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The stability and numerical analysis of martensitic microstructure

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The elastic energy density in the geometrically nolinear theory of martensite is minimized on multiple, rotationally invariant energy wells. For such energy densities, the gradients of energy-minimizing sequences can oscillate between the energy wells to approach the lowest energy. In this paper, we describe a stability theory for this microstructure, and we apply this stability theory to the finite element approximation of microstructure.

1 Introduction

Martensitic crystals are crystals which can undergo a phase transformation from a high temperature, solid phase (austenite) to a low temperature, less symmetric solid phase (martensite). This transformation is utilized in many new technologies that are based on the "shape-memory" property [28].

A geometrically nonlinear elasticity theory for the equilibrium configuration of martensitic crystals has been given by [3, 4, 15–17, 19]. In this theory, an energy-minimizing deformation is an equilibrium configuration of the crystal. However, the elastic energy density for a martensitic crystal has multiple, symmetry-related, rotationally invariant energy wells. For some boundary conditions, the deformation can only attain the minimum energy by the oscillation of its gradient between the energy wells on an infinitesimal scale.

We shall give a brief survey of this theory in §2 and §3 below. We refer the reader to [24] for a comprehensive introduction to the geometrically nonlinear theory of martensitic crystals, to microstructure, and to its numerical approximation.

In §4, we give a survey of the basic results on the stability of martensitic microstructure, and in §5 we give applications of this theory to the finite element approximation of martensitic microstructure. More detailed treatments and full proofs of the results are given in [7, 20–23]. An analysis of the stability and numerical approximation of microstructure in micromagnetics is given in [25]. Related results on the approximation of nonconvex variational problems can be found in [8, 9, 18, 27].

2 The Geometrically Nonlinear Theory of Martensite

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

$$\mathcal{E}(y) = \int_\Omega \phi(\nabla y(x))\, dx, \tag{1}$$

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

$$W^\phi = \left\{ y \in C(\bar{\Omega}; \mathbb{R}^3) : \int_\Omega \phi(\nabla y(x))\, dx < \infty \right\}. \tag{2}$$

The elastic energy density attains its minimum value (below the transformation temperature) on a set

$$\mathcal{U} \equiv \mathrm{SO}(3)U_1 \cup \cdots \cup \mathrm{SO}(3)U_N, \tag{3}$$

where SO(3) is the group of proper rotations defined by

$$\mathrm{SO}(3) = \left\{ Q \in \mathbb{R}^{3\times 3} : Q^T = Q^{-1} \text{ and } \det Q = 1 \right\},$$

and where the symmetry-related matrices, $U_1, \cdots, U_N$, for $N > 1$, represent the martensitic variants. The martensitic variants $U_1, \cdots, U_N$ are linear transformations which transform the lattice of the austenitic phase into the lattice of the martensitic phase.

Thus, we have (after adding a constant to the energy density) that

$$\begin{aligned} \phi(F) \geq 0, \qquad & \forall F \in \mathbb{R}^{3\times 3}, \\ \phi(F) = 0 \quad \text{if and only if} \quad & F \in \mathcal{U} \equiv \mathrm{SO}(3)U_1 \cup \cdots \cup \mathrm{SO}(3)U_N. \end{aligned}$$

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

$$\phi(F) \geq \kappa \|F - \pi(F)\|^2, \qquad \forall F \in \mathbb{R}^{3\times 3}, \tag{4}$$

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

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

In the above and in the following we use the matrix norm defined by

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

We have given an analysis of the stability of microstructure and of its numerical approximation for the following three phase transformations.

