

MULTISCALE RESOLUTION IN THE COMPUTATION OF CRYSTALLINE MICROSTRUCTURE

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ABSTRACT. This paper addresses the numerical approximation of microstructures in crystalline phase transitions without surface energy. It is shown that branching of different variants near interfaces of twinned martensite and simple austenite phases leads to reduced energies in finite element approximations. Such behavior of minimizing deformations is understood for an extended model that involves surface energies. Moreover, the closely related question of the role of different growth conditions of the employed bulk energy is discussed. By explicit construction of discrete deformations in lowest order finite element spaces we prove upper bounds for the energy and thereby clarify the question of the dependence of the convergence rate upon growth conditions and lamination orders. For first order laminates the estimates are optimal.

Keywords: finite element method, non-convex minimization, multi-well problem, microstructure, multiscale analysis, nonlinear elasticity

Subject Classification: 65K10, 65M50, 65N30, 73C50, 73S10

1. INTRODUCTION

The mathematical model of phase transitions in crystalline solids leads to the minimization of a non-quasiconvex functional over a space of admissible deformations. Following the work of [1, 2] we consider the variational problem: *Find* $u \in \mathcal{A}$ *such that* $I(u) = \inf_{v \in \mathcal{A}} I(v)$. Here,

$$\mathcal{A} := \left\{ v \in W^{1,p}(\Omega; \mathbb{R}^n) : v(x) = Fx \text{ for all } x \in \partial\Omega \right\},$$

where $\Omega \subseteq \mathbb{R}^n$, $n = 2, 3$, is a bounded Lipschitz domain, $F \in \mathbb{R}^{n \times n}$ is a given homogeneous deformation gradient and serves as the boundary data. For $v \in W^{1,p}(\Omega; \mathbb{R}^n)$ the energy functional $I : W^{1,p}(\Omega; \mathbb{R}^n) \rightarrow \mathbb{R}$ is defined by

$$I(v) := \int_{\Omega} W_{\theta}(\nabla v) dx.$$

W_{θ} is a temperature-dependent, continuous energy density such that, for all $G \in \mathbb{R}^{n \times n}$, there holds

$$c_1 |G|^p - c_2 \leq W_{\theta}(G) \leq c_2 (|G|^p + 1)$$

with constants $c_1, c_2 > 0$ and $p \geq 1$. Different choices of W_θ model various phase transitions in crystalline solids. We refer to [17] for the Ericksen-James energy density that describes a cubic to tetragonal phase transition and restrict ourselves to temperature independent energy densities of the form

$$W_\theta(G) = W(G) = \text{dist}(G, \{F_1, \dots, F_N\})^p, \quad G \in \mathbb{R}^{n \times n},$$

with a positive integer N and given (compatible) wells $F_1, \dots, F_N \in \mathbb{R}^{n \times n}$.

It is due to non-quasiconvexity of W that the variational problem does in general not admit solutions and infimizing sequences reveal the most important information of the physical situation. A conforming finite element scheme replaces \mathcal{A} by a finite-dimensional subspace \mathcal{A}_h and the resulting minimization problem admits a solution. For a family of finite element spaces $(\mathcal{A}_h)_{h>0}$ there holds $\lim_{h \rightarrow 0} \inf_{v_h \in \mathcal{A}_h} I(v_h) \rightarrow \inf_{v \in \mathcal{A}} I(v)$, i.e., finite element schemes yield infimizing sequences. Our main result concerns the decay rate of the energies and its dependence on the number $N \geq 2$ of wells and the exponent $p \geq 1$. We assume throughout this work that F lies in the lamination convex hull $\{F_j : j = 1, \dots, N\}^{lc}$ (cf. [19] and Section 4 for a definition of K^{lc}) of $\{F_j : j = 1, \dots, N\}$ so that $\inf_{v \in \mathcal{A}} I(v) = 0$.

The a priori analysis in [17] for $N = 2$ states

$$\inf_{v_h \in \mathcal{A}_h} I(v_h) \leq Ch^{1/2},$$

independently of p . Here, h is the maximal meshsize of the underlying triangulation and throughout this paper C is a generic, h -independent constant. It is shown in [9] that this estimate is sharp for $p = 1$ in the sense that there exists a triangulation of the domain $\Omega := (0, 1)^2 \subseteq \mathbb{R}^2$ and matrices $F_1, F_2 \in \mathbb{R}^{2 \times 2}$ such that $\inf_{v_h \in \mathcal{A}_h} I(v_h) \geq Ch^{1/2}$. In case that $N \geq 2$, the analysis in [14] shows

$$\inf_{v_h \in \mathcal{A}_h} I(v_h) \leq Ch^{\frac{1}{1+L}},$$

where $L \geq 1$ is the lamination level which is related to F and F_1, \dots, F_N (cf. Section 4). In all cited works, finite element minimizers are constructed (iteratively) by a lamination process and appropriate cut-off functions to satisfy the (averaged) boundary condition.

In physical experiments one observes branching of different variants near interfaces [22], and this effect has been analyzed in the continuous case in [12] for energy densities that involve a surface energy term. For $n = 2$ we show that finite element deformations which exhibit similar branching

structures on mesh dependent scales give rise to significantly reduced energies. In particular, we find an explicit dependence of branching structures on growth conditions.

Theorem 1.1. *If $n = 2$, $F \in \{F_1, \dots, F_N\}^{lc}$ with lamination level L , and if h is sufficiently small we have*

$$(1.1) \quad \inf_{v_h \in \mathcal{A}_h} I(v_h) \leq C h^{\frac{p}{p+L}} \left(1 + \log(h^{\frac{1-p}{p+L}})\right)^L.$$

It is assumed that a similar estimate holds for $n = 3$. We draw the following conclusions from our analysis: (i) We observe that the scale induced by the finite element space may be regarded as a scale arising from a surface energy. (ii) Finite element minimizers exhibit multiscale phenomena with branching structures close to the boundary and interfaces. (iii) The result is in agreement with the widely accepted conjecture that growth conditions are related to the amount of energy stored in interfaces between different phases and that they affect the geometry of branchings near interfaces. In particular, branching structures of constructed deformations disappear for the case $p = 1$ which fits with the known constructions mentioned above. (iv) The case of incompatible wells that has been analysed in [7] corresponds to the limit $L \rightarrow \infty$.

In the case of two compatible energy wells our construction may be summarized as follows. We choose a coarse lamination in the interior of the domain of scale $\mathcal{O}(h^{1/(p+1)})$. In a boundary layer of thickness $\mathcal{O}(h^{p/(p+1)})$ we choose a fine lamination of scale $\mathcal{O}(h^{p/(p+1)})$. To interpolate between the coarse and the fine lamination we introduce a branching or refinement region of thickness $\mathcal{O}(1)$. In this refinement region the deformation gradient is not an element of $\{F_1, F_2\}$ but is close enough to the wells. The growth condition for the energy density enters the estimate through the distance of the deformation gradient to the wells in this region and thus determines the geometry of the branching. We then employ a sharp cut-off function in the boundary layer to satisfy the boundary conditions. Finally, we use a nodal interpolation operator and prove the estimate (1.1) for the resulting discrete deformation.

The techniques of [9] to prove inverse estimates for $p = L = 1$ may be generalised to the case $p > 1$ and show that our estimate is sharp for simple laminates in the sense of the following theorem. The idea of the proof is to use a special criss-cross triangulation and then to count the number of triangles on which the discrete deformation gradient does not equal one of the two wells. This number is estimated by changes of the gradient from one well to the other along lines that are orthogonal to the direction in which oscillations occur. We refer to [9] for details.

Theorem 1.2. *There exist $F_1, F_2 \in \mathbb{R}^{2 \times 2}$, $F = (F_1 + F_2)/2$, and a triangulation \mathcal{T} of $\Omega = (0, 1)^2$ such that, for each $v_h \in \mathcal{A}_h$ satisfying*

$$I(v_h) \leq C h^{\frac{p}{p+1}} \left(1 + \log(h^{\frac{1-p}{p+1}}) \right)$$

there holds

$$I(v_h) \geq C' h^{\frac{p}{p+1}} \left(1 + \log(h^{\frac{1-p}{p+1}}) \right)^{-\frac{1}{p}}. \quad \square$$

We stress that our analysis is of theoretical interest: It is unlikely that a numerical scheme will find a correct minimizer. Using a priori knowledge, branching has been observed in numerical experiments in [16]. For the efficient computation of generalized formulations and their relation to the original problem we refer to [3, 4, 5, 13].

The rest of the paper is organized as follows: In Section 2 we introduce some notation and definitions and prove a basic lemma that shows our energy estimate (1.1) for simple laminates ($N = 2$) and allows for iteration ($N > 2$). The application of this lemma to a three well problem is performed in Section 3 to illustrate one iteration step. In Section 4 we show estimate (1.1) as the main result of this work.

