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APPROXIMATION OF A MARTENSITIC LAMINATE WITH VARYING VOLUME FRACTIONS*

Bo Li[1] and Mitchell Luskin[2]

Abstract. We give results for the approximation of a laminate with varying volume fractions for multi-well energy minimization problems modeling martensitic crystals that can undergo either an orthorhombic to monoclinic or a cubic to tetragonal transformation. 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.

Résumé. Nous considérons des problèmes de minimisation d'énergie avec de multiples puits de potentiel. De tels problèmes modélisent, pour des cristaux martensitiques, des transitions de phase d'un réseau orthorhombique à monoclinique, ou d'un réseau cubique à tétragonal, par exemple.
Des résultats d'approximation des structures laminaires correspondantes, avec fractions volumiques variables, sont donnés. Des suites minimisantes, avec déformations compatibles avec les conditions au bord, sont construites et permettent l'obtention de plusieurs estimations d'erreur concernant l'approximation de la déformation macroscopique limite en fonction de l'énergie élastique.
Finalement, nous décrivons des résultats concernant l'approximation par éléments finis de la structure laminaire avec fractions volumiques variables.

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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 $\mathrm{SO}(3)U_1 \cup \cdots \cup \mathrm{SO}(3)U_N$ where $U_1, \cdots, U_N$ for $N > 1$ are symmetry-related transformation strains representing distinct variants of the martensite and 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 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

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[1]Department of Mathematics, University of California, Los Angeles, 405 Hilgard Avenue, Los Angeles, CA 90095-1555, USA. e-mail: `bli@math.ucla.edu`

[2]School of Mathematics, University of Minnesota, 206 Church Street, S.E., Minneapolis, MN 55455, USA. e-mail: `luskin@math.umn.edu`

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 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 is 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 [22]. For constant volume fractions, an analysis for a nonconforming finite element approximation was given in [23].

A theory of numerical analysis for the microstructure in nonconvex variational problems was developed in [12, 13], and extended in [7–9, 17, 26]. Analyses of the approximation of relaxed variational problems have been given in [6, 16, 27–29, 31]. We refer to the recent article [24] 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 Sections 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 Section 6, we give error estimates for the approximation by quasi-optimal finite element deformations.

2. Energy minimization problems

In this section, we give a summary of the properties and known results for the orthorhombic to monoclinic and cubic to tetragonal martensitic transformations [2, 3, 24].

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

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

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 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 connected, bounded, open set 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 $\phi : \mathbb{R}^{3\times 3} \to \mathbb{R}$, where $\mathbb{R}^{3\times 3}$ denotes the set of all 3×3 real matrices. The elastic energy of a deformation $y : \Omega \to \mathbb{R}^3$ is given by

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

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

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

We assume that the energy density ϕ is minimized on the energy wells

$$\mathcal{U}_i = \mathrm{SO}(3) U_i, \quad i \in K,$$

where $K = \{1, 2\}$ for the orthorhombic to monoclinic transformation and $K = \{1, 2, 3\}$ for the cubic to tetragonal transformation. Thus, we may assume after adding a constant to the energy density that

$$\begin{aligned} \phi(F) \geq 0, &\qquad \forall F \in \mathbb{R}^{3\times 3}, \\ \phi(F) = 0 \quad \text{if and only if} &\quad F \in \mathcal{U} \equiv \cup \{\mathcal{U}_i : i \in K\}. \end{aligned} \tag{2.2}$$

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

$$\phi(F) \geq \kappa \|F - \pi(F)\|^2, \qquad \forall F \in \mathbb{R}^{3\times 3}, \tag{2.3}$$

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 easy to see that

$$\det F = d_1 d_2 d_3 > 0, \qquad \forall F \in \mathcal{U} \equiv \cup \{\mathcal{U}_i : i \in K\}, \tag{2.4}$$

for the orthorhombic to monoclinic transformation, and that

$$\det F = \eta_1^2 \eta_2 > 0, \qquad \forall F \in \mathcal{U} \equiv \cup \{\mathcal{U}_i : i \in K\}, \tag{2.5}$$

for the cubic to tetragonal transformation.