2.1 The Orthorhombic to Monoclinic Transformation

We first gave a stability analysis and numerical analysis of the approximation of the martensitic microstructure for the orthorhombic to monoclinic transformation [23]. The orthorhombic to monoclinic transformation has two rotationally invariant energy wells ($N = 2$). The energy wells for an orthorhombic to monoclinic transformation are determined by the martensitic variants

$$U_1 = (I + \eta e_2 \otimes e_1)D, \qquad U_2 = (I - \eta e_2 \otimes e_1)D, \tag{5}$$

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 diagonal, positive definite, linear transformation 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 $d_1, d_2, d_3 > 0$. We recall that the tensor $a \otimes n$ for $a, n \in \mathbb{R}^3$ defines the linear transformation $(a \otimes n)v = (n \cdot v)a$ for $v \in \mathbb{R}^3$.

2.2 The Cubic to Tetragonal Transformation

We next gave an analysis of stability and numerical approximation for the cubic to tetragonal transformation [21]. The cubic to tetragonal transformation has three rotationally invariant energy wells ($N = 3$). We note that the analysis of the stability of microstructure becomes more difficult as the number of energy wells increases since additional wells give the crystal additional freedom to deform without the cost of additional energy. We also note that although it can be shown that all problems with two rotationally invariant energy wells with a rank-one connection (see below) are equivalent [3], the analysis of the cubic to tetragonal transformation must utilize the specific form of the martensitic variants U_1, U_2, U_3.

The energy wells for a cubic to tetragonal transformation are determined by the martensitic variants

$$\begin{gathered} U_1 = \eta_1 I + (\eta_2 - \eta_1) e_1 \otimes e_1, \qquad U_2 = \eta_1 I + (\eta_2 - \eta_1) e_2 \otimes e_2, \\ U_3 = \eta_1 I + (\eta_2 - \eta_1) e_3 \otimes e_3, \end{gathered} \tag{6}$$

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 $\mathbb{R}^3$.

2.3 The Cubic to Orthorhombic Transformation

We have recently extended our stability analysis to the cubic to orthorhombic transformation [7]. The fact that the energy density for the cubic to orthorhombic transformation has six wells ($N = 6$) makes this problem significantly more difficult than the cubic to tetragonal transformation which has three wells ($N = 3$).

The uniqueness of the microstructure for the cubic to orthorhombic transformation, which had been an open problem, is a consequence of this stability analysis. This analysis also gives some rigorous justification for the assumption made by all of the analytical and computational research on the Chu-James experiment that the deformation gradient takes values in only two of the wells [1, 2, 10].

The six transformation matrices are given by [4, 5, 10]

$$U_1 = \begin{pmatrix} \zeta & 0 & 0 \\ 0 & \xi & \eta \\ 0 & \eta & \xi \end{pmatrix}, \qquad U_2 = \begin{pmatrix} \zeta & 0 & 0 \\ 0 & \xi & -\eta \\ 0 & -\eta & \xi \end{pmatrix},$$
$$U_3 = \begin{pmatrix} \xi & 0 & \eta \\ 0 & \zeta & 0 \\ \eta & 0 & \xi \end{pmatrix}, \qquad U_4 = \begin{pmatrix} \xi & 0 & -\eta \\ 0 & \zeta & 0 \\ -\eta & 0 & \xi \end{pmatrix}, \tag{7}$$
$$U_5 = \begin{pmatrix} \xi & \eta & 0 \\ \eta & \xi & 0 \\ 0 & 0 & \zeta \end{pmatrix}, \qquad U_6 = \begin{pmatrix} \xi & -\eta & 0 \\ -\eta & \xi & 0 \\ 0 & 0 & \zeta \end{pmatrix}.$$

The material parameters ξ, η, and ζ are defined by

$$\xi = \frac{\alpha + \gamma}{2}, \qquad \eta = \frac{\alpha - \gamma}{2}, \qquad \zeta = \beta,$$

where α, β, and γ are the transformation strains, that is, the principal strains of a linear transformation that transforms the cubic lattice to the orthorhombic lattice. We can assume without loss of generality that

$$\eta > 0, \qquad \xi > \eta, \qquad \zeta > 0. \tag{8}$$

We can assume the first one by renumbering the variants if necessary and the last two by the requirement that a transformation matrix is always symmetric positive definite.