2. BASIC LEMMA

In this and in the following two sections we assume that $\Omega \subseteq \mathbb{R}^2$ is a convex, piecewise affine, bounded Lipschitz domain. Moreover, we assume that \mathcal{T} is a regular triangulation of Ω .

Definition 2.1. For $\omega \subseteq \mathbb{R}^n$ and $n, n^\perp \in \mathbb{R}^n$, $|n| = |n^\perp| = 1$, $n \cdot n^\perp = 0$, the *diameter of ω in direction n* is defined by the minimal distance of two half-spaces, given by points z_1, z_2 and the normal n , that exclude ω , i.e.,

$$d_n(\omega) := \inf \left\{ \text{dist}(H_1, H_2) : H_j = \{x \in \mathbb{R}^n : (-1)^j(x - z_j) \cdot n \leq 0\}, \right. \\ \left. H_j \cap \omega = \emptyset, z_j \in \mathbb{R}^n, j = 1, 2 \right\}.$$

The *maximal length of a line segment in ω parallel to n^\perp* is defined by

$$\ell_{n^\perp}(\omega) := \sup \{ |s| : s \in \mathbb{R}, x \in \omega, x + sn^\perp \in \omega \}.$$

Remark 2.1. The quantity $s^{-1}d_n(\omega)$ describes how many line segments parallel to n^\perp and in distances $s > 0$ can be arranged in ω while $\ell_{n^\perp}(\omega)$ is the maximal length of such line segments (cf. Figure 1).

Lemma 2.1 (Basic Lemma). *Let $\omega \subseteq \mathbb{R}^2$ be a convex bounded Lipschitz domain with piecewise affine boundary. Moreover, let τ be a regular triangulation that covers ω and let h be the maximal diameter of elements in τ . Let $F = \lambda F_1 + (1 - \lambda)F_2$ for $F_1, F_2 \in \mathbb{R}^{2 \times 2}$ satisfying $F_1 - F_2 = a \otimes n$ for $a, n \in \mathbb{R}^2$, $|n| = 1$, and $\lambda \in (0, 1)$. Assume that $n^\perp \in \mathbb{R}^2$ satisfies $|n^\perp| = 1$ and $n \cdot n^\perp = 0$. If h is small enough there exists $y_h \in \mathcal{S}^1(\tau)^2$ with $y_h(x) = Fx$ for all $x \in \partial\omega$ and such that for $\alpha \in [0, 1]$, $\gamma \in [0, \alpha]$, and $\delta \in [\alpha, 1]$ with $\frac{\delta - \alpha}{\delta - \gamma} \geq \frac{p-1}{p}$ and $h^\alpha, h^\gamma, h^\delta \leq \text{diam}(\omega)$, there holds*

$$\begin{aligned} \int_{\omega} \text{dist}(\nabla y_h(x), \{F_1, F_2\})^p dx \\ \leq C \left(|\partial\omega| h^\delta + d_n(\omega) (h^{p\alpha - (p-1)\gamma} + h^{1+\gamma-\alpha} \log(h^{\alpha-\delta})) \right. \\ \left. + d_n(\omega) \ell_{n^\perp}(\omega) h^{1-\alpha} \right). \end{aligned}$$

Remark 2.2. The three terms on the right hand side of the estimate of the lemma reflect energy contributions that arise from a boundary layer, branching structures, and internal layer interfaces, respectively. Notice that only the second contribution shows dependence on the growth parameter $p \geq 1$.

As a direct consequence we obtain an improved energy estimate for simple laminates.

Theorem 2.1. *Under the assumptions of Lemma 2.1 (with $\omega = \Omega$ and $\tau = \mathcal{T}$) there holds*

$$\int_{\Omega} \text{dist}(\nabla y_h(x), \{F_1, F_2\})^p dx \leq C h^{p/(p+1)} (1 + \log(h^{(1-p)/(p+1)})).$$

Proof. Choosing $\alpha = 1/(p+1)$, $\delta = p/(p+1)$, and $\gamma = 0$, the assertion follows from Lemma 2.1. \square

Remark 2.3. The logarithmic term vanishes for $p = 1$. This reflects the fact that no branching is needed then and we recover the results of [17].

Proof of Lemma 2.1. Let $\alpha \in [0, 1]$, $\gamma \in [0, \alpha]$, and $\delta \in [\alpha, 1]$. For $k \in \mathbb{Z}$ define

$$\begin{aligned} \omega_k^1 &:= \{x \in \omega : kh^\alpha < x \cdot n \leq (k + \lambda)h^\alpha\}, \\ \omega_k^2 &:= \{x \in \omega : (k + \lambda)h^\alpha < x \cdot n \leq (k + 1)h^\alpha\}, \end{aligned}$$

and $\omega_k := \omega_k^1 \cup \omega_k^2$ (cf. Figure 1).

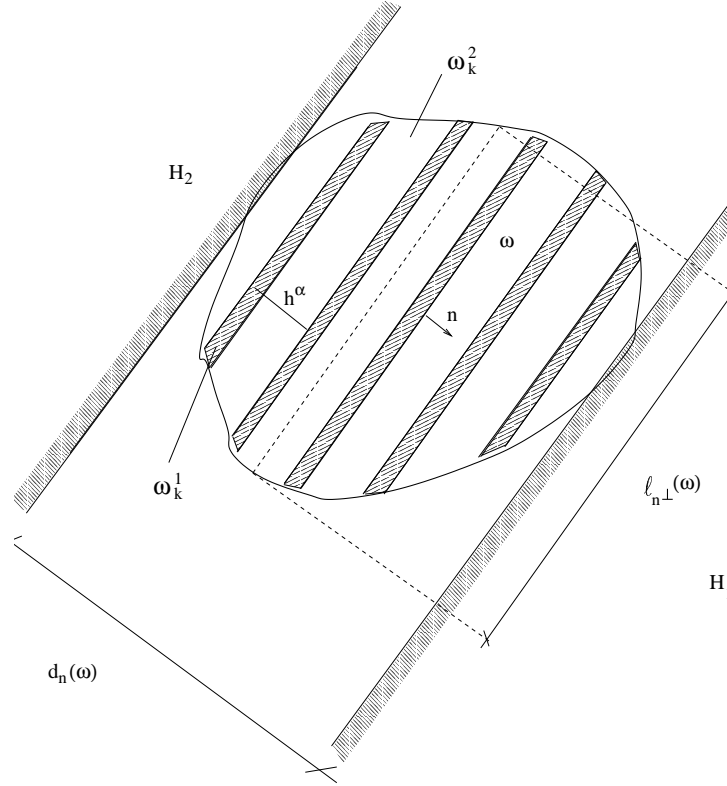


FIGURE 1. Decomposition of ω and quantities $d_n(\omega)$, $\ell_{n^\perp}(\omega)$.

Step 1: Construction of laminates in the interior of ω . For $x \in \omega$, we define a deformation \tilde{y}_0 , with χ_I being the 1-periodic extension of the characteristic function of $I \subseteq (0, 1)$ on $(0, 1)$ to \mathbb{R} , by

$$\tilde{y}_0(x) := F_1 x - a \int_0^{x \cdot n} \chi_{(\lambda, 1)}(t/h^\alpha) dt.$$

The mapping \tilde{y}_0 has the following properties.

- (i) There holds $\tilde{y}_0 \in W^{1, \infty}(\omega)$.
- (ii) There holds $\nabla \tilde{y}_0 = F_1 - \chi_{(\lambda, 1)}\left(\frac{x \cdot n}{h^\alpha}\right) a \otimes n = F_1$ in ω_k^1 and $\nabla \tilde{y}_0 = F_2$ in ω_k^2 for each $k \in \mathbb{Z}$ with $\omega_k^1 \neq \emptyset$ respectively $\omega_k^2 \neq \emptyset$. Thereby, ω is divided into at most $2d_n(\omega)h^{-\alpha}$ convex subdomains ω_k^j , $j = 1, 2$, in which $\nabla \tilde{y}_0$ is constant. The separating interfaces have a maximal length $\ell_{n^\perp}(\omega)$.
- (iii) For all $m, m^\perp \in \mathbb{R}^2$, $|m| = |m^\perp| = 1$, $m \cdot m^\perp = 0$, with $m \nparallel n$

there holds $\ell_{m^\perp}(\omega_k^j) \leq Ch^\alpha$ (where C depends on m and n) and $d_m(\omega_k^j) \leq d_m(\omega)$, $j = 1, 2$ and k such that $\omega_k^j \neq \emptyset$.

The properties (i) and (ii) follow directly from the definition of \tilde{y}_0 . Since each domain ω_k^j lies between two hyperplanes which are orthogonal to n^\perp and which have a distance h^α from each other and since $m^\perp \not\parallel n^\perp$ we have $\ell_{m^\perp}(\omega^\ell) \leq Ch^\alpha$, i.e., we have (iii).

