Approximation of a Laminated Microstructure for a Rotationally Invariant, Double Well Energy Density

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Abstract

We give error estimates for the approximation of a laminated microstructure which minimizes the energy $\int_\Omega \phi(\nabla v(x))\,dx$ for a rotationally invariant, double well energy density $\phi(A)$. We present error estimates for the convergence of the deformation in L^2, the convergence of directional derivatives of the deformation in the "twin planes," the weak convergence of the deformation gradient, the convergence of the microstructure (or Young measure) of the deformation gradients, and the convergence of nonlinear integrals of the deformation gradient.

1 Introduction

Martensitic crystals are often found in nature and in the laboratory in a simple laminated state where the crystal structure alternates between two symmetry-related variants (Burkart and Reid (1953) and Basinski and Christian (1954)). These observations are now well explained by a continuum theory for martensitic crystals based on energy minimization for an energy density which attains a minimum value at several symmetry-related deformation gradients (Ericksen (1986, 1987) and Ball and James (1987, 1992)). It is usually also desired that such an energy density be rotationally invariant or frame-indifferent (Ball and James (1987, 1992)), so the energy density attains its minimum value on multiple, rotationally invariant energy wells. The simple laminated state found in

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nature is modeled in the continuum theory by energy minimizing sequences of deformations which have layers (with width converging to zero) in which the deformation gradient is nearly constant and across which the deformation gradient oscillates between the energy wells so that the effective energy density becomes the relaxed energy density (see, for example, Kinderlehrer and Pedregal (1991) and Kohn (1991)).

We consider in this paper an energy density with two rotationally invariant energy wells (Kohn (1991) and Ball and James (1992)). The resulting mathematical model gives the laminated microstructure described above. For prescribed boundary conditions which are compatible with this simple laminate, it has been proven by Ball and James (1992) that the limiting microstructure (or Young measure) of the deformation gradients for energy minimizing sequences is unique. Although this problem has been widely utilized as a test problem for the numerical approximation of microstructure (see, for example, Collins and Luskin (1989), Collins, Luskin, and Riordan (1991, 1993), and Collins (1993)), there has not previously been given a proof of convergence or error estimates for any approximation method.

We denote the reference domain for our crystal by Ω, which is assumed to be a polygonal domain in $\mathbb{R}^3$. We will consider deformations $v : \Omega \to \mathbb{R}^3$ and corresponding deformation gradients $\nabla v(x) : \Omega \to \mathbb{R}^{3\times 3}$ where $\mathbb{R}^{3\times 3}$ denotes the space of 3×3 matrices.

We assume that the energy density $\phi : \mathbb{R}^{3\times 3} \to \mathbb{R}$ is a continuous, nonnegative function. For energy minimizing deformation gradients $F^+ \in \mathbb{R}^{3\times 3}$ and $F^- \in \mathbb{R}^{3\times 3}$, we define rotationally invariant energy wells by

$$\mathcal{U}^+ \equiv \mathrm{SO}(3)\mathcal{F}^+ \qquad \text{and} \qquad \mathcal{U}^- \equiv \mathrm{SO}(3)\mathcal{F}^-$$

where SO(3) denotes the space of proper rotations. We then assume that ϕ attains its minimum value only on the rotationally invariant set

$$\mathcal{U} \equiv \mathcal{U}^+ \cup \mathcal{U}^-,$$

so that

$$\begin{aligned} \phi(A) \geq 0 \qquad & \text{for all } A \in \mathbb{R}^{3\times 3}, \\ \phi(A) = 0 \qquad & \text{if and only if} \qquad A \in \mathcal{U}. \end{aligned}$$

Since F^+ and F^- represent symmetry-related states (Ball and James (1987, 1992)), we assume that they satisfy the condition

$$\det F^+ = \det F^- > 0 \tag{1}$$

and the Hadamard condition that there exist $a \in \mathbb{R}^3$ and $n \in \mathbb{R}^3$, $a,\ n \neq 0$ such that

$$F^+ = F^- + a \otimes n \tag{2}$$

where $a \otimes n \in \mathbb{R}^{3\times 3}$ is the tensor product of a and n defined by $(a \otimes n)_{ij} = a_i n_j$. We will assume without loss of generality (by rescaling a) that

$$|n| = 1.$$

We shall see in § 3 that the Hadamard condition (2) allows the existence of a continuous deformation with planar interfaces with normal n (which are called "twin planes" in the physical theory) separating layers in which the deformation gradient is either F^+ or F^-.

We wish to approximate the microstructure for a simple laminate. Boundary conditions that are compatible for a simple laminate (which is described in more detail in § 3) are given by

$$v(x) = Fx \qquad \text{for all } x \in \partial\Omega,$$

where

$$F = \lambda^+ F^+ + \lambda^- F^-$$

for $\lambda^+,\ \lambda^- \in \mathbb{R}$ satisfying

$$\lambda^+ + \lambda^- = 1 \qquad \text{and} \qquad 0 < \lambda^\pm < 1.$$

Thus, we seek to approximate the problem

$$\inf \left\{ \mathcal{E}(v) : v \in W^{1,\infty}(\Omega;\mathbb{R}^3) \cap C^F(\bar{\Omega};\mathbb{R}^3) \right\}$$

where the bulk energy of the crystal, $\mathcal{E}(v)$, is defined by

$$\mathcal{E}(v) = \int_\Omega \phi\left(\nabla v(x)\right)\, dx, \tag{3}$$

and where the affine space of continuous functions, $C^F(\bar{\Omega};\mathbb{R}^3)$, is defined by

$$C^F(\bar{\Omega};\mathbb{R}^3) = \left\{ v(x) \in C(\bar{\Omega};\mathbb{R}^3) : v(x) = Fx \text{ for } x \in \partial\Omega \right\} .$$

A theory for the numerical analysis of microstructure was first given by Collins, Kinderlerher, and Luskin (1991) and Collins and Luskin (1991) to analyze the minimization of the energy

$$\hat{\mathcal{E}}(v) = \int_0^1 \left[\phi(v'(x)) + |v(x) - Fx|^2\right]\, dx$$

where $\phi(s) : \mathbb{R} \to \mathbb{R}$ is a double well energy density (see also Luskin (1991)). This theory has been used to analyze the three-dimensional microstructure in micromagnetics (Luskin and Ma (1992)) and extended to some multi-dimensional problems for energy densities which have point energy wells (and so are not rotationally invariant) by Chipot (1991) and by Chipot and Collins (1992).

