that*

$$
\begin{aligned}
&\left|\int_\Omega \{f(x, \nabla y(x)) - [(1-\lambda(x\cdot n))f(x,F_0) + \lambda(x\cdot n)f(x,F_1)]\}\, dx\right| \\
&\qquad \le C\|f\|_{\mathcal{V}}\left[\mathcal{E}(y)^{\frac{1}{4}} + \mathcal{E}(y)^{\frac{1}{2}}\right], \quad \forall y \in W_\lambda^\phi,\ \forall f \in \mathcal{V}. \qquad (5.12)
\end{aligned}
$$

Proof. We have the decomposition

$$
\begin{aligned}
&\int_\Omega \{f(x, \nabla y(x)) - [(1-\lambda(x\cdot n))f(x,F_0) + \lambda(x\cdot n)f(x,F_1)]\}\, dx \\
&\quad = \int_\Omega [f(x, \nabla y(x)) - f(x, \Pi(\nabla y(x)))]\, dx \\
&\qquad + \int_\Omega \{f(x, \Pi(\nabla y(x))) - [(1-\lambda(x\cdot n))f(x,F_0) + \lambda(x\cdot n)f(x,F_1)]\}\, dx \\
&\quad = \mathcal{J}_1 + \mathcal{J}_2. \qquad (5.13)
\end{aligned}
$$

The first term $\mathcal{J}_1$ can be estimated by Theorem 5.1 as follows:

$$
\begin{aligned}
|\mathcal{J}_1| &\le \int_\Omega \left[\operatorname*{ess\,sup}_{F\in\mathbb{R}^{3\times3}} \|\nabla_F f(x,F)\|\right] \|\nabla y(x) - \Pi\left(\nabla y(x)\right)\| \, dx \\
&\le \left\{\int_\Omega \left[\operatorname*{ess\,sup}_{F\in\mathbb{R}^{3\times3}} \|\nabla_F f(x,F)\|\right]^2 dx\right\}^{\frac{1}{2}} \left[\int_\Omega \|\nabla y(x) - \Pi\left(\nabla y(x)\right)\|^2 \, dx\right]^{\frac{1}{2}} \\
&\le C\,\|f\|_{\mathcal{V}} \left[\mathcal{E}(y)^{\frac{1}{4}} + \mathcal{E}(y)^{\frac{1}{2}}\right]. \qquad (5.14)
\end{aligned}
$$

By (2.3) and the definition of $\Pi : \mathbb{R}^{3\times3} \to \{F_0, F_1\}$, we have the identity

$$
\begin{aligned}
&f\left(x, \Pi(F)\right) - \left[(1-\lambda(x\cdot n)) f(x,F_0) + \lambda(x\cdot n) f(x,F_1)\right] \\
&\quad = \tfrac{1}{|a|^2}\left\{a\cdot\left[\Pi(F) - \nabla y_\lambda(x)\right] n\right\} G_f(x), \\
&\qquad \forall F\in\mathbb{R}^{3\times3}, \text{ for almost all } x\in\Omega,
\end{aligned}
$$

leading to

$$
\begin{aligned}
\mathcal{J}_2 &= \int_\Omega \{f\left(x, \Pi\left(\nabla y(x)\right)\right) \\
&\qquad - \left[(1-\lambda(x\cdot n)) f(x,F_0) + \lambda(x\cdot n) f(x,F_1)\right]\} \, dx \\
&= \frac{1}{|a|^2}\int_\Omega \left\{a\cdot\left[\Pi\left(\nabla y(x)\right) - \nabla y_\lambda(x)\right] n\right\} G_f(x)\, dx \\
&= \frac{1}{|a|^2}\int_\Omega \left\{a\cdot\left[\Pi\left(\nabla y(x)\right) - \nabla y(x)\right] n\right\} G_f(x)\, dx \\
&\qquad + \frac{1}{|a|^2}\int_\Omega \left\{a\cdot\left[\nabla y(x) - \nabla y_\lambda(x)\right] n\right\} G_f(x)\, dx \\
&= \frac{1}{|a|^2}\int_\Omega \left\{a\cdot\left[\Pi\left(\nabla y(x)\right) - \nabla y(x)\right] n\right\} G_f(x)\, dx \\
&\qquad - \frac{1}{|a|^2}\int_\Omega \left\{a\cdot\left[y(x) - y_\lambda(x)\right]\right\} \left\{\nabla G_f(x)\cdot n\right\} \, dx,
\end{aligned}
$$