We will first modify \tilde{y}_0 in a neighbourhood of $\partial\omega$ and then apply a sharp cut-off function so that it satisfies the boundary condition. Finally, we prove the asserted estimate for $y_h := \mathcal{I}_h y$, the nodal interpolant of y .

Step 2: Construction of branchings for “twinned martensite - simple austenite” interfaces. For $A \subseteq \mathbb{R}^2$ let

$$d_{n^\perp}(x, A) := \inf_{t \in \mathbb{R}: x + tn^\perp \in A} |t|$$

denote the distance of $x \in \mathbb{R}^2$ to $A \subseteq \mathbb{R}^2$ in the direction of n^\perp (if it exists) and let t be the unit tangent to $\partial\omega$. For each connectivity component $\Gamma_{r,k}$, $r = 1, 2$, of $\partial\omega \cap \partial\omega_k$ we define a function $\tilde{y}_{r,k}$ in a neighbourhood of $\Gamma_{r,k}$ as follows.

(a) Assume that $\Gamma_{r,k}$ is affine, $t|_{\Gamma_{r,k}} \not\parallel n^\perp$, and $\ell_{n^\perp}(\omega_k) \geq 5h^\gamma$. The domain

$$B_{r,k} := \omega_k \cap \{x \in \omega : d_{n^\perp}(x, \Gamma_{r,k}) \leq h^\delta + 2h^\gamma\},$$

is assumed to be connected and we decompose it as follows. Let

$$\omega_{r,k}^{K+1} := \{x \in B_{r,k} : d_{n^\perp}(x, \Gamma_{r,k}) \leq h^\delta\}.$$

Here, $K \in \mathbb{N}$, $\bar{\varepsilon} \in [0, 1)$ satisfy $K = \log_2(h^{\alpha-\delta}) + \bar{\varepsilon}$. For $j = 0, \dots, K$ set

$$\omega_{r,k}^j := \left\{ x \in B_{r,k} : \sum_{\ell=1}^{K-j} \frac{h^\gamma}{2^{K-\ell+1}} < d_{n^\perp}(x, \Gamma_{r,k}) - h^\delta \leq \sum_{\ell=1}^{K-j+1} \frac{h^\gamma}{2^{K-\ell+1}} \right\}$$

$$\omega_{r,k}^{-1} := \left\{ x \in B_{r,k} : h^\delta + \sum_{\ell=0}^K \frac{h^\gamma}{2^\ell} < d_{n^\perp}(x, \Gamma_{r,k}) \right\}$$

(cf. Figure 3). For $0 \leq s \leq 1$ the intervals $I_1(s)$ and $I_2(s)$ are defined by (cf. Figure 2)

$$I_1(s) = s \frac{\lambda}{4} + (1-s) \frac{\lambda}{2} + \left(0, \frac{1-\lambda}{2}\right),$$

$$I_2(s) = s \left(1 - \frac{\lambda}{4}\right) + (1-s) \left(1 - \frac{\lambda}{2}\right) - \left(\frac{1-\lambda}{2}, 0\right).$$

An important fact for the subsequent construction of branching laminates is that $I_1(1) = \frac{1}{2}(I_1(0) \cup I_2(0))$. With the help of I_1 and I_2 the mapping

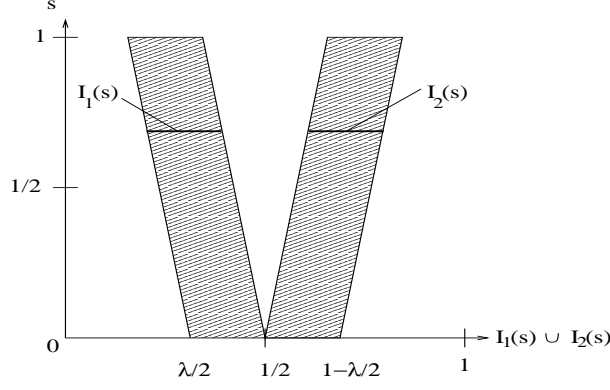


FIGURE 2. Intervals $I_1(s)$ and $I_2(s)$ for the definition of branchings near the boundary.

$\tilde{y}_{r,k} : B_{r,k} \rightarrow \mathbb{R}^2$ is, with

$$d_j(x) = \frac{2^j}{h^\gamma} d_{n^\perp} \left(x, \partial\omega_{r,k}^j \cap \partial\omega_{r,k}^{j-1} \right)$$

for values $0 \leq j \leq K$, defined as follows,

$$\tilde{y}_{r,k}(x) := F_1 x - \begin{cases} a \int_0^{x \cdot n} \chi_{(\lambda,1)} \left(\frac{s}{h^\alpha} \right) ds, & x \in \omega_{r,k}^{-1}, \\ a \int_0^{x \cdot n} \chi_{I_1(d_j(x)) \cup I_2(d_j(x))} \left(\frac{2^j s}{2h^\alpha} \right) ds, & x \in \omega_{r,k}^j, \\ a \int_0^{x \cdot n} \chi_{I_1(1) \cup I_2(1)} \left(\frac{2^K s}{2h^\alpha} \right) ds, & x \in \omega_{r,k}^{K+1}. \end{cases}$$

Figure 3 illustrates, how the function $\tilde{y}_{r,k}$ is constructed with the help of I_1, I_2 and with scaling and periodification to obtain a self-similar pattern for $\tilde{y}_{r,k}$ (cf. the construction in [12]).

(a1) There holds $\tilde{y}_{r,k} \in W^{1,\infty}(B_{r,k})$.

(a2) For all $x \in \omega_{r,k}^j$, $j = 0, \dots, K$, we have

$$\begin{aligned} \nabla \tilde{y}_{r,k}(x) &= F_1 - \chi_{I_1(d_j(x)) \cup I_2(d_j(x))} (2^j x \cdot n / (2h^\alpha)) a \otimes n \\ &\quad + \frac{\lambda}{2} h^{\alpha-\gamma} (\chi_{I_2(d_j(x))} (2^j x \cdot n / (2h^\alpha)) \\ &\quad \quad \quad + \chi_{I_1(d_j(x))} (2^j x \cdot n / (2h^\alpha))) a \otimes n^\perp. \end{aligned}$$

The mapping $\tilde{y}_{r,k}$ divides $\omega_{r,k}^j$ into at most $3 \cdot 2^j$ convex domains $\omega_{r,k}^{j,\ell}$, $\ell = 1, \dots, L_j \leq 3 \cdot 2^j$, of measure $\sim h^\alpha h^\gamma / 2^{2j}$ in which $\nabla \tilde{y}_{r,k}$ is constant. The joint boundaries have a maximal length $Ch^\gamma / 2^j$.

(a3) For all $m, m^\perp \in \mathbb{R}^2$, $|m| = |m^\perp| = 1$, $m \cdot m^\perp = 0$, with $m \nparallel n$ there holds $\ell_{m^\perp}(\omega_{r,k}^{j,\ell}) \leq Ch^\alpha / 2^j$ and $d_m(\omega_{r,k}^{j,\ell}) \leq Ch^\gamma / 2^j$, $j = 1, \dots, K$ and

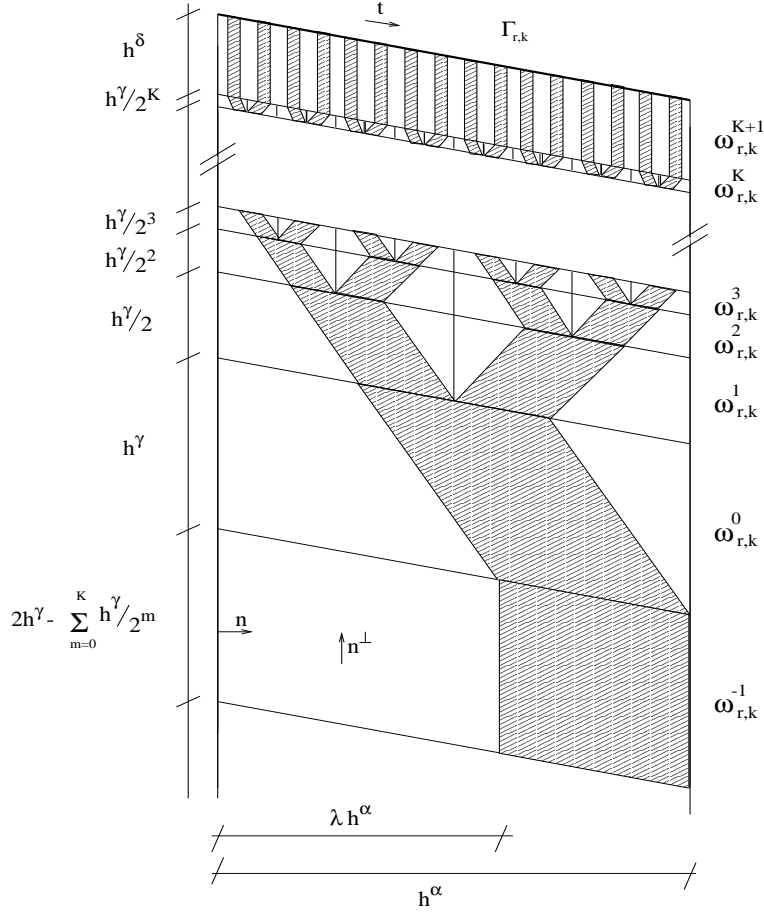


FIGURE 3. Partition of $B_{r,k}$ and branching of the domains in which $\nabla \tilde{y}_{r,k} = F_1$ (blank) respectively $\nabla \tilde{y}_{r,k} \approx F_2$ (shaded).