We note that every function in $W^{1,\infty}(\Omega)$ is equal almost everywhere to a unique Lipschitz continuous function defined on $\bar{\Omega}$ [1]. For simplicity in what follows, we shall consider only the Lipschitz continuous representatives of functions in $W^{1,\infty}(\Omega)$. Thus, we shall consider functions in $W^{1,\infty}(\Omega)$ to be Lipschitz continuous and defined everywhere, although the gradients of functions in $W^{1,\infty}(\Omega)$ can only be defined almost everywhere (denoted a.e.).

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 ∇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

$$F_1 - F_0 = a \otimes n \tag{2.6}$$

for some non-zero vector $a \in \mathbb{R}^3$. We next present a lemma that classifies all possible simple laminates formed by pairs of variants up to multiplication of rotations for the martensitic crystals in our discussion [2,3,24]. The lemma states that there is no rank-one connection between $\mathcal{U}_i$ and itself; and that for any $i, j \in K, i \neq j$, there are exactly two rank-one connections between $\mathcal{U}_i$ and $\mathcal{U}_j$.

Lemma 2.1. *(1) For each $i \in K$, there do not exist matrices $R_1 U_i$ and $R_2 U_i$ with distinct $R_1, R_2 \in SO(3)$ that are rank-one connected.*

(2) For any $i, j \in K, i \neq j$, there are exactly two distinct $Q \in SO(3)$ such that

$$QU_i - U_j = a \otimes n$$

for some $a, n \in \mathbb{R}^3, |n| = 1$, respectively.

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.

We shall also assume that $F_0, F_1 \in \mathcal{U}$ are rank-one connected as in (2.6), so

$$(1-\lambda)F_0 + \lambda F_1 = F_0 + \lambda a \otimes n, \qquad \lambda \in \mathbb{R}. \tag{2.7}$$

By Lemma 2.1, we can assume without loss of generality that $F_1 \in \mathcal{U}_1$ and $F_0 \in \mathcal{U}_2$, and we can 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. We note that it can be shown under the hypotheses of Lemma 2.1 that if $\lambda \neq 0$ and $\lambda \neq 1$ then [2,3,24]

$$(1-\lambda)F_0 + \lambda F_1 = F_0 + \lambda a \otimes n \notin \mathcal{U}.$$

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 $y \in W^{1,\infty}(\Omega, \mathbb{R}^3)$ be such that*

$$\nabla y(x) = (1-\lambda(x))F_0 + \lambda(x)F_1 \qquad a.e.\ x \in \Omega,$$

for the volume fraction $\lambda \in L^\infty(\Omega)$ satisfying $0 \leq \lambda(x) \leq 1$. We have that there exist unique $l \in W^{1,\infty}(\Omega)$ and $\hat{y} \in \mathbb{R}^3,\ \hat{y} \cdot a = 0$, such that

$$\begin{aligned} y(x) &= F_0 x + l(x)a + \hat{y}, \qquad && x \in \Omega, \\ \nabla l(x) &= \lambda(x) n && a.e.\ x \in \Omega. \end{aligned}$$

If $\tilde{\Omega} \subset \Omega$ is a subdomain with the property that $\{\, x \in \tilde{\Omega} : x \cdot n = \xi \,\}$ is connected for each $\xi \in \mathbb{R}$, then there exist $\tilde{l} \in W^{1,\infty}(\mathbb{R})$ and $\tilde{\lambda} \in L^\infty(\mathbb{R})$ such that

$$\begin{aligned} l(x) &= \tilde{l}(x \cdot n), \qquad && x \in \tilde{\Omega}, \\ \lambda(x) &= \tilde{\lambda}(x \cdot n) && a.e.\ x \in \tilde{\Omega}, \\ \tilde{l}'(s) &= \tilde{\lambda}(s) && a.e.\ s \in \mathbb{R}. \end{aligned}$$

Proof. The proof is identical to the proof of Proposition 1 in [2] for the case when λ is a characteristic function. It follows by noting that if $w \in \mathbb{R}^3,\ w \cdot a = 0$, then

$$\nabla \left[(y(x) - F_0 x) \cdot w \right] = 0 \qquad \text{a.e. } x \in \Omega.$$