A two-dimensional, rotationally invariant, double well model with bulk energy

$$\hat{\mathcal{E}}(v) = \int_\Omega [\phi(\nabla v(x)) + |v(x) - Fx|^q]\, dx \tag{4}$$

for $\Omega \subset \mathbb{R}^2$ and $1 < q < \infty$ has been analyzed by Gremaud (1994) and by Chipot, Collins, and Kinderlehrer (1995). The term $|v(x) - Fx|^q$ in the integrand of (4) is not part of the physical elastic energy density, but is a "penalty term" which has been added as in the one-dimensional case for mathematical convenience to force the convergence of $v(x) \to Fx$ in $L^q(\Omega; \mathbb{R}^2)$ for energy minimizing sequences of deformations. However, in contrast to the one-dimensional case, for the multi-dimensional problem the microstructure (or Young measure) for minimizing sequences for the energy (3) is unique even if the elastic energy density does not include the term $|v(x) - Fx|^q$ (Ball and James (1992)). The results that we prove in this paper do not utilize a term $|v(x) - Fx|^q$ in the energy density, but rather show that the convergence of $v(x) \to Fx$ in $L^2(\Omega; \mathbb{R}^3)$ and the convergence of the microstructure depend only on minimizing the elastic energy (3).

The statements of our theorems and lemmas are given in § 2. The remaining sections give the proofs of the theorems and lemmas. An estimate for the minimization of the energy (Theorem 1) is given in § 3. The proofs of the L^2 convergence of the directional derivatives in the plane orthogonal to n (Theorem 2) and of the L^2 convergence of the deformation (Lemma 2) are given in § 4, the estimate for the weak convergence of the deformation gradient (Theorem 3) is given in § 5, the estimate for the convergence of the deformation gradient to the set $\{F^+, F^-\}$ (Theorem 4) is given in § 6, the estimate for the convergence of the microstructure (Theorem 5) is given in § 7, and the estimate for the convergence of nonlinear integrals of the deformation gradient (Theorem 6) is given in § 8.

2 Definitions and Main Results

We shall assume that ϕ grows quadratically away from the energy wells. To describe this precisely, we let $\pi : \mathbb{R}^{3\times 3} \to \mathcal{U}$ be a Borel measurable projection defined by

$$\|A - \pi(A)\| = \min_{B\in\mathcal{U}} \|A - B\|.$$

We note that such a projection exists since $\mathcal{U}$ is compact, although the projection is not uniquely defined at $A \in \mathbb{R}^{3\times 3}$ where the minimum above is attained at more than one $B \in \mathcal{U}$. We shall assume that there exists $\kappa > 0$ such that

$$\phi(A) \ge \kappa \|A - \pi(A)\|^2 \qquad \text{for all } A \in \mathbb{R}^{3\times 3} \tag{5}$$

where we use the matrix norm

$$\|A\|^2 \equiv \sum_{i,j=1}^{3} A_{ij}^2 \qquad \text{for } A \in \mathbb{R}^{3\times 3}.$$

It will also be useful to define the operators $R(A) : \mathbb{R}^{3\times 3} \to \mathrm{SO}(3)$ and $\Pi : \mathbb{R}^{3\times 3} \to \{F^+, F^-\}$ by the relation

$$\pi(A) = R(A)\Pi(A) \qquad \text{for all } A \in \mathbb{R}^{3\times 3}. \tag{6}$$

The operators $R(A)$ and $\Pi(A)$ are easily seen to be uniquely defined by the relation (6).

We shall define the properties required for our finite element spaces abstractly so that they can be applied to the different finite element spaces which have been used to compute microstructure. We assume that τ_h for $0 < h < h_0$ is a family of decompositions of Ω into polyhedra $\{K\}$ such that (Quarteroni and Valli (1994)):

1. $\bar{\Omega} = \cup_{K\in\tau_h} K$;
2. interior $K_1 \cap$ interior $K_2 = \emptyset$ if $K_1 \neq K_2$ for $K_1,\ K_2 \in \tau_h$;
3. if $S = K_1 \cap K_2 \neq \emptyset$ for $K_1 \neq K_2,\ K_1,\ K_2 \in \tau_h$, then S is a common face, edge, or vertex of K_1 and K_2;
4. diam $K \le h$ for all $K \in \tau_h$.

We denote our family of finite element spaces by

$$\mathcal{M}_h^F \subset C^F(\bar{\Omega} : \mathbb{R}^3) \cap W^{1,\infty}(\Omega; \mathbb{R}^3) \qquad \text{for } 0 < h < h_0.$$

We assume that there exists an interpolation operator $\mathcal{I}_h : C^F(\bar{\Omega}; \mathbb{R}^3) \to \mathcal{M}_h^F$ such that

$$\text{ess sup}_{x\in\Omega} \|\nabla \mathcal{I}_h v(x)\| \le C\, \text{ess sup}_{x\in\Omega} \|\nabla v(x)\| \tag{7}$$

for all $v \in W^{1,\infty}(\Omega; \mathbb{R}^3) \cap C^F(\bar{\Omega}; \mathbb{R}^3)$, where the constant C in (7) and below will always denote a generic positive constant which is independent of h. We also assume that

$$\mathcal{I}_h v(x)|_K = v(x)|_K \text{ for } K \in \tau_h \text{ such that } v(x)|_K \in \left\{P^1(K)\right\}^3 \tag{8}$$

where $\left\{P^1(K)\right\}^3 \equiv P^1(K) \times P^1(K) \times P^1(K)$ and $P^1(K)$ denotes the space of linear polynomials defined on K.

The most widely-used finite element methods based on continuous, piecewise polynomial spaces have Lagrange interpolation operators $\mathcal{I}_h$ which satisfy (7) (for quasi-regular meshes) and (8) (Ciarlet (1978) and Quarteroni and Valli (1994)). In particular, (7) and (8) are valid for the trilinear elements defined on rectangular parellelepipeds which have been extensively used to compute laminated microstructure (Collins and Luskin (1989), Collins, Luskin, and Riordan (1991, 1993), and Collins (1993)), as well as for linear elements defined on tetrahedra.