$\ell = 1, \dots, L_j$.

(a4) There holds $|\tilde{y}_{r,k}(x) - Fx| \leq Ch^\alpha/2^K \leq Ch^\delta$ for all $x \in \omega_{r,k}^{K+1}$.

(a5) There holds $\tilde{y}_{r,k}|_{\partial B_{r,k} \cap \omega} = \tilde{y}_0|_{\partial B_{r,k} \cap \omega}$ and $\tilde{y}_0 = \tilde{y}_{r,k}$ in $\omega_{r,k}^{-1}$.

The assertions (a1), (a3), (a4), and (a5) follow from elementary manipulations. To prove (a2) we remark that for $I \subseteq (0, 1)$ and

$$G(x) = a \int_0^u \chi_{f(x)+I}(s/d) ds = da \int_0^{u/d} \chi_{f(x)+I}(s) ds$$

there holds

$$\nabla G(x) = -d\chi_{f(x)+I}(u/d) a \otimes \nabla f(x).$$

Then (a2) follows since $\nabla d_j = 2^j n^\perp / h^\gamma$.

We may now define a continuous mapping $\tilde{y}_1 \in W^{1,\infty}(\omega)$ by setting, for $x \in \omega$,

$$\tilde{y}_1(x) := \begin{cases} \tilde{y}_{r,k}(x) & \text{if } x \in B_{r,k}, \\ \tilde{y}_0(x) & \text{otherwise.} \end{cases}$$

(b) If $\Gamma_{r,k}$ fails to be affine but $t|_{\Gamma_{r,k}} \not\parallel n^\perp$ and $\ell_{n^\perp}(\omega_k) \geq 5h^\gamma$ then ω_k can be divided into finitely many subdomains $\hat{\omega}_k^\ell$ such that $\Gamma_{r,k} \cap \partial\hat{\omega}_k^\ell$ is affine so that we have situation (a) for each of those subdomains after introducing a new coarse lamination of scale $\mathcal{O}(h^\alpha)$ in each $\hat{\omega}_k^\ell$. We assume that the lamination matches the lines that separate the domains $\hat{\omega}_k^\ell$. We then modify \tilde{y}_1 to a continuous function $\tilde{y}_2 \in W^{1,\infty}(\omega)$ as in (a).

(c) Assume that there exists a subset of $\Gamma_{r,k}$ on which $t \parallel n^\perp$. Then, since ω is convex, $\Gamma_{r,k} \cap \{x \in \mathbb{R}^2 : x \cdot n = kh^\alpha\} = \emptyset$ or $\Gamma_{r,k} \cap \{x \in \mathbb{R}^2 : x \cdot n = (k+1)h^\alpha\} = \emptyset$. Without loss of generality we will consider the latter case which is sketched in the left plot of Figure 4. Since we may assume $\ell_{n^\perp}(\omega_k) \geq 5h^\gamma$ we may proceed as follows. We introduce a boundary region ω_k^{BL} of thickness h^δ as depicted in the left plot of Figure 4. In the remaining part of ω_k we introduce one lamination of scale $\mathcal{O}(h^\alpha)$ such that the lines separating $\omega_k \setminus \omega_k^{BL}$ from ω_{k-1} and ω_k^{BL} are matched by the laminates. We then define a branching of the laminate as in (a). Finally we modify \tilde{y}_2 to a function $\tilde{y}_3 \in W^{1,\infty}(\omega)$ as in (a) and such that $\tilde{y}_3(x) = Fx$ for all $x \in \omega_k^{BL}$.

(d) Assume now that $\ell_{n^\perp}(\omega_k) \leq 5h^\gamma$. Note that the number 5 is not essential in the analysis so that by decreasing it appropriately we may assume that this case only happens when $\omega_{k\pm(m+1)} = \emptyset$ for some m and such that the domains $\omega_{k+1}, \dots, \omega_{k+m}$ (or $\omega_{k-1}, \dots, \omega_{k-m}$) satisfy $\ell_{n^\perp}(\omega_{k+j}) \sim \ell_{n^\perp}(\omega_{k+j+1}) + h^\alpha$, $j = 1, \dots, m-1$. We then define $\tilde{\omega}_k := \cup_{j=0}^m \omega_{k+j}$ and partition $\tilde{\omega}_k$ as follows. Let $M := \log_2(h^{\gamma-\delta}) + \bar{\varepsilon}$, $M \in \mathbb{N}$, $\bar{\varepsilon} \in [0, 1]$, and define for $j = 1, \dots, M$,

$$\hat{\omega}_k^j := \left\{ x \in \omega : kh^\alpha + \sum_{\ell=1}^{j-1} h^\gamma/2^\ell \leq x \cdot n \leq kh^\alpha + \sum_{\ell=1}^j h^\gamma/2^\ell \right\}.$$

Since we may assume that $d_n(\tilde{\omega}_k) = \mathcal{O}(h^\gamma)$ (note that $\partial\Omega$ is piecewise affine) we may also assume that

$$\omega_k^{BL} := \left\{ x \in \omega : kh^\alpha + \sum_{\ell=1}^M h^\gamma/2^\ell \leq x \cdot n \right\}$$

is non-empty and satisfies $\ell_{n^\perp}(\omega_k^{BL}) \sim h^\gamma/2^M \leq Ch^\delta$ and $d_n(\omega_k^{BL}) \sim h^\delta$. The decomposition of $\tilde{\omega}_k$ is depicted in the right plot of Figure 4. In each $\hat{\omega}_k^j$, $j = 1, \dots, M$, we introduce a lamination of scale $Ch^\alpha/2^{sj}$ with $s = \frac{\alpha-\delta}{\gamma-\delta} \in [0, 1]$ and a constant $C > 0$ so that the lines separating $\hat{\omega}_k^j$ from $\hat{\omega}_k^{j-1}$ and $\hat{\omega}_k^{j+1}$ are matched by lamination interfaces. We then define

a branching towards the boundary as in (a) (or (b)) but with scales $h^\gamma/2^{j+\ell}$ and $h^\alpha/2^{j^{s+\ell}}$, $\ell = 1, \dots, K_j$, with $K_j = \log_2(2^{-j^s}h^{\alpha-\delta}) + \varepsilon_j$, instead of $h^\gamma/2^\ell$ and $h^\alpha/2^\ell$, $\ell = 1, \dots, K$. Notice that the branching region refines a lamination of scale $\mathcal{O}(h^\alpha/2^{sj})$ to a lamination of scale $\mathcal{O}(h^\alpha/2^{j^{s+K_j}}) = \mathcal{O}(h^\delta)$. Finally we modify \tilde{y}_3 in $\tilde{\omega}_k$ to a function $\tilde{y}_4 \in W^{1,\infty}(\omega)$ as above and such that $\tilde{y}_4(x) = Fx$ for all $x \in \omega_k^{BL}$.

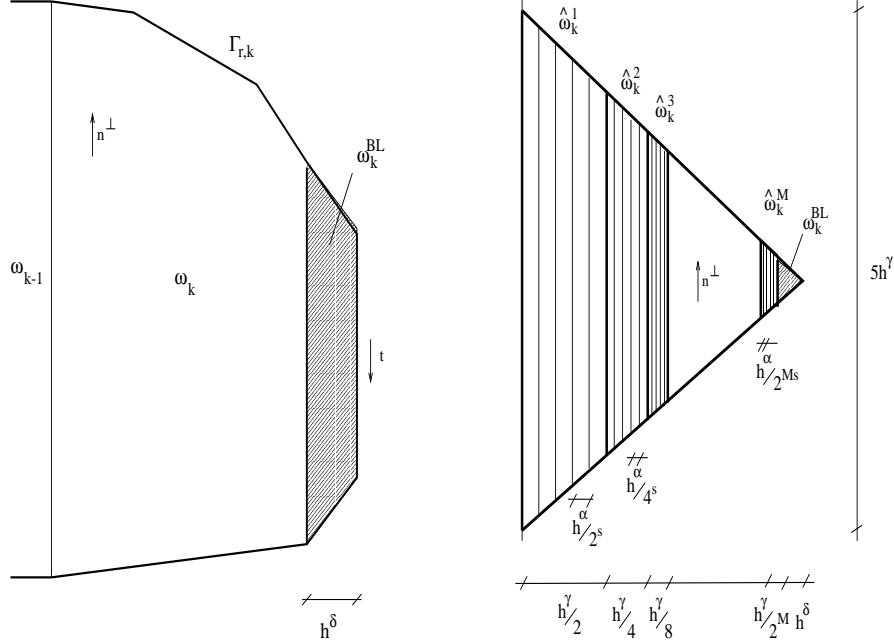


FIGURE 4. Partitions of ω_k if $t \parallel n^\perp$ (left plot) and if $\ell_{n^\perp}(\omega_k) \leq 5h^\gamma$ (right plot).