$\square$

In this paper, we consider the minimization of the elastic energy (2.1) with respect to deformations $y \in W^\phi$ which are constrained by $y(x) = y_\lambda(x)$ for $x \in \partial\Omega$ where

$$\begin{aligned} y_\lambda(x) &= F_0 x + l(x)a, \qquad && x \in \Omega, \\ \nabla l(x) &= \lambda(x) n && \text{a.e. } x \in \Omega, \end{aligned} \tag{2.8}$$

and where $l \in W^{1,\infty}(\Omega)$ and $\lambda \in L^\infty(\Omega)$ satisfies $0 \leq \lambda(x) \leq 1$. Our energy minimization problem is to minimize the energy (2.1) in the set of admissible deformations defined by

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

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

$$y_\lambda(x) = F_0 x + \left[\int_0^{x \cdot n} \tilde{\lambda}(s) ds + \zeta \right] a, \qquad x \in \Omega, \tag{3.1}$$

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

We construct in two steps a family of deformations $\hat{u}_\gamma \in W^{1,\infty}(\mathbb{R}^3;\mathbb{R}^3)$, $\gamma \in (0,\gamma_0]$, 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 $\hat{u}_\gamma \in W^\phi_\lambda$, $\gamma \in (0,\gamma_0]$, by modifying u_γ 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

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

Define the piecewise constant function $\tilde{\lambda}_\gamma : \mathbb{R} \to \mathbb{R}$ by

$$\tilde{\lambda}_\gamma(s) = \lambda^{(i)}_\gamma \qquad \text{if } s \in I^{(i)}_\gamma,\ i \in \mathbb{Z},$$

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

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

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

$$\left| \int_I \left[\chi_\gamma(s) - \tilde{\lambda}(s)\right] ds \right| \le 2\gamma. \tag{3.2}$$

Define now

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

Obviously, $u_\gamma \in W^{1,\infty}(\mathbb{R}^3;\mathbb{R}^3)$. Moreover, we have by (2.6) that

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

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

$$|u_\gamma(x) - y_\lambda(x)| \le 2|a|\gamma, \qquad x \in \mathbb{R}^3. \tag{3.4}$$

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

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

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

$$\begin{array}{ll} 0 \le \psi_\gamma(x) \le 1, & x \in \Omega, \\ \psi_\gamma(x) = 1, & x \in \Omega_\gamma, \\ \psi_\gamma(x) = 0, & x \in \partial\Omega, \\ |\nabla \psi_\gamma(x)| \le (\upsilon\gamma)^{-1} & \text{a.e. } x \in \Omega. \end{array} \tag{3.5}$$

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

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

It is easy to verify that

$$\nabla \hat{u}_\gamma(x) = [u_\gamma(x) - y_\lambda(x)] \otimes \nabla \psi_\gamma(x) + \psi_\gamma(x) \nabla u_\gamma(x) + (1 - \psi_\gamma(x))\, \nabla y_\lambda(x) \tag{3.6}$$

for almost all $x \in \Omega$. By (3.3) – (3.6), we have for all $\gamma \in (0, \gamma_0]$ that

$$\|\nabla \hat{u}_\gamma(x)\| \le C \qquad \text{a.e. } x \in \Omega, \tag{3.7}$$

where C here and below is a constant independent of γ, and that

$$\nabla \hat{u}_\gamma(x) \in \{F_0, F_1\} \qquad \text{a.e. } x \in \Omega_\gamma. \tag{3.8}$$

Therefore, $\hat{u}_\gamma \in W^\phi_\lambda$ for any $\gamma \in (0, \gamma_0]$ by the continuity of the energy density ϕ. Moreover, $\operatorname{meas}(\Omega \backslash \Omega_\gamma) = \mathrm{O}(\gamma)$ as $\gamma \to 0$ since Ω is a Lipschitz domain, so by (3.7), (3.8), and (2.2) we have

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

By the rank-one connection (2.6), 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 (2.4) and (2.5)) 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

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

where

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

Thus,

$$\det\left[\psi_\gamma(x) \nabla u_\gamma(x) + (1 - \psi_\gamma(x)) \nabla y_\lambda(x)\right] = \det F_0 = \det F_1 > 0 \qquad \text{a.e. } x \in \Omega.$$

Choosing $\upsilon > 0$ large enough, we can therefore conclude from (3.4) – (3.6) that

$$\det \nabla \hat{u}_\gamma(x) \geq C > 0 \qquad \text{a.e. } x \in \Omega,\ \forall \gamma \in (0, \gamma_0]. \tag{3.9}$$

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 corollary.