For completeness, we will give in § 3 an extension of the proof by Chipot, Collins and Kinderlehrer (1995) for the minimization of the energy $\mathcal{E}(v)$ over continuous, piecewise linear functions to the minimization of the energy $\mathcal{E}(v)$ over the more general family of finite element spaces $\mathcal{M}_h^F$.

Theorem 1 *There exists an optimal approximate deformation, $u_h \in \mathcal{M}_h^F$, such that*

$$\mathcal{E}(u_h) = \min_{v_h \in \mathcal{M}_h^F} \mathcal{E}(v_h) \leq Ch^{1/2}. \tag{9}$$

The following results will be given for an arbitrary $v_h(x) \in \mathcal{M}_h^F$. This allows the applicability of the results to the local minima with small energy which are typically computed rather than a global minimum (Collins (1993)). We also note that the results hold for arbitrary $v(x) \in W^{1,\infty}(\Omega;\mathbb{R}^3) \cap C^F(\bar{\Omega};\mathbb{R}^3)$, so the results are also applicable to more general approximation procedures.

The following lemma shows that the deformation gradients of minimizing sequences converge to the union of the energy wells $\mathcal{U} = \mathcal{U}^+ \cup \mathcal{U}^-$. It follows trivially from (5).

Lemma 1 *We have the estimate*

$$\int_\Omega \|\nabla v_h(x) - \pi(\nabla v_h(x))\|^2 \, dx \leq \kappa^{-1}\mathcal{E}(v_h) \qquad \text{for all } v_h \in \mathcal{M}_h^F.$$

The next theorem demonstrates that the directional derivatives orthogonal to n of sequences of energy minimizing deformations converge strongly.

Theorem 2 *For all $v_h \in \mathcal{M}_h^F$ and for all $w \in \mathbb{R}^3$ such that*

$$w \cdot n = 0 \quad \textit{and} \qquad |w| = 1,$$

we have that

$$\int_\Omega |(\nabla v_h(x) - F)w|^2 \, dx \leq C\mathcal{E}(v_h)^{1/2} + C\mathcal{E}(v_h).$$

The convergence of the deformation in L^2 will then follow from the Poincaré inequality and Theorem 2 (see § 4).

Lemma 2 *The deformations $v_h(x) \in \mathcal{M}_h^F$ can be approximated by Fx at a rate given by*

$$\int_\Omega |v_h(x) - Fx|^2 \, dx \leq C\mathcal{E}(v_h)^{1/2} + C\mathcal{E}(v_h). \tag{10}$$

It follows directly from the inequality (10) in Lemma 2 that we can give error estimates for the convergence of $v_h(x) \to Fx$ in $L^2(\Omega; \mathbb{R}^3)$ for finite element approximations to the minimization of elastic energies (3) which do not include the term $|v(x) - Fx|^2$ in the energy density.

The next theorem demonstrates that $\nabla v_h(x)$ converges weakly to F. We will consider $\omega \subset \Omega$ to be a smooth domain if it has a sufficiently smooth boundary $\partial\omega$ so that the divergence theorem and trace theorem used in its proof are valid.

Theorem 3 *For any smooth domain $\omega \subset \Omega$, we have for all $v_h \in \mathcal{M}_h^F$ that*

$$\left\| \int_\omega (\nabla v_h(x) - F)\, dx \right\| \le C\mathcal{E}(v_h)^{1/8} + C\mathcal{E}(v_h)^{1/2}.$$

The proof of Theorem 3 shows that the constants C in Theorem 3 are independent of h and converge to zero as the diameter of ω converges to zero if, for example, ω is obtained by scaling and translating a reference domain.

The following theorem shows that the deformation gradients of minimizing sequences converge to the set $\{ F^+,\ F^- \}$.

Theorem 4 *For all $v_h \in \mathcal{M}_h^F$, we have the estimate*

$$\int_\Omega \|\nabla v_h(x) - \Pi(\nabla v_h(x))\|^2\, dx \le C\mathcal{E}(v_h)^{1/2} + C\mathcal{E}(v_h).$$

Next, for any smooth domain $\omega \subset \Omega$, $\rho > 0$, and $v_h \in \mathcal{M}_h^F$, we define the sets

$$\begin{aligned} \omega_\rho^+ &= \omega_\rho^+(v_h) = \{ x \in \omega : \Pi(\nabla v_h(x)) = F^+ \text{ and } \|F^+ - \nabla v_h(x)\| < \rho \}\ , \\ \omega_\rho^- &= \omega_\rho^-(v_h) = \{ x \in \omega : \Pi(\nabla v_h(x)) = F^- \text{ and } \|F^- - \nabla v_h(x)\| < \rho \}\ . \end{aligned}$$

We will then use Theorem 3 and Theorem 4 to prove the following theorem which describes the convergence of the microstructure (or Young measure) of the deformation gradients of energy minimizing sequences. Theorem 5 states that in any smooth domain $\omega \subset \Omega$ and for any energy minimizing sequence the volume fraction that $\nabla v_h(x)$ is near F^+ converges to λ^+ and the volume fraction that $\nabla v_h(x)$ is near F^- converges to $\lambda^- = 1 - \lambda^+$.

Theorem 5 *We have for any smooth domain $\omega \subset \Omega$, $\rho > 0$, and $v_h \in \mathcal{M}_h^F$ that*

$$\left| \frac{\text{meas}(\omega_\rho^+(v_h))}{\text{meas}(\omega)} - \lambda^+ \right| \le C\mathcal{E}(v_h)^{1/8} + C\mathcal{E}(v_h)^{1/2}, \tag{11}$$

$$\left| \frac{\text{meas}(\omega_\rho^-(v_h))}{\text{meas}(\omega)} - \lambda^- \right| \le C\mathcal{E}(v_h)^{1/8} + C\mathcal{E}(v_h)^{1/2}. \tag{12}$$

It can be seen from the proof of Theorem 5 that the constants C in the estimates (11) and (12) are independent of h, but depend on ω and ρ.