Step 3: Definition of the global continuous and discrete deformations.

We now have to modify \tilde{y}_4 such that it satisfies the boundary conditions. Let $\rho \in C^1(\omega)$ satisfy $\rho = 0$ in a boundary layer of thickness $\mathcal{O}(h)$, $\rho = 1$ outside a boundary layer of thickness $\mathcal{O}(h^\delta)$ and $|\nabla\rho(x)| \leq C/h^\delta$ for all $x \in \omega$. Define, for all $x \in \omega$,

$$y(x) = (1 - \rho(x))Fx + \rho(x)\tilde{y}_4(x).$$

Then $y \in W^{1,\infty}(\omega)$ satisfies $y(x) = Fx$ for all $x \in \partial\omega$ and we extend y to $\cup\tau \setminus \omega$ by Fx . Let $y_h := \mathcal{I}_h y$ denote the nodal interpolant of y which, by choice of ρ , also satisfies the boundary condition. There holds $y_h|_T = y|_T$ if $T \in \tau$ and $\nabla y|_T$ is constant. Since we assume that τ is regular we also have that $\|\nabla \mathcal{I}_h v\|_{L^\infty(\cup\tau)} \leq C\|\nabla v\|_{L^\infty(\cup\tau)}$ for all $v \in W^{1,\infty}(\cup\tau) \cap C(\cup\tau)$.

Step 4: Estimation of the energy of the discrete deformation. To estimate

$$\int_{\omega} \text{dist}(\nabla y_h(x), \{F_1, F_2\})^p dx$$

we divide the integral into several contributions.

I. For all $x \in \omega_{r,k}^{K+1}$ and $x \in \omega_k^{BL}$ (i.e., in a boundary layer of thickness h^δ) we have, by choice of ρ ,

$$\begin{aligned} |\nabla y(x)| &\leq |(Fx - \tilde{y}_4(x))\nabla\rho(x)| + |\rho(x)(F + \nabla\tilde{y}_4(x))| \\ &\leq C(h^{-\delta}|Fx - \tilde{y}_4(x)| + 1), \end{aligned}$$

hence

$$\begin{aligned} \text{dist}(\nabla y_h(x), \{F_1, F_2\}) &\leq |\nabla y_h(x) - \nabla y(x)| + |\nabla y(x)| + \min_{j=1,2} |F_j| \\ &\leq C(1 + h^{-\delta}|Fx - \tilde{y}_4(x)|). \end{aligned}$$

Since the union of all domains $\omega_{r,k}^{K+1}$ and ω_k^{BL} defines a strip along $\partial\omega$ of width h^δ , property (a4) ensures $|Fx - \tilde{y}_4(x)| \leq h^\delta$ while $\tilde{y}(x) = Fx$ in ω_k^{BL} as defined in (c) and (d) of Step 2 so that

$$\int_{(\cup\omega_{r,k}^{K+1}) \cup (\cup\omega_k^{BL})} \text{dist}(\nabla y_h(x), \{F_1, F_2\})^p dx \leq C|\partial\omega|h^\delta.$$

II. In the branchings defined in (a) of Step 2 the energy in $\omega_{r,k}^0 \cup \dots \cup \omega_{r,k}^K$ can be estimated as follows. In a distance $\geq h$ from the line segments in whose neighbourhood ∇y is not constant there holds by (a2) of Step 2, $\nabla y_h(x) = \nabla\tilde{y}_{r,k} \in \{F_1, F_2\} + \mathcal{O}(h^{\alpha-\gamma})$. In an h -neighbourhood of the line segments, there holds, since $\alpha \geq \gamma$, $|\nabla y_h(x) - F_j| \leq C$, $j = 1, 2$. The K interfaces separating domains $\omega_{r,k}^j$ have a maximal length h^α and contribute in an h -neighbourhood to the energy. In each of the domains $\omega_{r,k}^j$, $j = 0, \dots, K$ there are 2^j line segments of length $h^\gamma/2^j$. For one domain $B_{r,k}$ we have, using $|\cup_{j=0, \dots, K} \omega_{r,k}^j| \leq Ch^{\alpha+\gamma}$,

$$\begin{aligned} \int_{B_{r,k}} \text{dist}(\nabla y_h(x), \{F_1, F_2\})^p dx \\ \leq C \int_{B_{r,k}} h^{p(\alpha-\gamma)} dx + C \sum_{\ell=0}^K 2^{\ell+1} h h^\gamma / 2^\ell + CKhh^\alpha \\ \leq C(h^{(p+1)\alpha-(p-1)\gamma} + Khh^\gamma + Khh^\alpha). \end{aligned}$$

Since there are at most $Cd_n(\omega)h^{-\alpha}$ many domains $B_{r,k}$ as in (a) and since $\gamma \leq \alpha$ it follows that

$$\begin{aligned} \int_{\cup B_{r,k}} \text{dist}(\nabla y_h(x), \{F_1, F_2\})^p dx \\ \leq Cd_n(\omega)(h^{p\alpha-(p-1)\gamma} + h^{1+\gamma-\alpha} \log_2(h^{\alpha-\delta})). \end{aligned}$$

III. There are at most $d_n(\omega)h^{-\alpha}$ many line segments in the interior of ω (i.e., away from the branching regions) that separate domains ω_k^1 and ω_k^2 . In their h -neighbourhood ∇y is non-constant. Since those line segments have a maximal length $\ell_{n^\perp}(\omega)$ they lead to an energy contribution

$$\int_{\{x \in \omega: x \notin B_{r,k}\} \cup (\cup \omega_{r,k}^{-1})} \text{dist}(\nabla y_h(x), \{F_1, F_2\})^p dx \leq C d_n(\omega) \ell_{n^\perp}(\omega) h^{1-\alpha}.$$

IV. The boundary regions defined in (c) of Step 2 can be estimated as in I.-III. Note that the number of such domains is independent of h .

V. Assume now the situation from (d) of Step 2. In each $\hat{\omega}_k^j$, $j = 1, \dots, M$, there are $h^\gamma h^{-\alpha} 2^{j(s-1)}$ many line segments of length $h^\gamma / 2^j$ which contribute to the energy in an h -neighbourhood. Moreover, from the branchings in $\hat{\omega}_k^j$ we obtain a contribution (cf. II.)

$$h^{\gamma-\alpha} 2^{j(s-1)} h^{p(\alpha-\gamma)} 2^{pj(1-s)} h^{\gamma+\alpha} 2^{-j(s+1)}.$$

Note that by assumption we have $1 \geq s \geq (p-1)/p$ so that $p(1-s) - 1 \leq 0$. The line segments in the branching regions lead to an energy

$$h^{\gamma-\alpha} 2^{j(s-1)} \log_2(2^{-sj} h^{\alpha-\delta}) h^{1+\gamma} 2^{-j}$$

and we have $\log_2(2^{-sj} h^{\alpha-\delta}) \leq \log_2(h^{\alpha-\delta})$. The summation over the domains $\hat{\omega}_k^1, \dots, \hat{\omega}_k^M$ and noting that the boundary layer ω_k^{BL} contributes an amount $|\partial\omega| h^\delta$ shows

$$\begin{aligned} \int_{\hat{\omega}_k} \text{dist}(\nabla y_h(x), \{F_1, F_2\})^p dx &\leq C |\partial\omega| h^\delta + C \sum_{j=1}^M h^{\gamma-\alpha} 2^{j(s-1)} \\ &\quad \times (h^{p(\alpha-\gamma)} 2^{pj(1-s)} h^{\gamma+\alpha} 2^{-(1+s)j} + \log_2(h^{\alpha-\delta}) h^{1+\gamma} 2^{-j} + h^{1+\gamma} 2^{-j}) \\ &\leq C |\partial\omega| h^\delta + C h^\gamma (h^{p\alpha-(p-1)\gamma} + \log_2(h^{\alpha-\delta}) h^{1+\gamma-\alpha} + h^{1+\gamma-\alpha}). \end{aligned}$$

Since $h^\gamma \leq C d_n(\omega)$ and $h^\gamma \leq C \ell_{n^\perp}(\omega)$ the right-hand side is bounded by the same quantities as in I., II., and III.

The summation of the contributions in I.-V. proves the assertion of the lemma. \square

3. APPLICATION TO A THREE-WELL PROBLEM

The explicit dependence of the energy estimate in Lemma 2.1 on various quantities related to ω allows for an iterative application. Layers within layers without branching (or transition layers) are depicted in Figure 5. We will proceed analogously but with appropriate branching at the boundary and at interfaces between different variants.