Corollary 3.1. *We 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 also suppose that there exist $\tilde{\lambda}_i \in L^\infty(\mathbb{R})$ for $i = 1, \ldots, M$ such that

$$\lambda(x) = \tilde{\lambda}_i(x \cdot n) \qquad a.e.\ x \in \Omega_i.$$

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

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

Proof. We construct deformations $\hat{u}_{i\gamma}$ defined on $\bar{\Omega}_i$ for $i = 1, \ldots, M$ such that

$$\hat{u}_{i\gamma}(x) = y_\lambda(x), \qquad x \in \partial\Omega_i,$$

by the technique of Theorem 3.1 applied to Ω_i, and we then construct $\hat{u}_\gamma \in W^\phi_\lambda$ by

$$\hat{u}_\gamma(x) = \hat{u}_{i\gamma}(x), \qquad x \in \Omega_i,\ i = 1, \ldots, M.$$

□

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 follows immediately from the growth rate of the energy density around the energy wells (2.3).

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*

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

for all $w \in \mathbb{R}^3$ satisfying $w \cdot n = 0$ and $|w| = 1$.

Proof. We first prove the lemma for the orthorhombic to monoclinic transformation. We have that

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

Fix $w \in \mathbb{R}^3$ with $w \cdot n = 0$ and $|w| = 1$. By (2.6) and (2.7), we have that

$$\nabla y_\lambda(x) w = F_0 w = F_1 w \qquad \text{a.e. } x \in \Omega, \tag{4.1}$$

leading to

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

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

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

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

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

Next, we prove the lemma for the cubic to tetragonal transformation. Recall that in this case the normal n is given as $n = (e_1 + e_2)/\sqrt{2}$. Set

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

We can easily verify 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 $\{w \in \mathbb{R}^3 : w \cdot n = 0\}$. □

We next give 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.

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 $|w| = 1$. It follows from the Poincaré inequality [25, 34] that

$$\int_\Omega |z(x)|^2 \, dx \le C \left[\int_{\partial\Omega} |z(x)|^2 \, dS + \int_\Omega |\nabla z(x) w|^2 \, dx\right], \tag{4.5}$$

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 obtain the desired result by Theorem 4.1 with $w \in \mathbb{R}^3$ so chosen that $w \cdot n = 0$ and $|w| = 1$. $\square$

The next corollary states that the *infimum* of the energy is not generally attained on W_λ^ϕ.

Corollary 4.1. *There does not exist $y \in W_\lambda^\phi$ such that $\mathcal{E}(y) = 0$ if*

$$\text{meas}\{\, x \in \Omega : 0 < \lambda(x) < 1 \,\} > 0. \tag{4.6}$$

Proof. We assume that there exist $y \in W_\lambda^\phi$ such that $\mathcal{E}(y) = 0$. By Theorem 4.2, we have that $y = y_\lambda$. It follows from (4.6) that there is an integer $p \ge 3$ such that the set

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

has positive measure. On the other hand, the set

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

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

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

$\square$

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*

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

Proof. We have from the divergence theorem and the Cauchy-Schwarz inequality that

$$\begin{aligned} \left\| \int_\omega [\nabla y(x) - \nabla y_\lambda(x)] \, dx \right\| &= \left\| \int_{\partial\omega} [y(x) - y_\lambda(x)] \otimes \nu \, dS \right\| \\ &\leq \int_{\partial\omega} |y(x) - y_\lambda(x)| \, dS \leq (\text{meas}_2\, \partial\omega)^{\frac{1}{2}} \left(\int_{\partial\omega} |y(x) - y_\lambda(x)|^2 \, dS \right)^{\frac{1}{2}}, \end{aligned} \tag{4.7}$$