We note that Gremaud (1994) and Chipot, Collins, and Kinderlehrer (1995) do not give estimates for the sets $\omega_\rho^\pm(v_h)$, but rather give estimates (for the problem $\int_\Omega [\phi(\nabla v(x)) + |v(x) - Fx|^q]\, dx$ with $\Omega \subset \mathbb{R}^2$) for the sets

$$\hat{\omega}_\rho^+(v_h) = \{\, x \in \omega : \pi(\nabla v_h(x)) \in \mathcal{U}^+ \text{ and } \|\pi(\nabla v_h(x)) - \nabla v_h(x)\| < \rho \}\ ,$$
$$\hat{\omega}_\rho^-(v_h) = \{\, x \in \omega : \pi(\nabla v_h(x)) \in \mathcal{U}^- \text{ and } \|\pi(\nabla v_h(x)) - \nabla v_h(x)\| < \rho \}\ .$$

Thus, their estimates give the volume fraction that $\nabla v_h(x)$ is near the wells $\mathcal{U}^+ = \mathrm{SO}(3)F^+$ and $\mathcal{U}^- = \mathrm{SO}(3)F^-$, whereas Theorem 5 gives an estimate for the approximation of the Young measure since it gives the volume fraction that $\nabla v_h(x)$ is near F^+ and F^-. It is easy to see from Theorem 5 that

$$\left| \frac{\mathrm{meas}\big(\hat{\omega}_\rho^\pm(v_h)\big)}{\mathrm{meas}(\omega)} - \lambda^\pm \right| \le C\mathcal{E}(v_h)^{1/8} + C\mathcal{E}(v_h)^{1/2}$$

since $\lambda^+ + \lambda^- = 1$ and since by the definition of π we have that $\omega_\rho^\pm(v_h) \subset \hat{\omega}_\rho^\pm(v_h)$ and $\hat{\omega}_\rho^+(v_h) \cap \hat{\omega}_\rho^-(v_h) = \emptyset$.

We next use the analysis introduced in Collins and Luskin (1991) to show that nonlinear integrals of $\nabla v_h(x)$ (which approximate macroscopic thermodynamic variables) can be estimated. For linear transformations $\mathcal{L} : \mathbb{R}^{3\times 3} \to \mathbb{R}$ we define the operator norm

$$\|\mathcal{L}\| = \max_{\|A\|=1} |\mathcal{L}(A)|,$$

so for Lipschitz functions $g(A) : \mathbb{R}^{3\times 3} \to \mathbb{R}$ we can define the function norm

$$\left\| \frac{\partial g}{\partial A} \right\|_{L^\infty} = \mathrm{ess\ sup}_{B \in \mathbb{R}^{3\times 3}} \left\| \frac{\partial g}{\partial A}(B) \right\|.$$

We obtain estimates for the Sobolev space $\mathcal{V}$ of measurable functions $f(x, A) : \Omega \times \mathbb{R}^{3\times 3} \to \mathbb{R}$ such that

$$\int_\Omega \left[\left\| \frac{\partial f}{\partial A}(x, \cdot) \right\|_{L^\infty}^2 + |\nabla G(x) \cdot n|^2 + G(x)^2 \right] dx < \infty$$

where

$$G(x) = f(x, F^+) - f(x, F^-).$$

We observe that if $f(x, A) \in \mathcal{V}$, then $f(x, A)$ is Lipschitz continuous as a function of $A \in \mathbb{R}^{3\times 3}$ for almost all $x \in \Omega$.

Theorem 6 *For all $v_h \in \mathcal{M}_h^F$ and all functions $f(x,A) \in \mathcal{V}$, we have that*

$$\left| \int_\Omega f\left(x, \nabla v_h(x)\right) - \left[\lambda^+ f(x,F^+) + \lambda^- f(x,F^-)\right]\, dx \right|$$
$$\leq C \left\{ \int_\Omega \left[\left\| \frac{\partial f}{\partial A}(x,\cdot) \right\|_{L^\infty}^2 + |\nabla G(x)\cdot n|^2 + G(x)^2 \right] dx \right\}^{1/2} \left(\mathcal{E}(v_h)^{1/4} + \mathcal{E}(v_h)^{1/2} \right)$$

where

$$G(x) = f(x,F^+) - f(x,F^-).$$

Finally, it follows directly from using the estimate in Theorem 1 that we can obtain the following error estimates for an optimal approximate deformation $u_h \in \mathcal{M}_h^F$ satisfying (9).

Lemma 3 *For deformations $u_h(x)$ which minimize the energy $\mathcal{E}(v)$ in $\mathcal{M}_h^F$ and for all $w \in \mathbb{R}^3$ such that*

$$w \cdot n = 0 \quad \text{and} \quad |w| = 1,$$

we have that

$$\int_\Omega |(\nabla u_h(x) - F)w|^2\, dx \leq Ch^{1/4}.$$

Lemma 4 *Any deformation $u_h(x) \in \mathcal{M}_h^F$ which minimizes the energy $\mathcal{E}(v)$ in $\mathcal{M}_h^F$ is approximated by Fx at a rate given by*

$$\int_\Omega |u_h(x) - Fx|^2\, dx \leq Ch^{1/4}.$$

Lemma 5 *We have for any smooth domain $\omega \subset \Omega$ that if the deformation $u_h(x)$ minimizes the energy $\mathcal{E}(v)$ in $\mathcal{M}_h^F$, then*

$$\left| \frac{\operatorname{meas}\left(\omega_\rho^+(u_h)\right)}{\operatorname{meas}(\omega)} - \lambda^+ \right| \leq Ch^{\frac{1}{16}}, \qquad \left| \frac{\operatorname{meas}\left(\omega_\rho^-(u_h)\right)}{\operatorname{meas}(\omega)} - \lambda^- \right| \leq Ch^{\frac{1}{16}}.$$