Theorem 3.1. *Suppose that $F = \lambda(\rho F_{11} + (1-\rho)F_{12}) + (1-\lambda)F_2$ for $F_{11}, F_{12}, F_2 \in \mathbb{R}^{2 \times 2}$ and $\rho, \lambda \in (0, 1)$. Moreover, assume that $F_1 - F_2 = a \otimes n$ for $a, n \in \mathbb{R}^2$ and $|n| = 1$, where $F_1 = \rho F_{11} + (1-\rho)F_{12}$ such that*

there exist $b, m \in \mathbb{R}^2$, $|m| = 1$, $m \nparallel n$, with $F_{11} - F_{12} = b \otimes m$. If h is small enough there exists $y_h \in \mathcal{S}^1(\mathcal{T})^2$ satisfying $y_h(x) = Fx$ for all $x \in \partial\Omega$ such that there holds

$$\int_{\Omega} \text{dist}(\nabla y_h(x), \{F_{11}, F_{12}, F_2\})^p dx \leq Ch^{p/(p+2)} (1 + \log(h^{(1-p)/(p+2)}))^2.$$

Proof. We start as in the proof of Lemma 2.1 and define with $F_1, F_2, (\alpha, \gamma, \delta) = (\alpha_1, \gamma_1, \delta_1)$, and $\omega = \Omega$ a function \tilde{y} by performing Steps 1-3 in the proof of Lemma 2.1. To each subdomain $\omega \subseteq \Omega$ outside the boundary layers ω_k^{BL} or $\omega_{r,k}^{K+1}$, and such that $\nabla \tilde{y}|_{\omega} = F_1$, we want to apply Lemma 2.1 with appropriate scales $(\alpha_2, \gamma_2, \delta_2)$ (if necessary choosing the coarsest scale of the branchings in ω as $(h^{\alpha_2}/2^j, h^{\gamma_2}/2^j)$ for some $j \geq 0$), F_{11}, F_{12} , and ρ . This defines a mapping $y_h|_{\omega}$ satisfying $y_h(x) = F_1 x$ for all $x \in \partial\omega$. Since $\tilde{y}(x) = F_1 x + a$ for all $x \in \omega$ and some $a \in \mathbb{R}^2$ the mapping

$$\tilde{y}(x) = \begin{cases} y_h(x) + a & \text{for } x \in \omega, \\ \tilde{y}(x) & \text{for } x \in \Omega \setminus \omega, \end{cases}$$

is continuous. The nodal interpolant of \tilde{y} then satisfies $\nabla \mathcal{I}_h \tilde{y} = \nabla y_h$ in $\omega \setminus \{x \in \omega : \text{dist}(x, \partial\omega) > Ch\}$. To estimate the energy of this mapping, we have to give an upper bound for the energy coming from those subdomains in which we modified \tilde{y} . From the part of Ω that we do not modify we get the contributions of Lemma 2.1 (with exponents $(\alpha_1, \gamma_1, \delta_1)$ and domain Ω). We now estimate the energy coming from subdomains ω as above.

Step 1: Domains ω away from the branchings. The mapping \tilde{y} in the proof of Lemma 2.1 defines at most $d_n(\Omega)h^{-\alpha_1}$ many domains ω_k^1 such that $d_m(\omega_k^1) \leq C$ and $\ell_{m^\perp}(\omega_k^1) \leq Ch^{\alpha_1}$ in which $\nabla \tilde{y} = F_1$. Lemma 2.1 then defines for each such domain ω_k^1 a function $y_h|_{\omega_k^1}$, such that for $\alpha_1 \leq \gamma_2 \leq \alpha_2 \leq \delta_2$ there holds

$$\begin{aligned} \int_{\cup \omega_k^1} \text{dist}(\nabla y_h(x), \{F_{11}, F_{12}\})^p dx &\leq Ch^{-\alpha_1} \max\{d_m(\omega_k^1), |\partial\omega|\} \\ &\times (h^{\delta_2} + (h^{p\alpha_2 - (p-1)\gamma_2} + h^{1+\gamma_2-\alpha_2} \log_2(h^{\alpha_2-\delta_2})) + h^{1-\alpha_2+\alpha_1}). \end{aligned}$$

Step 2: Domains in branching regions. In the branchings close to the boundary of Ω there are domains $\omega_{r,k}^{j,\ell}$, $j = 0, \dots, K$, with $K = \log_2(h^{\alpha_1-\delta_1}) + \bar{\varepsilon}$ and $\ell = 1, \dots, L_j \leq 3 \cdot 2^j$, in which $\nabla \tilde{y} = F_1$ and $d_m(\omega_{r,k}^{j,\ell}) \leq Ch^{\gamma_1}/2^j$, $\ell_{m^\perp}(\omega_{r,k}^{j,\ell}) \leq Ch^{\alpha_1}/2^j$ and $|\partial\omega_{r,k}^{j,\ell}| \leq Ch^{\gamma_1}/2^j$. To such domains we apply Lemma 2.1 with scales $(h^{\alpha_2}/2^j, h^{\gamma_2}/2^j, h^{\delta_2})$. We have to ensure that $h^{\alpha_2}/2^j \geq Ch^{\delta_2}$, $j = 1, \dots, K$. Since $2^K \leq Ch^{\alpha_1-\delta_1}$ this is guaranteed if

$\alpha_1 - \delta_1 = \alpha_2 - \delta_2$. We then obtain mappings $y_h|_{\omega_{r,k}^{j,\ell}}$ such that

$$\begin{aligned} \int_{\omega_{r,k}^{j,\ell}} \text{dist}(\nabla y_h(x), \{F_{11}, F_{12}\})^p dx &\leq Ch^{\gamma_1} / 2^j \\ &\times \left(h^{\delta_2} + h^{p\alpha_2 - (p-1)\gamma_2} / 2^j + h^{1+\gamma_2 - \alpha_2} \log_2(2^{-j} h^{\alpha_2 - \delta_2}) + h^{1-\alpha_2 + \alpha_1} \right). \end{aligned}$$

Note that $0 \leq \log_2(2^{-j} h^{\alpha_2 - \delta_2}) \leq \log_2(h^{\alpha_2 - \delta_2})$. The summation of all such domains shows, since there are at most $d_n(\Omega)h^{-\alpha_1}$ many domains $B_{r,k}$, in which branchings between F_1 and F_2 are needed,

$$\begin{aligned} \int_{\cup \omega_{r,k}^{j,\ell}} \text{dist}(\nabla y_h(x), \{F_{11}, F_{12}\})^p dx &\leq Ch^{-\alpha_1} \sum_{j=0}^K 2^{j+1} h^{\gamma_1} / 2^j \\ &\times \left(h^{\delta_2} + h^{p\alpha_2 - (p-1)\gamma_2} / 2^j + h^{1+\gamma_2 - \alpha_2} \log_2(h^{\alpha_2 - \delta_2}) + h^{1-\alpha_2 + \alpha_1} \right) \\ &\leq CKh^{\gamma_1 - \alpha_1} \left(h^{\delta_2} + h^{p\alpha_2 - (p-1)\gamma_2} + h^{1+\gamma_2 - \alpha_2} \log_2(h^{\alpha_2 - \delta_2}) + h^{1-\alpha_2 + \alpha_1} \right). \end{aligned}$$

Step 3: Domains within corner domains. We now estimate the energy stemming from replacing a gradient F_1 by a laminate in corner domains as considered in (d) in the proof of Lemma 2.1. Here, a domain ω in which a gradient equals F_1 satisfies

$$|\partial\omega| \leq Ch^{\gamma_1} / 2^{j+k}, \quad d_m(\omega) \leq Ch^{\gamma_1} / 2^{j+k}$$

and

$$\ell_{m^\perp}(\omega) \leq Ch^{\alpha_1} / 2^{sj+k}$$

for $j = 1, \dots, M \leq \log_2(h^{\gamma_1 - \delta_1})$ and $k = 1, \dots, K_j \leq \log_2(2^{-sj} h^{\alpha_1 - \delta_1}) \leq \log_2(h^{\alpha_1 - \delta_1})$. The lamination in ω using gradients F_{11} and F_{12} is then on a scale $h^{\gamma_2} / 2^{j+k}$ and $h^{\alpha_2} / 2^{sj+k}$ and the branching starts on that scale and refines the lamination by successively dividing $h^{\alpha_2} / 2^{sj+k}$ and $h^{\gamma_2} / 2^{j+k}$ by 2 until $h^{\alpha_2} / 2^{sj+k+m} = h^{\delta_2}$. Since $p - ps - 1 \leq 0$ and $s = \frac{\delta_1 - \alpha_1}{\delta_1 - \gamma_1} \leq 1$ we obtain a contribution

$$\begin{aligned} \int_{\omega} \text{dist}(\nabla y_h(x), \{F_{11}, F_{12}\})^p dx &\leq Ch^{\gamma_1} / 2^{j+k} \left[h^{\delta_2} + h^{p\alpha_2 - (p-1)\gamma_2} 2^{j(p-ps-1)} 2^{-k} \right. \\ &\quad \left. + h^{1+\gamma_2 - \alpha_2} \log_2(2^{-sj} h^{\alpha_2 - \delta_2}) 2^{j(s-1)} + h^{1-\alpha_2 + \alpha_1} \right] \\ &\leq Ch^{\gamma_1} / 2^{j+k} \\ &\times \left(h^{\delta_2} + h^{p\alpha_2 - (p-1)\gamma_2} 2^{-k} + h^{1+\gamma_2 - \alpha_2} \log_2(2^{-sj} h^{\alpha_2 - \delta_2}) + h^{1-\alpha_2 + \alpha_1} \right) \end{aligned}$$