3 Microstructure

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

$$F_1 - F_0 = a \otimes n \tag{9}$$

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 [3, 4, 6, 7, 10, 24]. The lemma states that there is no rank-one connection between $\mathrm{SO}(3)U_i$ and itself; and that for any $i, j,\ i \neq j$, there are exactly two rank-one connections between $\mathrm{SO}(3)U_i$ and $\mathrm{SO}(3)U_j$.

Lemma 3.1 *The following result holds for the orthorhombic to monoclinic transformation* (5)*, the cubic to tetragonal transformation* (6)*, and the cubic to orthorhombic transformation* (7)*.*

(1) For each i, there do not exist matrices R_1U_i and R_2U_i with distinct $R_1, R_2 \in SO(3)$ that are rank-one connected.

(2) For any $i, j,\ i \neq j$, 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. In this case, we also have for any $\lambda \in (0, 1)$ that

$$\lambda QU_i + (1-\lambda)U_j \notin SO(3)U_1 \cup \cdots \cup SO(3)U_N. \tag{10}$$

If F_0 and F_1 are rank-one connected as in (9), then we can construct a continuous deformation having parallel planar interfaces

$$S_i = \{x \in \Omega : x \cdot n = s_i\}$$

for $s_1 < \cdots < s_m$ with the same normal n separating the layers in which the deformation gradient alternates between F_0 and F_1 by

$$w(x) = F_0 x + \left[\int_0^{x\cdot n} \chi(s)\ ds\right] a, \tag{11}$$

where $\chi(s) : \mathbb{R} \to \mathbb{R}$ is the characteristic function

$$\chi(s) = \begin{cases} 0 \text{ if } x \in (s_{2l}, s_{2l+1}) \text{ for } 0 \leq 2l \leq m \text{ where } l \in \mathbb{Z}, \\ 1 \text{ if } x \in (s_{2l+1}, s_{2l+2}) \text{ for } 1 \leq 2l+1 \leq m \text{ where } l \in \mathbb{Z}, \end{cases}$$

where we take $s_0 = -\infty$ and $s_{m+1} = \infty$. This deformation satisfies the property that

$$\nabla w(x) = F_0 + \chi(x \cdot n) a \otimes n = \begin{cases} F_0 \text{ for all } x \text{ such that } \chi(x \cdot n) = 0, \\ F_1 \text{ for all } x \text{ such that } \chi(x \cdot n) = 1. \end{cases}$$

Deformations $w(x)$ of the form (11) with layer thickness $s_{i+1} - s_i$ small for $i = 1, \dots, m$ are the simplest examples of *microstructure*.

In this paper, we consider the minimization of the elastic energy (1) with respect to deformations $y \in W^{1,\infty}(\Omega; \mathbb{R}^3)$ which are constrained by $y(x) = y_\lambda(x)$ for $x \in \partial\Omega$ where [21]

$$\begin{aligned} y_\lambda(x) &= F_0 x + l(x) a, \qquad && x \in \Omega, \\ \nabla l(x) &= \lambda(x) n && \text{a.e. } \ x \in \Omega, \end{aligned} \tag{12}$$

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 (1) in the set of admissible deformations defined by

$$W^{1,\infty}_\lambda(\Omega; \mathbb{R}^3) = \left\{ y \in W^{1,\infty}(\Omega; \mathbb{R}^3) : y = y_\lambda \text{ on } \partial\Omega \right\}.$$

We note that

$$\nabla y_\lambda(x) = F_0 + \lambda(x) a \otimes n,$$

so by (10) we have that

$$\phi\left(\nabla y_\lambda(x)\right) > 0 \quad \text{for all } x \text{ such that } \quad 0 < \lambda(x) < 1.$$

Hence, we have that

$$\mathcal{E}(y_\lambda) > 0$$

if $\text{meas}\left\{ x \in \Omega : 0 < \lambda(x) < 1 \right\} > 0$.