Lemma 6 *If the deformation $u_h(x)$ minimizes the energy $\mathcal{E}(v)$ in $\mathcal{M}_h^F$ and $f(x,A) \in \mathcal{V}$, then we have that*

$$\left| \int_\Omega f\left(x, \nabla u_h(x)\right) - \left[\lambda^+ f(x,F^+) + \lambda^- f(x,F^-)\right]\, dx \right|$$
$$\leq C \left\{ \int_\Omega \left[\left\| \frac{\partial f}{\partial A}(x,\cdot) \right\|_{L^\infty}^2 + |\nabla G(x)\cdot n|^2 + G(x)^2 \right] dx \right\}^{1/2} h^{1/8}$$

where

$$G(x) = f(x,F^+) - f(x,F^-).$$

3 Estimates for the Energy

Proof of Theorem 1. We will now describe a construction of $v_h(x) \in \mathcal{M}_h^F$ such that

$$\mathcal{E}(v_h) = \int_\Omega \phi(\nabla v_h(x))\, dx \le C h^{1/2}.$$

We first define the deformation $w_h(x) : \Omega \to \mathbb{R}^3$ by

$$w_h(x) = F^- x + \left[\int_0^{x\cdot n} \chi\left(\frac{s}{h^{1/2}}\right)\, ds \right] a \tag{13}$$

where $\chi(s) : \mathbb{R} \to \mathbb{R}$ is a characteristic function with period 1 such that

$$\chi(s) = \begin{cases} 1 & \text{for all } 0 \le s \le \lambda^+, \\ 0 & \text{for all } \lambda^+ < s < 1. \end{cases}$$

Note that

$$|w_h(x) - Fx| \le C h^{1/2} \qquad \text{for all } x \in \Omega. \tag{14}$$

We also have that

$$\nabla w_h(x) = F^- + \chi\left(\frac{x\cdot n}{h^{1/2}}\right) a \otimes n, \qquad x \in \Omega,$$

so

$$\nabla w_h(x) = \begin{cases} F^+ & \text{if } j h^{1/2} < x \cdot n < (j + \lambda^+) h^{1/2} \text{ for some } j \in \mathbb{Z}, \\ F^- & \text{if } (j+\lambda^+) h^{1/2} < x \cdot n < (j+1) h^{1/2} \text{ for some } j \in \mathbb{Z}. \end{cases} \tag{15}$$

Next, we define the subset

$$\Omega_h^1 = \left\{ x \in \Omega : \operatorname{dist}(x, \partial\Omega) > h^{1/2} \right\},$$

and we define the function $\psi_h(x) : \Omega \to \mathbb{R}$ by

$$\psi_h(x) = \begin{cases} 1 & \text{for all } x \in \Omega_h^1, \\ h^{-1/2} \operatorname{dist}(x, \partial\Omega) & \text{for all } x \in \Omega \setminus \Omega_h^1. \end{cases}$$

The function $\psi_h(x)$ is easily seen to satisfy the following properties:

$$\begin{aligned} 0 \le \psi_h(x) \le 1 & \qquad \text{for all } x \in \Omega, \\ \psi_h(x) = 1 & \qquad \text{for all } x \in \Omega_h^1, \\ \psi_h(x) = 0 & \qquad \text{for all } x \in \partial\Omega, \\ |\nabla \psi_h(x)| \le C h^{-1/2} & \qquad \text{for all } x \in \Omega. \end{aligned} \tag{16}$$

We then define the deformation $\hat{v}_h(x) : \Omega \to \mathbb{R}^3$ by

$$\hat{v}_h(x) = \psi_h(x) w_h(x) + (1 - \psi_h(x)) F x \qquad \text{for all } x \in \Omega,$$

so we have for $x \in \Omega$ that

$$\nabla \hat{v}_h(x) = (w_h(x) - Fx) \otimes \nabla \psi_h(x) + \psi_h(x) \nabla w_h(x) + (1 - \psi_h(x))\, F.$$

It then follows from (14), (15), and (16) that

$$\begin{aligned} \nabla \hat{v}_h(x) = \nabla w_h(x) \in \mathcal{U}, &\quad x \in \Omega_h^1, \\ \|\nabla \hat{v}_h(x)\| \le C, &\quad x \in \Omega, \\ \hat{v}_h(x) = Fx, &\quad x \in \partial\Omega. \end{aligned}$$

Finally, we define the deformation $v_h(x) \in \mathcal{M}_h^F$ by

$$v_h(x) = \mathcal{I}_h\left(\hat{v}_h(x)\right).$$

It follows from the definition of the interpolation operator $\mathcal{I}_\langle$ that

$$v_h(x) = \hat{v}_h(x) = w_h(x) \qquad \text{for all } x \in \Omega_h \tag{17}$$

for (recalling that $|n|$=1)

$$\Omega_h = \Omega_h^2 \setminus \, ,\, _h$$

where

$$\begin{aligned} \Omega_h^2 &= \left\{ x \in \Omega : \text{dist}(x, \partial\Omega) > h^{1/2} + h \right\}, \\ ,\, _h &= \textstyle\bigcup_{j \in \mathbb{Z}} \left\{ x \in \Omega_h^2 : |x \cdot n - j h^{1/2}| \le h \text{ or } |x \cdot n - (j + \lambda^+) h^{1/2}| \le h \right\}. \end{aligned}$$

Now $\text{meas}(\Omega \setminus \Omega_h^2) \le C h^{1/2}$ since $\Omega \setminus \Omega_h^2$ is a layer of width $h^{1/2} + h$ around the boundary of Ω, and $\text{meas}(,\, _h) \le C h^{1/2}$ since $,\, _h$ is the union of $\mathcal{O}(h^{-1/2})$ planar layers of thickness h. (Note that only $\mathcal{O}(h^{-1/2})$ of the sets in the definition of $,\, _h$ are non-empty.) So, since $\Omega \setminus \Omega_h = \left\{ \Omega \setminus \Omega_h^2 \right\} \cup \, ,\, _h$, we have that

$$\text{meas}\left(\Omega \setminus \Omega_h\right) \le C h^{1/2}, \tag{18}$$

and we have by (7), (15), and (17) that

$$\begin{aligned} \nabla v_h(x) \in \mathcal{U}, &\quad x \in \Omega_h, \\ \|\nabla v_h(x)\| \le C, &\quad x \in \Omega. \end{aligned} \tag{19}$$

Since ϕ is continuous, it is bounded on bounded sets in $\mathbb{R}^{3\times 3}$. Thus, it follows from (18) and (19) that

$$\begin{aligned} \left| \int_\Omega \phi\left(\nabla v_h(x)\right)\, dx \right| &= \left| \int_{\Omega_h} \phi\left(\nabla v_h(x)\right)\, dx + \int_{\Omega \setminus \Omega_h} \phi\left(\nabla v_h(x)\right)\, dx \right| \\ &= \int_{\Omega \setminus \Omega_h} \phi\left(\nabla v_h(x)\right)\, dx \le C h^{1/2}. \end{aligned}$$