We now have to sum all such domains ω . Noting that in each domain $\hat{\omega}_k^j$ there are $\frac{h^{\gamma_1} 2^{sj}}{2^j h^{\alpha_1}}$ many branching regions and laminates we find

$$\begin{aligned} \int_{\cup \omega} \text{dist}(\nabla y_h(x), \{F_{11}, F_{12}\})^p dx &\leq C \sum_{j=1}^M \frac{h^{\gamma_1} 2^{sj}}{2^j h^{\alpha_1}} \left(\sum_{k=j}^{K_j} 2^k \frac{h^{\gamma_1}}{2^{j+k}} \right) \\ &\times \left(h^{\delta_2} + h^{p\alpha_2 - (p-1)\gamma_2} + h^{1+\gamma_2 - \alpha_2} \log_2(2^{-sj} h^{\alpha_2 - \delta_2}) + h^{1 - \alpha_2 + \alpha_1} \right) \\ &\leq C h^{\gamma_1 - \alpha_1} \log_2(h^{\alpha_1 - \delta_1}) \\ &\times \left(h^{\delta_2} + h^{p\alpha_2 - (p-1)\gamma_2} + h^{1+\gamma_2 - \alpha_2} \log_2(2^{-sj} h^{\alpha_2 - \delta_2}) + h^{1 - \alpha_2 + \alpha_1} \right). \end{aligned}$$

Step 4: Estimation of the total energy. The two lamination processes lead to a total energy

$$\begin{aligned} \int_{\Omega} \text{dist}(\nabla y_h(x), \{F_{11}, F_{12}, F_2\})^p dx \\ \leq C \left[h^{\gamma_1} \log_2(h^{\alpha_1 - \delta_1}) \right. \\ \times \left(h^{\delta_2 - \alpha_1} + h^{p\alpha_2 - (p-1)\gamma_2 - \alpha_1} + h^{1+\gamma_2 - \alpha_2 - \alpha_1} \log_2(h^{\alpha_2 - \delta_2}) + h^{1 - \alpha_2} \right) \\ \left. + h^{\delta_1} + h^{p\alpha_1 - (p-1)\gamma_1} + h^{1+\gamma_1 - \alpha_1} \log_2(h^{\alpha_1 - \delta_1}) + h^{1 - \alpha_1} \right]. \end{aligned}$$

For $j = 1, 2$ we choose $\alpha_j = j/(p+2)$, $\gamma_j = (j-1)/(p+2)$, and $\delta_j = (p+j-1)/(p+2)$ and check that the assumptions on s and $\alpha_2 - \delta_2 = \alpha_1 - \delta_1$ are satisfied to conclude the proof. \square

Remark 3.1. In the previous proof we chose the first lamination such that we have gradients F_1 in the branching regions and then replaced F_1 by another lamination. Some care has to be taken if one also wants to replace F_2 since in the branching regions the deformation gradient is not exactly equal to F_2 . Instead, one has a gradient $F_2 + \tilde{F}_2$ with $\tilde{F}_2 = \mathcal{O}(h^{\alpha_1 - \gamma_1})$. One may then replace F_2 by a lamination and add \tilde{F}_2 after that process again. The resulting energy is then estimated with the help of the triangle inequality to obtain the same bound.

4. APPLICATION TO HIGHER-ORDER LAMINATES

We now perform the iterative lamination process for arbitrary lamination orders. We will assume that the boundary data lies in the lamination convex hull of $\{F_1, \dots, F_N\}$ in the following sense.

Definition 4.1. The homogeneous deformation $F \in \mathbb{R}^{n \times n}$ lies in the *lamination convex hull* of $\{F_1, \dots, F_N\}$ if there exist a positive integer L , $E_{j,k} \in$

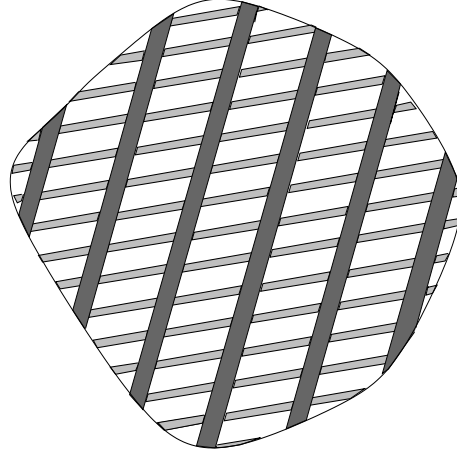


FIGURE 5. Iterated lamination in Ω (without branching or transition layers) using three different gradients.

$\mathbb{R}^{n \times n}$, $\varrho_{j,k} \in [0, 1]$, $a_{j,k} \in \mathbb{R}^n$, $n_{j,k} \in \mathbb{R}^n$, $|n_{j,k}| = 1$, $j = 0, 1, 2, \dots, L$, $k = 1, 2, \dots, 2^j$, such that $F = E_{0,1}$ and

$$\begin{aligned} E_{j,k} &= \varrho_{j,k} E_{j+1,2k-1} + (1 - \varrho_{j,k}) E_{j+1,2k}, \\ E_{j+1,2k} - E_{j+1,2k-1} &= a_{j,k} \otimes n_{j,k}, \\ E_{L,k} &\in \{F_1, \dots, F_N\}. \end{aligned}$$

To apply Lemma 2.1 we will also assume that two successive normals in the construction of the boundary data F in the lamination convex hull of $\{F_1, \dots, F_N\}$ are not parallel.

Theorem 4.1. *Assume that $F \in \mathbb{R}^{2 \times 2}$ lies in the lamination convex hull of $\{F_1, \dots, F_N\}$ and assume that if F is constructed as in Definition 4.1 for $j = 0, 1, \dots, L - 1$, $k = 1, 2, \dots, 2^j$, the normal $n_{j,k}$ is neither parallel to $n_{j+1,2k-1}$ nor to $n_{j+1,2k}$. If h is small enough there exists $y_h \in \mathcal{S}^1(\mathcal{T})^2$ satisfying $y_h(x) = Fx$ for all $x \in \partial\Omega$ and such that*

$$\inf_{v_h \in \mathcal{A}_h} I(v_h) \leq C h^{p/(p+L)} (1 + \log(h^{(1-p)/(p+L)}))^L.$$

Remark 4.1. Improved estimates for the approximation of volume fractions and Young measure support as well as for convergence of v_h in L^2 follow from the theorem. We refer to [18, 11].

Proof. As in the proof of Theorem 3.1 we define a deformation y_h by successively replacing a deformation gradient $E_{j,k}$ by $E_{j+1,2k-1}$ and $E_{j+1,2k}$ with the help of Lemma 2.1. If we ensure $\alpha_m - \delta_m = \alpha_1 - \delta_1$ and $\gamma_m - \delta_m = \gamma_1 - \delta_1$ for $m = 1, \dots, L$ we may set $s = \frac{\delta_1 - \alpha_1}{\delta_1 - \gamma_1} \in [0, 1]$ and assume that in a domain ω with $d_{n_{L-1,\ell}}(\omega) \leq Ch^{\alpha_{L-2}}$ or $d_{n_{L-1,\ell}}(\omega) \leq Ch^{\gamma_{L-1}}/2^k$ and $\ell_{n_{L-1,\ell}}(\omega) \leq Ch^{\alpha_{L-1}}/2^{k'+k''}$ for $k'+k'' = k$, where $k \leq \log_2(h^{\alpha_{L-1}-\delta_{L-1}})$,

we replaced a gradient $E_{L-1,\ell}$ by a lamination and branching of $E_{L,2\ell}$ and $E_{L,2\ell+1}$. Suppose (and check later) that $h^{\alpha_{L-2}} \sim h^{\gamma_{L-1}}$ so that we only have to consider the latter case. The domain ω contributes to the total energy the amount (cf. the proof of Theorem 3.1)

$$(4.1) \quad \int_{\omega} \text{dist}(\nabla y_h(x), \{E_{L,2k}, E_{L,2k-1}\})^p dx \leq Ch^{\gamma_{L-1}}/2^k \\ \times (h^{\delta_L} + h^{p\alpha_L - (p-1)\gamma_L} + h^{1+\gamma_L - \alpha_L} \log_2(h^{\alpha_L - \delta_L}) + h^{1-\alpha_L + \alpha_{L-1}}).$$