A special case of (12) is given by

$$y_\lambda(x) = F_0 x + \left[\int_0^{x \cdot n} \tilde{\lambda}(s) ds + \zeta \right] a, \qquad x \in \Omega, \tag{13}$$

for some $\zeta \in \mathbb{R}^3$ where $\lambda(x) = \tilde{\lambda}(x \cdot n)$ for $\tilde{\lambda}(s) \in L^\infty(\mathbb{R})$. If $y_\lambda(x)$ has the form (13), then we show in [21] that there exist a family of deformations $\hat{u}_\gamma \in W^{1,\infty}_\lambda(\Omega;\mathbb{R}^3)$, $\gamma \in (0,\gamma_0]$, for any fixed $\gamma_0 > 0$, such that

$$\lim_{\gamma \to 0} \mathcal{E}(\hat{u}_\gamma) = 0. \tag{14}$$

The family of deformations $\hat{u}_\gamma \in W^{1,\infty}_\lambda(\Omega;\mathbb{R}^3)$ can be constructed to have the form (11) in the interior of Ω with layer thickness $s_{i+1} - s_i = \mathrm{O}(\gamma)$ as $\gamma \to 0$. The value of the deformations $\hat{u}_\gamma \in W^{1,\infty}_\lambda(\Omega;\mathbb{R}^3)$ in a boundary layer of thickness $\mathrm{O}(\gamma)$ as $\gamma \to 0$ is defined by interpolation to ensure that the boundary conditions are satisfied [21].

Even though we can construct deformations $y \in W^{1,\infty}_\lambda(\Omega;\mathbb{R}^3)$ with energy arbitrarily close to the mininum, we prove in [21] that there does not exist $y \in W^{1,\infty}_\lambda(\Omega;\mathbb{R}^3)$ such that $\mathcal{E}(y) = 0$ if

$$\text{meas}\,\{x \in \Omega : 0 < \lambda(x \cdot n) < 1\} > 0. \tag{15}$$

The results in the following section demonstrate the the gradients of energy-minimizing sequences of deformations must oscillate between the energy wells with a length scale which converges to zero.

4 The Stability of Microstructure

The results in this section hold for the orthorhombic to monoclinic transformation [21, 23],the cubic to tetragonal transformation [20, 21], and the cubic to orthorhombic transformation [7].

The first step in proving the stability of microstructure is the following theorem that gives an error bound for the L^2 approximation of the directional derivative of the limiting macroscopic deformation y_λ in any direction tangential to parallel layers of the laminate.

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

$$\int_\Omega |[\nabla y(x) - \nabla y_\lambda(x)]\, w|^2 \, dx \le C \left[\mathcal{E}(y)^{\frac{1}{2}} + \mathcal{E}(y)\right], \qquad \forall y \in W^{1,\infty}_\lambda(\Omega;\mathbb{R}^3), \tag{16}$$

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

The next result gives an error bound for the L^2 approximation of the limiting macroscopic deformation y_λ by admissible deformations $y \in W^{1,\infty}_\lambda(\Omega;\mathbb{R}^3)$. It follows directly from (16) and Poincaré's inequality.

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

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

We next give a result shows that the gradient of a low energy deformation must oscillate between F_0 and F_1. To describe the result, 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 also define the operators $\Theta : \mathbb{R}^{3\times 3} \to \mathrm{SO}(3)$ and $\Pi : \mathbb{R}^{3\times 3} \to \{F_0, F_1\}$ by the relation

$$\pi_{12}(F) = \Theta(F)\Pi(F), \qquad \forall F \in \mathbb{R}^{3\times 3}. \tag{17}$$

We can now give an estimate for the difference between $\nabla y(x)$ and $\Pi(\nabla y(x))$.

Theorem 4.3 *There exists a constant $C > 0$ such that*

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

We next give an estimate for the approximation of volume fractions. Our estimate states that for any energy minimizing sequence $\{y_k\}$ in $W^{1,\infty}_\lambda(\Omega;\mathbb{R}^3)$ and for almost all $x \in \Omega$, 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 $\lambda(x)$.