□

4 Strong Convergence of the Directional Derivatives in the Plane Orthogonal to n.

Proof of Theorem 2. We first observe that

$$F = \frac{1}{\text{meas}(\Omega)} \int_\Omega \nabla v_h(x)\, dx \qquad \text{for all } v_h \in \mathcal{M}_h^F$$

since $v_h(x) = Fx$ for $x \in \partial\Omega$. Since $F^+ = F^- + a \otimes n$, we have for $w \in \mathbb{R}^3$ orthogonal to n that

$$\begin{aligned} &F^+ w = F^- w = Fw, \\ &|\pi(A)w| = |F^+ w| = |F^- w| \qquad \text{for all } A \in \mathbb{R}^{3\times 3}. \end{aligned} \tag{20}$$

Hence, we have for any $w \in \mathbb{R}^3$ satisfying $w \cdot n = 0$ and $|w| = 1$ and any $\mu > 0$ that

$$\begin{aligned}
&\frac{1}{\text{meas}(\Omega)} \int_\Omega |(\nabla v_h(x) - F)w|^2\, dx \\
&\quad = \frac{1}{\text{meas}(\Omega)} \int_\Omega |\nabla v_h(x) w|^2\, dx - \frac{1}{\text{meas}(\Omega)} \int_\Omega |Fw|^2\, dx \\
&\quad = \frac{1}{\text{meas}(\Omega)} \int_\Omega |\nabla v_h(x) w|^2\, dx - |F^+ w|^2 \\
&\quad = \frac{1}{\text{meas}(\Omega)} \int_\Omega |[\nabla v_h(x) - \pi(\nabla v_h(x))]\, w + \pi(\nabla v_h(x))\, w|^2\, dx - |F^+ w|^2 \\
&\quad \le \frac{1}{\text{meas}(\Omega)} \int_\Omega \left(1 + \frac{1}{\mu}\right) |[\nabla v_h(x) - \pi(\nabla v_h(x))]\, w|^2\, dx \\
&\qquad\qquad + \frac{1}{\text{meas}(\Omega)} \int_\Omega (1+\mu)\, |\pi(\nabla v_h(x))\, w|^2\, dx - |F^+ w|^2 \\
&\quad \le \frac{\mu + 1}{\mu\, \text{meas}(\Omega)} \int_\Omega \|\nabla v_h(x) - \pi(\nabla v_h(x))\|^2\, dx + \mu |F^+ w|^2 \\
&\quad \le \frac{(\mu+1)\mathcal{E}(v_h)}{\mu\kappa\, \text{meas}(\Omega)} + \mu |F^+ w|^2.
\end{aligned}$$

The result now follows by setting $\mu = \mathcal{E}(v_h)^{1/2}$. $\square$

We now show that the convergence of the deformation in L^2 follows directly from the Poincaré inequality (Wloka(1987)) and Theorem 2.

Proof of Lemma 2. Since $v_h \in \mathcal{M}_h^F$, we have that $v_h(x) - Fx = 0$ for $x \in \partial\Omega$. So, for $w \in \mathbb{R}^3$ such that $|w| = 1$ we have by integration by parts and the Cauchy-Schwarz inequality that

$$\begin{aligned}
&\int_\Omega |v_h(x) - Fx|^2\, dx = -\int_\Omega \left(\nabla |v_h(x) - Fx|^2 \cdot w\right)(w \cdot x)\, dx \\
&\quad \le 2 \max_{x\in\Omega} |w \cdot x| \left\{ \int_\Omega |v_h(x) - Fx|^2\, dx \right\}^{1/2} \left\{ \int_\Omega |(\nabla v_h(x) - F)w|^2\, dx \right\}^{1/2}.
\end{aligned}$$

Hence, we have the Poincaré inequality that for $w \in \mathbb{R}^3$ such that $|w| = 1$

$$\int_\Omega |v_h(x) - Fx|^2 \, dx \le C \int_\Omega |(\nabla v_h(x) - F)w|^2 \, dx. \tag{21}$$

The result of Lemma 2 follows from Theorem 2 and (21) with w choosen so that $w \cdot n = 0$ and $|w| = 1$. □

5 Weak Convergence of the Deformation Gradient

Proof of Theorem 3. We have by the divergence theorem and the Cauchy-Schwarz inequality that

$$\begin{aligned} \left\| \int_\omega (\nabla v_h(x) - F) \, dx \right\| &= \left\| \int_{\partial\omega} (v_h(x) - Fx) \otimes \nu \, dS \right\| \\ &\le \int_{\partial\omega} |v_h(x) - Fx| \, dS \\ &\le \mathrm{meas}_2(\partial\omega)^{1/2} \left(\int_{\partial\omega} |v_h(x) - Fx|^2 \, dS \right)^{1/2} \end{aligned} \tag{22}$$

where ν is the unit exterior normal to $\partial\omega$ and where $\mathrm{meas}_2(\partial\omega)$ is the surface area of $\partial\omega$. We then use the trace theorem (Adams (1975)) to obtain the estimate

$$\begin{aligned} &\int_{\partial\omega} \left|v_h(x) - Fx\right|^2 dS \\ &\quad\le C \left[\int_\omega |v_h(x) - Fx|^2 \, dx + \int_\omega \left| \nabla |v_h(x) - Fx|^2 \right| dx \right] \\ &\quad\le C \left[\int_\omega |v_h(x) - Fx|^2 \, dx + \int_\omega |v_h(x) - Fx| \cdot \|\nabla (v_h(x) - Fx)\| \, dx \right] \\ &\quad\le C \Bigg[\int_\omega |v_h(x) - Fx|^2 \, dx \\ &\qquad + \left(\int_\omega |v_h(x) - Fx|^2 \, dx \right)^{1/2} \left(\int_\omega \|\nabla (v_h(x) - Fx)\|^2 \, dx \right)^{1/2} \Bigg]. \end{aligned} \tag{23}$$

By the triangle inequality and Lemma 1, we have that

$$\begin{aligned} &\left(\int_\omega \|\nabla v_h(x) - F\|^2 \, dx \right)^{1/2} \\ &\quad\le \left(\int_\omega \|\nabla v_h(x) - \pi\left(\nabla v_h(x)\right)\|^2 \, dx \right)^{1/2} + \left(\int_\omega \|\pi\left(\nabla v_h(x)\right) - F\|^2 \, dx \right)^{1/2} \\ &\quad\le \kappa^{-1/2} \mathcal{E}(v_h)^{1/2} + C \mathrm{meas}(\omega)^{1/2} \end{aligned} \tag{24}$$

since $\|\pi(A)\| \leq C$ for all $A \in \mathbb{R}^{3\times 3}$ by the compactness of SO(3).