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

$$\begin{aligned} \int_{\partial\omega} \left| y(x) - y_\lambda(x) \right|^2 dS &\leq C \left[\int_\omega |y(x) - y_\lambda(x)|^2 \, dx + \int_\omega \left| \nabla |y(x) - \nabla y_\lambda(x)|^2 \right| dx \right] \\ &\leq C \left[\int_\omega |y(x) - y_\lambda(x)|^2 \, dx + \int_\omega |y(x) - y_\lambda(x)| \|\nabla [y(x) - y_\lambda(x)] \| \, dx \right] \\ &\leq C \Bigg[\int_\Omega |y(x) - y_\lambda(x)|^2 \, dx + \left(\int_\Omega |y(x) - y_\lambda(x)|^2 \, dx \right)^{\frac{1}{2}} \left(\int_\Omega \|\nabla y(x) - \nabla y_\lambda(x)\|^2 \, dx \right)^{\frac{1}{2}} \Bigg]. \end{aligned} \tag{4.8}$$

We also have by the triangle inequality and Lemma 4.1 that

$$\begin{aligned} \left(\int_\Omega \|\nabla y(x) - \nabla y_\lambda(x)\|^2 \, dx \right)^{\frac{1}{2}} &\leq \left(\int_\Omega \|\nabla y(x) - \pi(\nabla y(x))\|^2 \, dx \right)^{\frac{1}{2}} + \left(\int_\Omega \|\pi(\nabla y(x)) - \nabla y_\lambda(x)\|^2 \, dx \right)^{\frac{1}{2}} \\ &\leq C \left[\mathcal{E}(y)^{\frac{1}{2}} + 1 \right]. \end{aligned} \tag{4.9}$$

Hence, we obtain from using the inequality of Theorem 4.2 and (4.9) in (4.8) that

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

which, together with (4.7), 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

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

We note that $\pi_{12} = \pi$ for the orthorhombic to monoclinic transformation. Next, we 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 identity

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

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. It is easy to check that

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

For a fixed $y \in W_\lambda^\phi$, we set

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

Since $e_3 \cdot n = 0$, it follows from Lemma 4.2 that

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

Consequently, we have by Lemma 4.1 that

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

completing the proof. ∎

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*

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

Proof. We have for any $w \in \mathbb{R}^3$ such that $w \cdot n = 0$ the identity

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

Hence, we obtain from (5.1) that

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

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

$$\int_\Omega |[\Theta(\nabla y(x)) - I]\, F_0 w|^2\, dx \le 2\int_\Omega |[\pi_{12}(\nabla y(x)) - \pi(\nabla y(x))]\, w|^2\, dx + 2\int_\Omega |[\pi(\nabla y(x)) - \nabla y_\lambda(x)]\, w|^2\, dx$$
$$\le C\mathcal{E}(y)^{\frac{1}{2}}. \tag{5.3}$$

We next fix $w_1 \in \mathbb{R}^3$ 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. We have for $m = F_0 w_1 \times F_0 w_2$ that

$$Qm = QF_0 w_1 \times QF_0 w_2, \qquad \forall Q \in \mathrm{SO}(3).$$

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

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

We obtain from the above inequality and (5.3) that

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

Since $\{F_0 w_1, F_0 w_2, m\}$ is a basis for $\mathbb{R}^3$, it follows from (5.3) and (5.4) that

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

The proof is completed 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 terms by Lemma 5.1 and (5.5). ☐

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 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 $\lambda(x)$. The statement of the theorem utilizes the subsets

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

which are defined for any subset $\omega \subset \Omega$, $\rho > 0$, and $y \in W_\lambda^\phi$. We also denote the mean value of λ on ω by

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

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

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

and

$$\left|\frac{\operatorname{meas}\omega_\rho^0(y)}{\operatorname{meas}\omega} - (1-\hat\lambda_\omega)\right| + \left|\frac{\operatorname{meas}\omega_\rho^1(y)}{\operatorname{meas}\omega} - \hat\lambda_\omega\right| \le C\left[\mathcal{E}(y)^{\frac18} + \mathcal{E}(y)\right], \qquad \forall y \in W_\lambda^\phi. \tag{5.7}$$