We now have to count how many such domains ω there are. Let us set $\alpha_{-1} = \alpha_0 = \gamma_0 = \delta_0 := 0$ and $\tilde{\gamma}_j := \min\{\gamma_j, \alpha_{j-1}\}$, $j = 0, \dots, L$. After the first lamination there are, for $j_1 = k$, in branchings as defined in (a) in the proof of Lemma 2.1 and in corner domains, respectively,

$$h^{\tilde{\gamma}_0 - \alpha_1} 2^{j_1} + \sum_{\ell_1=0}^{j_1} \frac{h^{\tilde{\gamma}_1} 2^{s\ell_1}}{2^{\ell_1} h^{\alpha_1}} 2^{j_1 - \ell_1} \leq Ch^{\tilde{\gamma}_0 - \alpha_1} 2^{j_1}$$

many domains ω with $d_{n_{1,1}}(\omega) \leq Ch^{\tilde{\gamma}_1}/2^k$ respectively $d_{n_{1,2}}(\omega) \leq Ch^{\tilde{\gamma}_1}/2^k$. Since in such a domain we use a lamination of scale $h^{\alpha_2}/2^{j_1}$ and a branching starting on scales $h^{\alpha_2}/2^{j_1}$, $h^{\gamma_2}/2^{j_1}$ while the corner domains themselves start on a scale $h^{\gamma_2}/2^{j_1}$, we have

$$\sum_{j_1+j_2=k} h^{\tilde{\gamma}_0 - \alpha_1} 2^{j_1} \left(h^{\tilde{\gamma}_1 - \alpha_2} 2^{j_2} + \sum_{\ell_2=j_1}^{j_2} \frac{h^{\gamma_2} 2^{s\ell_2}}{2^{\ell_2} h^{\alpha_2}} 2^{j_2 - \ell_2} \right) \\ \leq C \sum_{j_1+j_2=k} h^{\tilde{\gamma}_0 - \alpha_1} 2^{j_1} h^{\tilde{\gamma}_1 - \alpha_2} 2^{j_2}$$

many domains ω with $d_{n_{2,m}}(\omega) \leq Ch^{\gamma_2}/2^k$ for $m = 1, \dots, 4$ after the second lamination. Iterating the argumentation we find that there are

$$\sum_{j_1+\dots+j_{L-1}=k} \prod_{\ell=1}^{L-1} (h^{\tilde{\gamma}_{\ell-1} - \alpha_{\ell}} 2^{j_{\ell}}) = 2^k \left(\prod_{\ell=1}^{L-1} h^{\gamma_{\ell-1} - \alpha_{\ell}} \right) \times \left(\sum_{j_1+\dots+j_{L-1}=k} 1 \right)$$

many domains ω in which we have a gradient on level $L-1$ and such that $d_{n_{L-1,m}}(\omega) \leq Ch^{\gamma_{L-1}}/2^k$ for $m = 1, \dots, 2^{L-1}$. Summing the energy contributions (4.1) for $k = 1, \dots, K \leq \log_2(h^{\alpha_{L-1} - \delta_{L-1}})$ we find, noting that $\sum_{k=1}^K \sum_{j_1+\dots+j_{L-1}=k} 1 \leq K^{L-1}$,

$$\int_{\cup \omega} \text{dist}(\nabla y_h(x), \{E_{L,2k}, E_{L,2k-1}\})^p dx \leq CK^{L-1} \left(\prod_{\ell=1}^{L-1} h^{\tilde{\gamma}_{\ell-1} - \alpha_{\ell}} \right) h^{\gamma_{L-1}} \\ \times (h^{\delta_L} + h^{p\alpha_L - (p-1)\gamma_L} + h^{1+\gamma_L - \alpha_L} \log_2(h^{\alpha_L - \delta_L}) + h^{1-\alpha_L + \alpha_{L-1}}).$$

Summing the contribution from each lamination step (since the binary tree might have a local depth $\leq L$) we obtain the following bound on the energy

$$I(y_h) \leq C \sum_{k=1}^L \left(\prod_{\ell=1}^{k-1} h^{\tilde{\gamma}_{\ell-1} - \alpha_{\ell}} \right) \log_2(h^{\alpha_{k-1} - \delta_{k-1}})^{k-1} \\ \times h^{\gamma_{k-1}} \left(h^{\delta_k} + (h^{p\alpha_k - (p-1)\gamma_k} + h^{1+\gamma_k - \alpha_k} \log_2(h^{\alpha_k - \delta_k})) + h^{1-\alpha_k + \alpha_{k-1}} \right).$$

For $j = 1, \dots, L$ we choose $\alpha_j = j/(p+L)$, $\gamma_j = (j-1)/(p+L)$, and $\delta_j = (p+j-1)/(p+L)$ so that

$$\left(\prod_{\ell=1}^{k-1} h^{\tilde{\gamma}_{\ell-1} - \alpha_{\ell}} \right) h^{\gamma_{k-1}} \log_2(h^{\alpha_{k-1} - \delta_{k-1}})^{k-1} = h^{-\alpha_{k-1}} \log_2(h^{(1-p)/(p+L)})^{k-1}.$$

We then have $\inf_{v_h \in \mathcal{A}_h} I(v_h) \leq Ch^{p/(p+L)}(1 + \log_2(h^{(1-p)/(p+L)}))^L$. \square

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REFERENCES

- [1] John M. Ball and Richard D. James, *Fine phase mixtures as minimizers of energy*, Arch. Rat. Mech. Anal. **100** (1987), 13-52.
- [2] John M. Ball and Richard D. James, *Proposed experimental tests of a theory of fine microstructure and the two-well problem*, Phil. Tras. R. Soc. Lond. A **338** (1992), 389-450.
- [3] Sören Bartels, *Numerical analysis of some non-convex variational problems*, PhD-Thesis, Universität Kiel (2001).
- [4] Carsten Carstensen and Petr Plecháč, *Numerical solution of the scalar double-well problem allowing microstructure*, Math. Comp. **66** (1997), 997-1026.
- [5] Carsten Carstensen and Thomáš Roubíček, *Numerical approximation of young measures in non-convex variational problems*. Numer. Math. **84** (2000), 395-415.
- [6] Michel Chipot and Charles Collins, *Numerical approximations in variational problems with potential wells*, SIAM J. Numer. Anal. **29** (1992), 1002-1019.
- [7] Michel Chipot, *The appearance of microstructures in problems with incompatible wells and their numerical approach* (English), Numer. Math. **83** (1999), 325-352.
- [8] Michel Chipot, Charles Collins, and David Kinderlehrer, *Numerical analysis of oscillations in multiple well problems*, Numer. Math. **70** (1995), 259-282.
- [9] Michel Chipot and Stefan Müller, *Sharp energy estimates for finite element approximations of non-convex problems*, MPI-Preprint no. **8**, Leipzig (1997).
- [10] Philippe G. Ciarlet, *The Finite Element Method for Elliptic Problems*, North-Holland, Amsterdam, (1978).
- [11] Matthias K. Gobbert and Andreas Prohl, *A discontinuous finite element method for solving a multi-well problem*, SIAM J. Numer. Anal. **37** (1999), 246-268.
- [12] Robert V. Kohn and Stefan Müller, *Branching of twins near an austenite/twinned martensite interface*, Phil. Mag. **66A**, (1994), 697-715.
- [13] Martin Kružík, *Numerical approach to double well problems*, SIAM J. Numer. Anal. **35** (1998), 1833-1849.

- [14] Bo Li, *Finite element analysis of a class of stress-free martensitic microstructures*, preprint (2000).
- [15] Bo Li and Mitchell Luskin, *Nonconforming Finite element approximation of crystalline microstructure*, Techn. Report **1420**, IMA, (1996).
- [16] Bo Li and Mitchell Luskin, *Theory and computation for the microstructure near the interface between twinned layers and a pure variant of martensite*, Preprint (1998).
- [17] Mitchell Luskin, *Approximation of a laminated microstructure for a rotationally invariant, double well energy density*, Numer. Math. **75** (1997), 205-221.
- [18] Mitchell Luskin, *On the computation of crystalline microstructure*, Acta Numerica (1996).
- [19] Stefan Müller, *Variational models for microstructure and phase transitions* (English), Springer. Lect. Notes Math. **1713** (1999), 85-210.
- [20] Pablo Pedregal, *On the numerical analysis of nonconvex variational problems*, Num. Math., **74** (1996), 325-336.
- [21] Andreas Prohl, *An adaptive finite element method for solving a double well problem describing crystalline microstructure*, M2AN, vol. **33** (1999), 781-796.
- [22] Thomas W. Shield, (www.aem.umn.edu/people/faculty/shield/needles) *Needles in Martensites*.

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