Hence, by using Lemma 2 and (24) in (23) we obtain

$$\int_{\partial\omega} \left|v_h(x) - Fx\right|^2 \leq C\mathcal{E}(v_h)^{1/4} + C\mathcal{E}(v_h) \qquad \text{for all } v_h \in \mathcal{M}_h^F. \tag{25}$$

The result of Theorem 3 now follows from using (25) in (22). □

6 Convergence of the Deformation Gradient to $\{F^+, F^-\}$

We have by (20) that for $w \in \mathbb{R}^3$ satisfying $w \cdot n = 0$

$$\Pi(A)w = F^+w = F^-w = Fw \qquad \text{for all } A \in \mathbb{R}^{3\times 3}. \tag{26}$$

Thus, it follows from (6) and (26) that for $w \cdot n = 0$

$$\begin{aligned}[R(A) - I]\, F^+w &= [R(A) - I]\, \Pi(A)w = [\pi(A) - F]\, w \\ &= [\pi(A) - A]\, w + [A - F]\, w \qquad \text{for all } A \in \mathbb{R}^{3\times 3}.\end{aligned} \tag{27}$$

We then obtain by applying the triangle inequality to (27) with $A = \nabla v_h(x)$ and estimating the two terms by Lemma 1 and Theorem 2 that

$$\begin{aligned}&\int_\Omega \left|[R(\nabla v_h(x)) - I]\, F^+w\right|^2 dx \\ &\quad\leq 2\int_\Omega \left|[\pi(\nabla v_h(x)) - \nabla v_h(x)]\, w\right|^2 dx + 2\int_\Omega \left|[\nabla v_h(x) - F]\, w\right|^2 dx \\ &\quad\leq C\mathcal{E}(v_h) + C\mathcal{E}(v_h)^{\frac{1}{2}} \qquad \text{for } w \cdot n = 0.\end{aligned} \tag{28}$$

Next, since F^+ is nonsingular by (1), we can choose $w_1 \in \mathbb{R}^3$ and $w_2 \in \mathbb{R}^3$ to satisfy

$$\begin{aligned}w_1 \cdot n = w_2 \cdot n = 0, \qquad F^+w_1 \cdot F^+w_2 = 0, \\ |F^+w_1| = |F^+w_2| = 1.\end{aligned} \tag{29}$$

Now, for

$$m = F^+w_1 \times F^+w_2, \tag{30}$$

we have that

$$Qm = QF^+w_1 \times QF^+w_2 \qquad \text{for all } Q \in \mathrm{SO}(3).$$

So, for all $A \in \mathbb{R}^{3\times 3}$ we have the identity

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

Hence, it follows from the above identity with $A = \nabla v_h(x)$ and the estimates (28) that

$$\int_\Omega |[R(\nabla v_h(x)) - I]\, m|^2 \, dx \le C\mathcal{E}(v_h)^{1/2} + C\mathcal{E}(v_h). \tag{31}$$

Since $\{F^+ w_1, F^+ w_2,\ m\}$ is a basis for $\mathbb{R}^3$ by (29) and (30), we have from (28) and (31) that

$$\int_\Omega \|[R(\nabla v_h(x)) - I]\|^2 \, dx \le C\mathcal{E}(v_h)^{1/2} + C\mathcal{E}(v_h) \qquad \text{for all } v_h \in \mathcal{M}_h^F. \tag{32}$$

Theorem 4 is now proven by applying the triangle inequality to the identity

$$\begin{aligned} A - \Pi(A) &= [A - \pi(A)] + [\pi(A) - \Pi(A)] \\ &= [A - \pi(A)] + [R(A) - I]\,\Pi(A) \qquad \text{for all } A \in \mathbb{R}^{3\times 3} \end{aligned}$$

with $A = \nabla v_h(x)$ and by estimating the two terms by Lemma 1 and (32). □

7 Convergence of the Microstructure

Proof of Theorem 5. We have that

$$\begin{aligned} &\left[\text{meas}(\omega_\rho^+) - \lambda^+ \text{meas}(\omega)\right] F^+ + \left[\text{meas}(\omega_\rho^-) - \lambda^- \text{meas}(\omega)\right] F^- \\ &\quad = \int_\omega (\Pi(\nabla v_h(x)) - F)\, dx - \int_{\omega - \{\omega_\rho^+ \cup \omega_\rho^-\}} \Pi(\nabla v_h(x))\, dx. \end{aligned}$$

Now by the triangle inequality, the Cauchy-Schwarz inequality, Theorem 3, and Theorem 4, we have that

$$\begin{aligned} &\left\| \int_\omega (\Pi(\nabla v_h(x)) - F)\, dx \right\| \\ &\quad \le \left\| \int_\omega (\Pi(\nabla v_h(x)) - \nabla v_h(x))\, dx \right\| + \left\| \int_\omega (\nabla v_h(x) - F)\, dx \right\| \\ &\quad \le \text{meas}(\omega)^{1/2} \left[\int_\omega \|\Pi(\nabla v_h(x)) - \nabla v_h(x)\|^2 \, dx \right]^{1/2} + C\mathcal{E}(v_h)^{1/8} + C\mathcal{E}(v_h)^{1/2} \\ &\quad \le C\mathcal{E}(v_h)^{1/8} + C\mathcal{E}(v_h)^{1/2} \qquad \text{for all } v_h \in \mathcal{M}_h^F. \end{aligned} \tag{33}$$