To state this result, for any subset $\omega \subset \Omega$, $\rho > 0$, and $y \in W^{1,\infty}_\lambda(\Omega;\mathbb{R}^3)$, we define the sets

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

and the mean value of λ on ω by

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

Theorem 4.4 *For any Lipschitz domain $\omega \subset \Omega$ and any $\rho > 0$ there exists a positive constant C such that*

$$\operatorname{meas}\left(\omega - \{\omega^0_\rho(y) \cup \omega^1_\rho(y)\}\right) \le C\left[\mathcal{E}(y)^{\frac{1}{2}} + \mathcal{E}(y)\right], \tag{18}$$

for all $y \in W^{1,\infty}_\lambda(\Omega;\mathbb{R}^3)$ *and*

$$\left|\frac{\operatorname{meas}\omega^0_\rho(y)}{\operatorname{meas}\omega} - (1-\tilde{\lambda}_\omega)\right| + \left|\frac{\operatorname{meas}\omega^1_\rho(y)}{\operatorname{meas}\omega} - \tilde{\lambda}_\omega\right| \le C\left[\mathcal{E}(y)^{\frac{1}{8}} + \mathcal{E}(y)\right] \qquad (19)$$

for all $y \in W^{1,\infty}_\lambda(\Omega;\mathbb{R}^3)$.

Our final result describes the convergence of nonlinear integrals of $\nabla y(x)$. We define $\mathcal{V}$ to be the Sobolev space of all functions $f \in L^2\left(\Omega \times \mathbb{R}^{3\times 3}\right)$ such that

$$\|f\|^2_{\mathcal{V}} = \int_\Omega \left[\operatorname*{ess\,sup}_{F\in\mathbb{R}^{3\times 3}} \|\nabla_F f(x,F)\|\right]^2 dx + \|G_f\|^2_{W^{1,2}(\Omega)} < \infty, \qquad (20)$$

where

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

Since thermodynamic variables such as the energy density and stress are nonlinear functions of $\nabla y(x)$, the following lemma allows us to define macroscopic or average values of the thermodynamics variables to deformations with microstructure.

Theorem 4.5 *There exists a constant* $C > 0$ *such that*

$$\begin{aligned}&\left|\int_\Omega \{f\,(x,\nabla y(x)) - [(1-\lambda(x))f(x,F_0) + \lambda(x)f(x,F_1)]\}\,dx\right|\\ &\le C\|f\|_{\mathcal{V}}\left[\mathcal{E}(y)^{\frac{1}{4}} + \mathcal{E}(y)^{\frac{1}{2}}\right], \quad \forall y \in W^{1,\infty}_\lambda(\Omega;\mathbb{R}^3),\ \forall f \in \mathcal{V}. \qquad (21)\end{aligned}$$

This result (21) and the previous result (18) demonstrate that $\nabla y(x)$ converges to $(1-\lambda(x))\delta_{F_0} + \lambda(x)\delta_{F_1}$ in the sense of the Young measure [4, 24].

5 The Finite Element Approximation of Microstructure

We shall assume in what follows that the reference configuration $\Omega \subset \mathbb{R}^3$ is a polyhedral domain. For a fixed positive maximal mesh diameter h_0, let τ_h, $0 < h \le h_0$, be a family of quasi-regular 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. For simplicity, 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, 26]. Deformations with microstructure are typically approximately piecewise linear, so the use of piecewise linear elements is a good choice of finite element space for the approximation of deformations with fine-scale microstructure.