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

$$\begin{aligned}\operatorname{meas}\left(\omega - \{\omega_\rho^0 \cup \omega_\rho^1\}\right) &\le \frac{1}{\rho}\int_{\omega-\{\omega_\rho^0\cup\omega_\rho^1\}} \|\Pi(\nabla y(x)) - \nabla y(x)\|\,dx \\ &\le \frac{\left[\operatorname{meas}\left(\omega - \{\omega_\rho^0\cup\omega_\rho^1\}\right)\right]^{\frac12}}{\rho}\left[\int_\Omega \|\Pi(\nabla y(x)) - \nabla y(x)\|^2\,dx\right]^{\frac12}.\end{aligned}$$

Consequently, we have

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

which together with Theorem 5.1 implies (5.6).

We have by (2.7) that

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

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

$$\begin{aligned}\left\|\int_\omega \left[\Pi(\nabla y(x)) - \nabla y_\lambda(x)\right]\,dx\right\| &\le \left\|\int_\omega \left[\Pi(\nabla y(x)) - \nabla y(x)\right]\,dx\right\| + \left\|\int_\omega \left[\nabla y(x) - \nabla y_\lambda(x)\right]\,dx\right\| \\ &\le (\operatorname{meas}\omega)^{\frac12}\left[\int_\Omega \|\Pi(\nabla y(x)) - \nabla y(x)\|^2\,dx\right]^{\frac12} + \left\|\int_\omega \left[\nabla y(x) - \nabla y_\lambda(x)\right]\,dx\right\| \\ &\le C\left[\mathcal{E}(y)^{\frac18} + \mathcal{E}(y)^{\frac12}\right]. \end{aligned}\tag{5.9}$$

We also have by (5.6) that

$$\left\|\int_{\omega-\{\omega_\rho^0\cup\omega_\rho^1\}} \Pi(\nabla y(x))\,dx\right\| \le C\operatorname{meas}\left(\omega - \{\omega_\rho^0\cup\omega_\rho^1\}\right) \le C\left[\mathcal{E}(y)^{\frac12} + \mathcal{E}(y)\right]. \tag{5.10}$$

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

The final theorem in this section gives an estimate for nonlinear functions of the deformation gradient. The estimate utilizes the Sobolev space $\mathcal{V}$ of all functions $f \in L^2\left(\Omega \times \mathbb{R}^{3\times3}\right)$ such that

$$\|f\|_{\mathcal{V}}^2 = \int_\Omega \left[\operatorname*{ess\,sup}_{F\in\mathbb{R}^{3\times3}} \|\nabla_F f(x,F)\|\right]^2\,dx + \|G_f\|_{W^{1,2}(\Omega)}^2 < \infty,$$

where

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

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

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

$$\begin{aligned} &\left|\int_\Omega \{f(x, \nabla y(x)) - [(1-\lambda(x)) f(x, F_0) + \lambda(x) f(x, F_1)]\} \, dx\right| \\ &\quad \le C\|f\|_{\mathcal{V}} \left[\mathcal{E}(y)^{\frac{1}{4}} + \mathcal{E}(y)^{\frac{1}{2}}\right], \qquad \forall y \in W^\phi_\lambda, \ \forall f \in \mathcal{V}. \end{aligned} \tag{5.11}$$

Proof. We have the decomposition

$$\begin{aligned} &\int_\Omega \{f(x, \nabla y(x)) - [(1-\lambda(x)) f(x, F_0) + \lambda(x) f(x, F_1)]\} \, dx \\ &\quad = \int_\Omega [f(x, \nabla y(x)) - f(x, \Pi(\nabla y(x)))] \, dx \\ &\qquad + \int_\Omega \{f(x, \Pi(\nabla y(x))) - [(1-\lambda(x)) f(x, F_0) + \lambda(x) f(x, F_1)]\} \, dx \\ &\quad = \mathcal{J}_1 + \mathcal{J}_2. \end{aligned} \tag{5.12}$$