Also, we observe that by the definition of $\omega_\rho^\pm(v_h)$,

$$\text{meas}\big(\omega - \{\omega_\rho^+ \cup \omega_\rho^-\}\big) \le \frac{1}{\rho} \int_{\omega - \{\omega_\rho^+ \cup \omega_\rho^-\}} \|\Pi(\nabla v_h(x)) - \nabla v_h(x)\| \, dx. \tag{34}$$

Hence, since $\|\Pi(A)\| = \|F^+\|$ or $\|F^-\|$ for all $A \in \mathbb{R}^{3\times 3}$, we can obtain from (34) and Theorem 4 that

$$\begin{aligned}
\left\| \int_{\omega - \{\omega_\rho^+ \cup \omega_\rho^-\}} \Pi\left(\nabla v_h(x)\right)\, dx \right\| &\le C\text{meas}\big(\omega - \{\omega_\rho^+ \cup \omega_\rho^-\}\big) \\
&\le \frac{C}{\rho} \int_{\omega - \{\omega_\rho^+ \cup \omega_\rho^-\}} \|\Pi\left(\nabla v_h(x)\right) - \nabla v_h(x)\|\, dx \\
&\le \frac{C\text{meas}(\omega)^{1/2}}{\rho} \left[\int_\omega \|\Pi\left(\nabla v_h(x)\right) - \nabla v_h(x)\|^2\, dx \right]^{1/2} \\
&\le C\mathcal{E}(v_h)^{1/4} + C\mathcal{E}(v_h)^{1/2}. \qquad (35)
\end{aligned}$$

Hence, we have from (33) and (35) that

$$\begin{aligned}
&\left\| \left[\text{meas}(\omega_\rho^+) - \lambda^+\text{meas}(\omega)\right] F^+ + \left[\text{meas}(\omega_\rho^-) - \lambda^-\text{meas}(\omega)\right] F^- \right\| \\
&\qquad \le C\mathcal{E}(v_h)^{1/8} + C\mathcal{E}(v_h)^{1/2}. \qquad (36)
\end{aligned}$$

The result of Theorem 5 now follows from the linear independence of F^+ and F^-. □

8 Convergence of Nonlinear Integrals of the Deformation Gradient

Proof of Theorem 6. We have that

$$\begin{aligned}
&\int_\Omega \left\{ f\left(x, \nabla v_h(x)\right) - \left[\lambda^+ f(x, F^+) + \lambda^- f(x, F^-)\right] \right\} dx \\
&\quad = \int_\Omega \left[f\left(x, \nabla v_h(x)\right) - f\left(x, \Pi\left(\nabla v_h(x)\right)\right) \right] dx \\
&\qquad + \int_\Omega \left\{ f\left(x, \Pi\left(\nabla v_h(x)\right)\right) - \left[\lambda^+ f(x, F^+) + \lambda^- f(x, F^-)\right] \right\} dx \\
&\quad = \mathcal{J}_1 + \mathcal{J}_2.
\end{aligned}$$

We estimate the term $\mathcal{J}_1$ by Theorem 4 as follows:

$$\begin{aligned}
|\mathcal{J}_1| &\le \int_\Omega \left\| \frac{\partial f}{\partial A}(x, \cdot) \right\|_{L^\infty} \|\nabla v_h(x) - \Pi\left(\nabla v_h(x)\right)\|\, dx \\
&\le \left[\int_\Omega \left\| \frac{\partial f}{\partial A}(x, \cdot) \right\|_{L^\infty}^2 dx \right]^{1/2} \left[\int_\Omega \|\nabla v_h(x) - \Pi\left(\nabla v_h(x)\right)\|^2\, dx \right]^{1/2} \\
&\le C \left[\int_\Omega \left\| \frac{\partial f}{\partial A}(x, \cdot) \right\|_{L^\infty}^2 dx \right]^{1/2} \left(\mathcal{E}(v_h)^{1/4} + \mathcal{E}(v_h)^{1/2} \right). \qquad (37)
\end{aligned}$$

Now we have for $G(x) = f(x, F^+) - f(x, F^-)$ that

$$
\begin{aligned}
f\left(x, \Pi\left(A\right)\right) &- \left[\lambda^+ f(x, F^+) + \lambda^- f(x, F^-)\right] \\
&= \frac{1}{|a|^2} \left\{a \cdot \left[\Pi(A) - F\right] n\right\} \left[f(x, F^+) - f(x, F^-)\right] \\
&= \frac{1}{|a|^2} \left\{a \cdot \left[\Pi(A) - F\right] n\right\} G(x),
\end{aligned} \tag{38}
$$

so we have from (38) and integration by parts that

$$
\begin{aligned}
\mathcal{J}_2 &= \int_\Omega \left\{f\left(x, \Pi\left(\nabla v_h(x)\right)\right) - \left[\lambda^+ f(x, F^+) + \lambda^- f(x, F^-)\right]\right\} \, dx \\
&= \frac{1}{|a|^2} \int_\Omega \left\{a \cdot \left[\Pi\left(\nabla v_h(x)\right) - F\right] n\right\} G(x) \, dx \\
&= \frac{1}{|a|^2} \int_\Omega \left\{a \cdot \left[\Pi\left(\nabla v_h(x)\right) - \nabla v_h(x)\right] n\right\} G(x) \, dx \\
&\quad + \frac{1}{|a|^2} \int_\Omega \left\{a \cdot \left[\nabla v_h(x) - F\right] n\right\} G(x) \, dx \\
&= \frac{1}{|a|^2} \int_\Omega \left\{a \cdot \left[\Pi\left(\nabla v_h(x)\right) - \nabla v_h(x)\right] n\right\} G(x) \, dx \\
&\quad - \frac{1}{|a|^2} \int_\Omega \left\{a \cdot \left[v_h(x) - Fx\right]\right\} \left\{\nabla G(x) \cdot n\right\} \, dx.
\end{aligned}
$$

We thus obtain from the Cauchy-Schwarz inequality, Lemma 2, and Theorem 4 that

$$
|\mathcal{J}_2| \le C \left\{\int_\Omega |\nabla G(x) \cdot n|^2 \, dx + \int_\Omega G(x)^2 \, dx\right\}^{1/2} \left(\mathcal{E}(v_h)^{1/4} + \mathcal{E}(v_h)^{1/2}\right). \tag{39}
$$

The result of Theorem 6 now follows from (37) and (39). □

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