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

$$
\begin{aligned}
|\mathcal{J}_2| &\le C\left\{\int_\Omega \left[|\nabla G_f(x)\cdot n|^2 + G_f(x)^2\right] dx\right\}^{\frac{1}{2}} \left[\mathcal{E}(y)^{\frac{1}{4}} + \mathcal{E}(y)^{\frac{1}{2}}\right] \\
&\le C\,\|f\|_{\mathcal{V}} \left[\mathcal{E}(y)^{\frac{1}{4}} + \mathcal{E}(y)^{\frac{1}{2}}\right]. \qquad (5.15)
\end{aligned}
$$

We finally obtain the inequality (5.12) from (5.13) – (5.15). $\square$

6. Finite Element Approximations

For simplicity we assume in what follows that the reference configuration $\Omega \subset \mathbb{R}^3$ is a polygonal domain. For a fixed positive number h_0, let τ_h, $0 < h \leq h_0$, be a family of tetrahedral finite element meshes of Ω, such that $\bar{\Omega} = \cup_{T \in \tau_h} T$, where h is the maximum diameter of any tetrahedron T in the mesh τ_h. We shall assume as usual that any face of any tetrahedron in a mesh τ_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 τ_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 τ_h [11, 29].

We can define the interpolation operator $\mathcal{I}_h : C(\bar{\Omega}; \mathbb{R}^3) \to \mathcal{A}_h$ for each $h \in (0, h_0]$ which interpolates the values at the vertices of the tetrahedral elements T of τ_h. We will assume that the family τ_h of finite meshes is quasi-regular [11, 29], so that

$$\operatorname{ess\,sup}_{x\in\Omega} \|\nabla \mathcal{I}_h y(x)\| \leq C \operatorname{ess\,sup}_{x\in\Omega} \|\nabla y(x)\| \tag{6.1}$$

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 $y \in C(\bar{\Omega}; \mathbb{R}^3)$ that

$$\mathcal{I}_h y(x)|_T = y(x)|_T \text{ for any } T \in \tau_h \text{ such that } y(x)|_T \in \left\{P^1(T)\right\}^3, \tag{6.2}$$

for $h \in (0, h_0]$, where $\left\{P^1(T)\right\}^3 \equiv P^1(T) \times P^1(T) \times P^1(T)$ 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 (2.13), we define the finite element deformation $y_{\lambda h} \in \mathcal{A}_h$ by

$$y_{\lambda h} = \mathcal{I}_h y_\lambda(x), \qquad x \in \bar{\Omega},$$

and define the finite element space of admissible deformations

$$\mathcal{A}_{\lambda h} = \left\{ y_h \in \mathcal{A}_h : y_h(x) = y_{\lambda h}(x),\ \forall x \in \partial\Omega \right\}.$$

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, 29] that

$$\|y_\lambda - y_{\lambda h}\|_{L^\infty(\partial\Omega; \mathbf{R}^3)} \leq Ch \|y_\lambda\|_{W^{1,\infty}(\partial\Omega; \mathbf{R}^3)}.$$

In what follows we shall use the result that $y_{\lambda h} \in \mathcal{A}_{\lambda h}$, $0 < h \leq h_0$, satisfies the condition

$$\|y_\lambda - y_{\lambda h}\|_{L^2(\partial\Omega;\mathbf{R}^3)} \leq Ch. \tag{6.3}$$

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 elastic energy $\mathcal{E}$ on the space $\mathcal{A}_{\lambda h}$.

Theorem 6.1. *There exists $y_h \in \mathcal{A}_{\lambda h}$ for each $h \in (0, h_0]$ such that*

$$\mathcal{E}(y_h) = \min_{z_h \in \mathcal{A}_{\lambda h}} \mathcal{E}(z_h) \leq Ch^{1/2}. \tag{6.4}$$

Proof. The existence of $y_h \in \mathcal{A}_{\lambda h}$ can be proved by the same argument as in the proof of Theorem 6.1 in [22]. To prove the inequality in (6.4) we follow the argument given in [23] to show that $\hat{y}_h = \mathcal{I}_h \hat{u}_\gamma \in \mathcal{A}_{\lambda h}$ with $\gamma = h^{1/2}$ satisfies

$$\mathcal{E}(\hat{y}_h) \leq Ch^{1/2}.$$

□

We next give a series of estimates for the finite element approximation of the deformation y_λ by deformation $y_h \in \mathcal{A}_{\lambda h}$. These estimates are parallel to those for the deformations $y \in W_\lambda^\phi$ 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*