We define the interpolation operator $\mathcal{I}_h : C(\bar{\Omega};\mathbb{R}^3) \to \mathcal{A}_h$ for each $h \in (0, h_0]$ to be the operator which interpolates the values at the vertices of the tetrahedral elements T of τ_h. We approximate the boundary data $y_\lambda \in W^{1,\infty}(\Omega;\mathbb{R}^3)$, given in (13), by defining the finite element deformation $y_{\lambda h} \in \mathcal{A}_h$ by

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

We can then define the finite element space of admissible deformations

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

We note that if $\lambda(x)$ is independent of x, then $\mathcal{A}_{\lambda h} \subset W^{1,\infty}_\lambda(\Omega;\mathbb{R}^3)$, but otherwise $\mathcal{A}_{\lambda h} \not\subset W^{1,\infty}_\lambda(\Omega;\mathbb{R}^3)$.

In §4, we gave various bounds for the approximation of the microstructure in terms of the elastic energy $\mathcal{E}$. Thus, to analyze the approximation of the microstructure by the finite element method, we need the following result on the minimization of the elastic energy $\mathcal{E}$ on the space $\mathcal{A}_{\lambda h}$.

Theorem 5.1 *There exists $y_h \in \mathcal{A}_{\lambda h}$ for each $h \in (0, h_0]$ such that*

$$\mathcal{E}(y_h) = \min_{z_h \in \mathcal{A}_{\lambda h}} \mathcal{E}(z_h) \le C h^{1/2}. \tag{22}$$

If $\lambda(x)$ is independent of x so that $\mathcal{A}_{\lambda h} \subset W^{1,\infty}_\lambda(\Omega;\mathbb{R}^3)$, then the result (22) can be used with the stability results in the previous section to immediately derive estimates for the finite element approximation of microstructure. We shall give results below for the more general case when $\lambda(x)$ is dependent on x and $\mathcal{A}_{\lambda h} \not\subset W^{1,\infty}_\lambda(\Omega;\mathbb{R}^3)$.

There are local minima for the problem

$$\inf_{y_h \in \mathcal{A}_{\lambda h}} \mathcal{E}(y_h) \tag{23}$$

which are approximations on different length scales to the same optimal microstructure [24]. In fact, the number of local minima of the problem (23) grows arbitrarily large as the mesh size $h \to 0$. For this reason, we give error estimates for finite element deformations $y_h \in \mathcal{A}_{\lambda h}$ that satisfy the quasi-optimality condition

$$\mathcal{E}(y_h) \le \alpha \inf_{z_h \in \mathcal{A}_{\lambda h}} \mathcal{E}(z_h) \tag{24}$$

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

The following estimates for the finite element approximation of the deformation y_λ by deformations $y_h \in \mathcal{A}_{\lambda h}$ are similar to those for the deformations $y \in W^{1,\infty}_\lambda(\Omega;\mathbb{R}^3)$ in the previous section, but additional terms are needed to account for the fact that $\mathcal{A}_{\lambda h} \not\subset W^{1,\infty}_\lambda(\Omega;\mathbb{R}^3)$.

Theorem 5.2 *We have for any $w \in \mathbb{R}^3$ such that $w \cdot n = 0$ and $|w| = 1$ that*

$$\int_\Omega |[\nabla y_h(x) - \nabla y_\lambda(x)]\, w|^2 \, dx \le C\left[\mathcal{E}(y_h)^{\frac{1}{2}} + \mathcal{E}(y_h) + \|y_\lambda - y_{\lambda h}\|_{L^2(\partial\Omega;\mathbb{R}^3)}\right], \tag{25}$$

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

Theorem 5.3 *We have*

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

We recall the operator $\Pi : \mathbb{R}^{3\times 3} \to \{F_0, F_1\}$ defined by (17). We then have the following extension to Theorem 4.3.

Theorem 5.4 *We have*

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

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

We recall that $\tilde{\lambda}_\omega$ is the average of λ on ω. We can then obtain the following extension of Theorem 4.4.

Theorem 5.5 *For any Lipschitz domain $\omega \subset \Omega$ and any $\rho > 0$ there exists a positive constant $C = C(\omega, \rho)$, independent of h, such that*

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

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

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

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

We next give the following extension of Theorem 4.5 for admissible finite element deformations.