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

$$\begin{aligned} |\mathcal{J}_1| &\le \int_\Omega \left[\operatorname*{ess\,sup}_{F \in \mathbb{R}^{3\times3}} \|\nabla_F f(x, F)\|\right] \|\nabla y(x) - \Pi(\nabla y(x))\| \, dx \\ &\le \left\{\int_\Omega \left[\operatorname*{ess\,sup}_{F \in \mathbb{R}^{3\times3}} \|\nabla_F f(x, F)\|\right]^2 dx\right\}^{\frac{1}{2}} \left[\int_\Omega \|\nabla y(x) - \Pi(\nabla y(x))\|^2 \, dx\right]^{\frac{1}{2}} \\ &\le C \|f\|_{\mathcal{V}} \left[\mathcal{E}(y)^{\frac{1}{4}} + \mathcal{E}(y)^{\frac{1}{2}}\right]. \end{aligned} \tag{5.13}$$

By (2.6) and the definition of $\Pi : \mathbb{R}^{3\times3} \to \{F_0, F_1\}$, 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 $F \in \mathbb{R}^{3\times3}$ and for almost all $x \in \Omega$, leading to

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

where we used the divergence theorem and the fact that $y(x) = y_\lambda(x)$ for any $y \in W^\phi_\lambda$ and for all $x \in \partial\Omega$. It next follows from the Cauchy-Schwarz inequality, Theorem 4.2, and Theorem 5.1 that

$$\begin{aligned} |\mathcal{J}_2| &\le C\left\{\int_\Omega \left[|\nabla G_f(x)\cdot n|^2 + G_f(x)^2\right]\,dx\right\}^{\frac{1}{2}}\left[\mathcal{E}(y)^{\frac{1}{4}} + \mathcal{E}(y)^{\frac{1}{2}}\right] \\ &\le C\,\|f\|_{\mathcal{V}}\left[\mathcal{E}(y)^{\frac{1}{4}} + \mathcal{E}(y)^{\frac{1}{2}}\right]. \end{aligned} \tag{5.14}$$

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

6. Finite element approximations

For simplicity, we shall 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 τ_h, $0 < h \le h_0$, 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 $\mathcal{A}_h$, $0 < h \le h_0$, be the corresponding family of piecewise linear, continuous finite element spaces with respect to the mesh τ_h [11, 30].

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 element meshes is quasi-regular [11, 30], so that

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

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

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

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.

Since Ω is the union of disjoint tetrahedra, we can assume in this section by Lemma 2.2 that there exist disjoint Lipschitz subdomains $\Omega_i \subset \Omega$ for $i = 1, \ldots, M$ with $\bar\Omega = \bigcup_{i=1}^M \bar\Omega_i$, $\tilde l_i \in W^{1,\infty}(\mathbb{R})$, $\tilde\lambda_i \in L^\infty(\mathbb{R})$, and $\hat y_i \in \mathbb{R}^3$, $\hat y_i \cdot a = 0$, such that

$$\begin{aligned} y_\lambda(x) &= F_0 x + \tilde l_i(x\cdot n)a + \hat y_i, && x \in \Omega_i, \\ \tilde l_i'(s) &= \lambda_i(s), && \text{a.e. } s \in \mathbb{R}. \end{aligned}$$

Recall from Section 2 that since $y_\lambda \in W^{1,\infty}(\Omega;\mathbb{R}^3)$, y_λ can be uniquely represented as a Lipschitz continuous function defined on $\bar\Omega$. So, we can then uniquely 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 we can define the finite element space of admissible deformations

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

We also note that the trace $y_\lambda|_{\partial\Omega} \in W^{1,\infty}(\partial\Omega;\mathbb{R}^3)$ is then well-defined, and it follows from well-known estimates for the interpolation error [11, 30] that

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

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

$$\|y_\lambda - y_{\lambda h}\|_{L^2(\partial\Omega;\mathbf{R}^3)} \le Ch. \tag{6.2}$$

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 $\mathcal{E}$ 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*

$$\mathcal{E}(y_h) = \min_{z_h\in\mathcal{A}_{\lambda h}} \mathcal{E}(z_h) \le Ch^{1/2}. \tag{6.3}$$