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

Proof. Fix $y_h \in \mathcal{A}_{\lambda h}$ 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

$$\int_\Omega |[\pi(\nabla y_h(x)) - \nabla y_\lambda(x)]\, w|^2 \, dx$$
$$\leq C\left[\mathcal{E}(y_h)^{\frac{1}{2}} + \|y_\lambda - y_{\lambda h}\|_{L^2(\Omega;\mathbb{R}^3)}\right]. \tag{6.6}$$

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

$$\begin{aligned}
&\int_\Omega |[\pi(\nabla y_h(x)) - \nabla y_\lambda(x)]\, w|^2\, dx \\
&\quad = 2F_0 w \cdot \int_\Omega [\nabla y_\lambda(x) - \pi(\nabla y_h(x))]\, w\, dx \\
&\quad = 2F_0 w \cdot \left\{ \int_\Omega [\nabla y_\lambda(x) - \nabla y_h(x)]\, dx + \int_\Omega [\nabla y_h(x) - \pi(\nabla y_h(x))]\, dx \right\} w \\
&\quad = 2F_0 w \cdot \left\{ \int_{\partial\Omega} [y_\lambda(x) - y_{\lambda h}(x)] \otimes \nu\, dS + \int_\Omega [\nabla y_h(x) - \pi(\nabla y_h(x))]\, dx \right\} w
\end{aligned}$$

This, together with Lemma 4.1 and the Cauchy-Schwarz inequality, leads to (6.6). $\square$

Theorem 6.3. *We have*

$$\begin{aligned}
\int_\Omega |y_h(x) - y_\lambda(x)|^2\, dx &\le C\left[\mathcal{E}(y_h)^{\frac{1}{2}} + \mathcal{E}(y_h)\right] \\
&\quad + \left[\|y_\lambda - y_{\lambda h}\|_{L^2(\partial\Omega;\mathbb{R}^3)} + \|y_\lambda - y_{\lambda h}\|^2_{L^2(\partial\Omega;\mathbb{R}^3)}\right], \qquad \forall y_h \in \mathcal{A}_{\lambda h}.
\end{aligned}$$

Proof. Fix $y_h \in \mathcal{A}_h$. 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 (4.6) and Theorem (6.2). $\square$

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*

$$\begin{aligned}
\left\| \int_\omega [\nabla y_h(x) - \nabla y_\lambda(x)]\, dx \right\| &\le C\left[\mathcal{E}(y_h)^{\frac{1}{8}} + \mathcal{E}(y_h)\right] \\
&\quad + C\left[\|y_\lambda - y_{\lambda h}\|^{\frac{1}{4}}_{L^2(\partial\Omega;\mathbb{R}^3)} + \|y_\lambda - y_{\lambda h}\|_{L^2(\partial\Omega;\mathbb{R}^3)}\right], \qquad \forall y_h \in \mathcal{A}_{\lambda h}.
\end{aligned}$$

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 (6.6).

Theorem 6.5. *We have*

$$\int_\Omega \|\nabla y_h(x) - \Pi(\nabla y_h(x))\|^2\, dx$$

$$\leq C\left[\mathcal{E}(y_h)^{\frac{1}{2}} + \mathcal{E}(y_h) + \|y_\lambda - y_{\lambda h}\|_{L^2(\partial\Omega;\mathbb{R}^3)}\right], \qquad \forall y_h \in \mathcal{A}_{\lambda h}.$$

Recall that $\tilde{\lambda}_\omega$ is the average of λ on ω. 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*

$$\operatorname{meas}\left(\omega - \{\omega_\rho^0(y_h) \cup \omega_\rho^1(y_h)\}\right) \leq C\left[\mathcal{E}(y_h)^{\frac{1}{2}} + \mathcal{E}(y_h) + \|y_\lambda - y_{\lambda h}\|_{L^2(\partial\Omega;\mathbb{R}^3)}\right]$$

and

$$\begin{aligned}&\left|\frac{\operatorname{meas}\omega_\rho^0(y_h)}{\operatorname{meas}\omega} - (1-\tilde{\lambda}_\omega)\right| + \left|\frac{\operatorname{meas}\omega_\rho^1(y_h)}{\operatorname{meas}\omega} - \tilde{\lambda}_\omega\right| \\ &\qquad \leq C\left[\mathcal{E}(y_h)^{\frac{1}{8}} + \mathcal{E}(y_h) + \|y_\lambda - y_{\lambda h}\|_{L^2(\partial\Omega;\mathbb{R}^3)}^{\frac{1}{4}} + \|y_\lambda - y_{\lambda h}\|_{L^2(\partial\Omega;\mathbb{R}^3)}\right]\end{aligned}$$

for any $y_h \in \mathcal{A}_{\lambda h}$.