Theorem 5.6 *We have*

$$\left|\int_\Omega \{f(x,\nabla y_h(x)) - [(1-\lambda(x))f(x,F_0) + \lambda(x)f(x,F_1)]\}\ dx\right|$$
$$\leq C\|f\|_{\mathcal{V}}\left[\mathcal{E}(y_h)^{\frac{1}{4}} + \mathcal{E}(y_h)^{\frac{1}{2}} + \|y_\lambda - y_{\lambda h}\|^{\frac{1}{2}}_{L^2(\partial\Omega;\mathbb{R}^3)} + \|y_\lambda - y_{\lambda h}\|_{L^2(\partial\Omega;\mathbb{R}^3)}\right] \tag{26}$$

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

We have that $\nabla y_\lambda = F_0 + \lambda a \otimes n \in L^\infty(\Omega;\mathbb{R}^3)$ since $\lambda \in L^\infty(\Omega)$. It then follows from well-known estimates for the interpolation error [11, 26] that

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

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

$$\|y_\lambda - y_{\lambda h}\|_{L^2(\partial\Omega;\mathbf{R}^3)} \leq Ch. \tag{27}$$

We can now substitute (22) and (27) into the theorems given in this section to obtain the following error estimates for quasi-optimal finite element deformations $y_h \in \mathcal{A}_{\lambda h}$.

Corollary 5.1 *We have*

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

for any $w \in \mathbb{R}^3$ such that $w \cdot n = 1$ and $|w| = 1$, and for any $y_h \in \mathcal{A}_{\lambda h}$ that satisfies the quasi-optimality condition (24)*.*

Corollary 5.2 *We have*

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

for any $y_h \in \mathcal{A}_{\lambda h}$ that satisfies the quasi-optimality condition (24)*.*

Corollary 5.3 *We have*

$$\int_\Omega \|\nabla y_h(x) - \Pi(\nabla y_h(x))\|^2\ dx \leq Ch^{\frac{1}{4}}$$

for any $y_h \in \mathcal{A}_{\lambda h}$ that satisfies the quasi-optimality condition (24)*.*

Corollary 5.4 *For any Lipschitz domain $\omega \subset \Omega$ and any $\rho > 0$ there exists a positive constant $C = C(\omega, \rho)$, independent of h, such that*

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

and

$$\left|\frac{\text{meas}\,\omega_\rho^0(y_h)}{\text{meas}\,\omega} - (1 - \tilde{\lambda}_\omega)\right| + \left|\frac{\text{meas}\,\omega_\rho^1(y_h)}{\text{meas}\,\omega} - \tilde{\lambda}_\omega\right| \leq Ch^{\frac{1}{16}}$$

for any $y_h \in \mathcal{A}_{\lambda h}$ that satisfies the quasi-optimality condition (24).

Corollary 5.5 *We have*

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

for any $f \in \mathcal{V}$ and any $y_h \in \mathcal{A}_{\lambda h}$ that satisfies the quasi-optimality condition (24).

5.1 Nonconforming elements

Continuous finite element spaces effectively approximate microstructure with layers that are parallel to the planes across which the finite element deformation gradients can be discontinuous, but they have difficulty approximating microstructure on the scale of the mesh when the layers are not oriented with respect to the mesh. Computational experiments with the continuous, piecewise linear element for a two-dimensional model have shown that numerical solutions for microstructure given by conforming spaces can have a layer thickness that is large compared to the grid if the layers are not oriented with respect to the mesh [12, 24].

Since nonconforming finite element approximations are not required to be globally continuous [11, 26], it is reasonable to think that they would be able to give a more accurate approximation to fine-scale microstructure when the microstructure is not aligned with the mesh [24]. We have demonstrated that all the estimates obtained in this section hold for the nonconforming element analyzed in [22].

Another promising approach has been to relax the constraints of continuous finite elements by using reduced integration on bilinear finite elements [14]. The theory given in §4 has been utilized in [13] to obtain results for the reduced integration approximation that are similar to those given in this section.

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