Proof. The existence of $y_h \in \mathcal{A}_{\lambda h}$ can be proven by the same argument as in the proof of Theorem 6.1 in [22]. To prove the inequality in (6.3) we follow the argument given in [24] to show that $\hat{y}_h = \mathcal{I}_h\hat{u}_\gamma \in \mathcal{A}_{\lambda h}$ with $\hat{u}_\gamma(x)$ defined by Corollary 3.1 and $\gamma = h^{1/2}$ satisfies

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

□

We next give a series of estimates for the finite element approximation of the deformation y_λ by deformations $y_h \in \mathcal{A}_{\lambda h}$. 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*

$$\int_\Omega |[\nabla y_h(x) - \nabla y_\lambda(x)]\,w|^2\,dx \le C\left[\mathcal{E}(y_h)^{\frac12} + \mathcal{E}(y_h) + \|y_\lambda - y_{\lambda h}\|_{L^2(\partial\Omega;\mathbb{R}^3)}\right], \qquad \forall y_h \in \mathcal{A}_{\lambda h}.$$

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

$$\int_\Omega |[\pi(\nabla y_h(x)) - \nabla y_\lambda(x)]\,w|^2\,dx \le C\left[\mathcal{E}(y_h)^{\frac12} + \|y_\lambda - y_{\lambda h}\|_{L^2(\partial\Omega;\mathbb{R}^3)}\right]. \tag{6.4}$$

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

$$\begin{aligned}
\int_\Omega |[\pi(\nabla y_h(x)) - \nabla y_\lambda(x)]\,w|^2\,dx &= 2F_0 w \cdot \int_\Omega [\nabla y_\lambda(x) - \pi(\nabla y_h(x))]\,w\,dx \\
&= 2F_0 w \cdot \left\{\int_\Omega [\nabla y_\lambda(x) - \nabla y_h(x)]\,dx + \int_\Omega [\nabla y_h(x) - \pi(\nabla y_h(x))]\,dx\right\} w \\
&= 2F_0 w \cdot \left\{\int_{\partial\Omega} [y_\lambda(x) - y_{\lambda h}(x)] \otimes \nu\,dS + \int_\Omega [\nabla y_h(x) - \pi(\nabla y_h(x))]\,dx\right\} w
\end{aligned} \tag{6.5}$$

This, together with Lemma 4.1 and the Cauchy-Schwarz inequality, leads to (6.4). □

Theorem 6.3. *We have*

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

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 (4.5) 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 of finite element approximations.

Theorem 6.4. *For any Lipschitz domain $\omega \subset \Omega$ we have that*

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

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*

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

Recall that $\hat{\lambda}_\omega$ 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 $\rho > 0$ we have that*

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

and

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

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*

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

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

Optimization techniques applied to the problem

$$\inf_{y_h \in \mathcal{A}_{\lambda h}} \mathcal{E}(y_h)$$

compute one of the many local minima given by approximations on different length scales to the same optimal microstructure [24]. For this reason, we give error estimates for finite element deformations $y_h \in \mathcal{A}_{\lambda h}$ that satisfy the following quasi-optimality condition

$$\mathcal{E}(y_h) \leq \alpha \inf_{z_h \in \mathcal{A}_{\lambda h}} \mathcal{E}(z_h) \tag{6.6}$$

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*

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

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 (6.6).

Corollary 6.2. *We have*

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

for any $y_h \in \mathcal{A}_{\lambda h}$ which satisfies the quasi-optimality condition (6.6).

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

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

for any $y_h \in \mathcal{A}_{\lambda h}$ which satisfies the quasi-optimality condition (6.6).

Corollary 6.4. *We have*

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

for any $y_h \in \mathcal{A}_{\lambda h}$ which satisfies the quasi-optimality condition (6.6).

Corollary 6.5. *For any Lipschitz domain $\omega \subset \Omega$ and any $\rho > 0$ we have*

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

and

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

for any $y_h \in \mathcal{A}_{\lambda h}$ which satisfies the quasi-optimality condition (6.6).

Corollary 6.6. *We have*

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

for any $f \in \mathcal{V}$ and any $y_h \in \mathcal{A}_{\lambda h}$ which satisfies the quasi-optimality condition (6.6).

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