Recall that the Sobolev space $\mathcal{V}$ consists of all functions $f \in L^2(\Omega \times \mathbb{R}^{3\times 3})$ that satisfy (5.11). 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*

$$\begin{aligned}&\left|\int_\Omega \{f(x, \nabla y_h(x)) - [(1-\lambda(x\cdot n))f(x,F_0) + \lambda(x\cdot n)f(x,F_1)]\}\,dx\right| \\ &\leq C\|f\|_{\mathcal{V}}\left[\mathcal{E}(y_h)^{\frac{1}{4}} + \mathcal{E}(y_h)^{\frac{1}{2}} + \|y_\lambda - y_{\lambda h}\|_{L^2(\partial\Omega;\mathbb{R}^3)}^{\frac{1}{2}} + \|y_\lambda - y_{\lambda h}\|_{L^2(\partial\Omega;\mathbb{R}^3)}\right]\end{aligned}$$

for all $y_h \in \mathcal{A}_{\lambda h}$ and all $f \in \mathcal{V}$.

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 [23]. 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

$$\mathcal{E}(y_h) \leq \alpha \inf_{z_h \in \mathcal{A}_{\lambda h}} \mathcal{E}(z_h) \tag{6.7}$$

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

It follows directly from the previous theorems in this section and (6.3) that we can obtain the following error estimates for a quasi-optimal finite element deformation $y_h \in \mathcal{A}_{\lambda h}$.

Corollary 6.1. *We have*

$$\int_\Omega |[\nabla y_h(x) - \nabla y_\lambda(x)]\, w|^2 \, dx \le C h^{\frac{1}{4}}$$

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* (6.7).

Corollary 6.2. *We have*

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

for any $y_h \in \mathcal{A}_{\lambda h}$ *which satisfies the quasi-optimality condition* (6.7).

Corollary 6.3. *If* $\omega \subset \Omega$ *is a Lipschitz domain, then there exists a positive constant* C, *independent of* h, *such that*

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

for any $y_h \in \mathcal{A}_{\lambda h}$ *which satisfies the quasi-optimality condition* (6.7).

Corollary 6.4. *We have*

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

for any $y_h \in \mathcal{A}_{\lambda h}$ *which satisfies the quasi-optimality condition* (6.7).

Corollary 6.5. *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*

$$meas\left(\omega - \left\{\omega_\rho^0(y_h) \cup \omega_\rho^1(y_h)\right\}\right) \le C h^{\frac{1}{4}}$$

and

$$\left| \frac{\operatorname{meas} \omega_\rho^0(y_h)}{\operatorname{meas} \omega} - (1 - \tilde{\lambda}_\omega) \right| + \left| \frac{\operatorname{meas} \omega_\rho^1(y_h)}{\operatorname{meas} \omega} - \tilde{\lambda}_\omega \right| \le C h^{\frac{1}{16}}$$

for any $y_h \in \mathcal{A}_{\lambda h}$ *which satisfies the quasi-optimality condition* (6.7).

Corollary 6.6. *We have*

$$\left| \int_\Omega \{ f(x, \nabla y_h(x)) - [(1 - \lambda(x \cdot n)) f(x, F_0) + \lambda(x \cdot n) f(x, F_1)] \} \, dx \right|$$

$$\leq C\|f\|_{\mathcal{V}} h^{\frac{1}{8}}$$

for any $f \in \mathcal{V}$ *and any* $y_h \in \mathcal{A}_{\lambda h}$ *which satisfies the quasi-optimality condition* (6.7).

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Bo Li, Department of Mathematics, University of California, Los Angeles, 405 Hilgard Avenue, Los Angeles, CA 90095-1555, U.S.A.

E-mail address: `bli@ucla.umn.edu`

Mitchell Luskin, School of Mathematics, University of Minnesota, 206 Church Street, S.E., Minneapolis, MN 55455, U.S.A.

E-mail address: `luskin@math.umn.edu`